Sub Topic: e.g. Laminar Flames

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Temperature measurements in the reaction zone of a small-scale hybrid rocket combustor using near-infrared tunable diode laser absorption spectroscopy

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Abstract: In this work, a Tunable Diode Laser Absorption Spectroscopy system operating in the near infrared spectrum (NIR) is outlined to be used for two-dimensional gas-phase temperature and concentration of water in the combustion zone of a paraffin wax slab simulating a hybrid rocket. The transient temperature field resulting from the regression of the slab surface will be tracked with the laser and results are used to locate the flame zone and extract surface regression rate. Experimental measurements are supported by two-dimensional numerical simulations which incorporate multi-phase effects caused by the melt layer. The TDLAS system was demonstrated on a flat flame burner used to calibrate the system and select optimal absorption transition pairs. The temperature profile extracted from the burner follows a temperature profile similar to what was expected, but the overall temperature values were noisy. This is believed to have resulted from the high sensitivity of the temperature equation relating to the integrated absorbance values, and absorption transition parameters. Further improvements to the TDLAS system will need to be made before being connected to the hybrid combustor.
Keywords: Laser absorption spectroscopy, Hybrid combustion, paraffin wax

1. Introduction

This work aims to utilize TDLAS to measure gas-phase temperature in the flame zone of a model hybrid rocket combustor and subsequently utilize the temperature measurements to understand the combustion process and regression rate of the solid fuel.

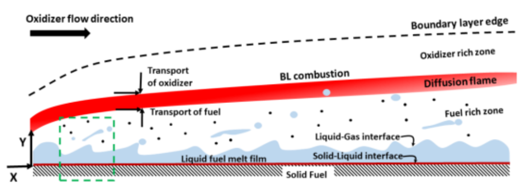


Figure 1. Physical phenomena associated with boundary layer combustion in a hybrid propulsion system.

A hybrid propulsion system provides an alternative to conventional solid and liquid systems. The benefits of utilizing a hybrid propulsion system is reviewed in the work of Kuo et. al [1]. The main drawback of employing a hybrid propulsion system, is low average fuel regression rate in comparison to a solid propulsion system. A hybrid propulsion system undergoes “boundary layer combustion”, wherein the flame is detached from the fuel surface and the fuel vapors are generated, by pyrolysis/vaporization, using the thermal energy from the flame (combustion zone), transported by dominant heat transfer modes - radiation and convection. The heat transfer to the fuel surface is further impeded by vapor generation at the surface, referred to as “Blocking effect”. Figure 1 shows a schematic representing the complex heat and mass transfer as well as energy release processes occurring during hybrid combustion. Optimizing the regression rate of liquefying fuels requires a detailed understanding of transport and combustion processes in the complex flow-field generated in the boundary layer of the solid fuel.

Tunable diode laser absorption spectroscopy (TDLAS) is a relatively low-cost, non-intrusive technique, capable of high-speed temperature measurements. The approach uses the concept that a gaseous medium strongly absorbs incident radiation at particular wavelengths. Incident radiation generated by the diode laser causes excitation of the molecules and a transition in vibrational state. This transition in vibrational state requires energy from the incident radiation to be absorbed by the molecules and the amount of energy absorbed is dependent on the temperature of the molecule and the selected wavelength of the incident light. The absorption transition is well described by the Beer-Lambert relation [2]:

$$I_\nu = I_{\nu,0}\exp[-S(T)g(\nu-\nu_0)Nl] \tag{1}$$

The key to making temperature measurements using TDLAS lies in measuring the absorption response of a molecule using two absorption transitions. Some fundamental assumptions are required for the two-line technique to be appropriate; both lines must experience the same pressure, mole fraction of target species, and path length. Taking this a step forward, the ratio of the measured integrated absorbance’s (R) can be related to the target molecule’s temperature (T), and can be determined as shown in Eqn. 2:

$$R = \frac{S_1(T)}{S_2(T)} = \frac{S_1(T_0)}{S_2(T_0)} exp\left[-\frac{hc\left(E_1''-E_2''\right)}{k}\left(\frac{1}{T}-\frac{1}{T_0}\right)\right] with\ T = \frac{\frac{hc}{k}\left(E_2''-E_1''\right)}{ln\frac{A_1}{A_2}+ln\frac{S_2(T_0)}{S_1(T_0)}+\frac{hc\left(E_2''-E_1''\right)}{k}\frac{}{T_0}} \tag{2}$$

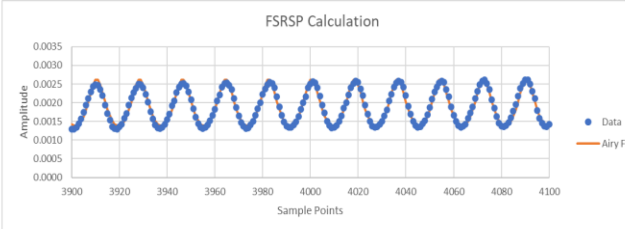
For an imaging volume with a uniform distribution of the target species (H_2O), at a uniform temperature, the solution given by Eqn. 2 would provide the average temperature along the laser path.

2. Methods

2.1 Flat-flame burner TDLAS setup

A McKenna burner (flat-flame burner) is used to validate TDLAS measurements and tune the respective lasers to produce accurate temperature data. This allows for the system to avoid atmospheric interference. The system was run at an equivalence ratio of 1 with both the methane and air at 20 psi. Data points were taken radially at 5mm increments at a height above the burner (HAB) of 7mm.

Two DFB diode lasers (NLK1E5EAAA & NLK1B5EAAA) with a center line wavelength of 1343 nm (7445 cm-1) and 1391 nm (7186 cm-1), respectively; with an output power of 10 mW are controlled using a laser diode controller (LDC 3900, ILX Lightwave). The controller provides both current and temperature control for the lasers as well as a through port for modulation. The laser current is modulated using a sawtooth signal operating at 10Hz with an amplitude of 0.45Vpp which scans the laser wavelength within a range of ~2 cm^{-1} near the central wavelength of the laser. A single collimating lens combines the two laser inputs and sends the incident beam through a flat flame burner to be recorded through a photodiode (InGaAs, Thorlabs SM05PD4A). The amplified output is scanned at 40kHz using a National Instruments DAQ system (BNC-2120) using LabView. A Fabry Perot interferometer (etalon) is used to determine the specific wavelengths of light produced by the two lasers by using multiple beam interference. This is necessary to calculate the integrated absorbance value in the correct units and will allow for simple calculation of the FSR value by fitting an Airy Function over the etalon output for each laser. P4 from the Airy Function provides the frequency of the of the etalon output.



$$Airy\ fit = P1 + P2 * \frac{1}{1 + P3(P4\sin^2(x - P5))} \quad (3)$$

$$FSR = \frac{1}{2nd}, \qquad FSRSP = \frac{\pi}{P4}, \qquad r = \frac{FSR}{FSRSP} \quad (4)$$

Figure 2. Airy function fitting for full spectral range calculation from the Silicon Etalon.

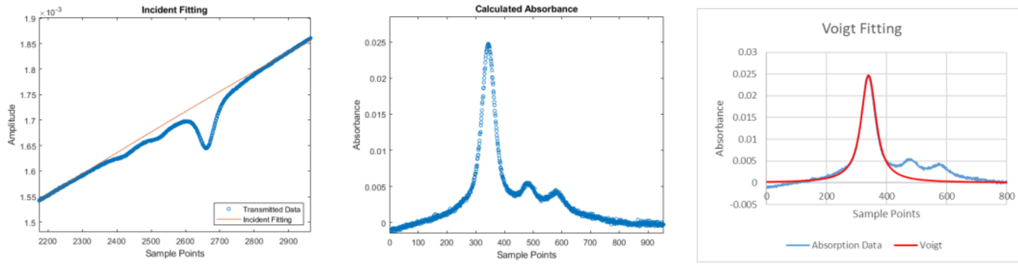


Figure 3. Sawtooth profile fitting with absorption transition (left), isolated absorption transition (center), and Voigt profile fitting (right)

A typical data set from the burner experiment looks like the absorption transition found in the left image of Figure 3. A third order polynomial has been fit using the non-absorbing wings of the data set to provide the basis of the incident beam behavior. The absorption transition captured can be converted to an absorbance response by using Beer-Lambert's law such as the image in the center of Figure 3. The absorbance response is then integrated over the set of sample points by using a Voigt fit. The Voigt fit corrects the noisy non absorbing wings that are connected to the absorbance response and helps with integration allowing the entire absorbance response to be stored as 5 simple parameter values. The ratio r calculated from the etalon is used to correct the integrated absorbance units. The reference lower energy level and line strengths at 296K are then pulled from the HITRAN database to calculate the temperature using the integrated absorbance values.

2.2 Model hybrid combustor TDLAS setup

Once the TDLAS system has been proven to provide accurate temperature behavior within the flat flame burner, the system will be added onto a custom slab model hybrid combustor. Optical quartz windows on each side of the paraffin wax slab will allow for the lasers to scan into the combustion zone of the combustor and provide temperature measurements within the target zone of Figure 4. Quartz was chosen because it has a high transmittance in the near infrared spectrum. This system can accommodate a range of solid fuels and flowrates to be used for a wide range of applications. At the time of this paper this system is currently being machined.

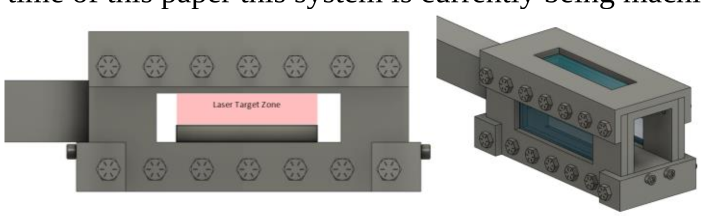


Figure 4. Model hybrid combustor setup.

2.3 Two-phase hybrid combustion simulation setup

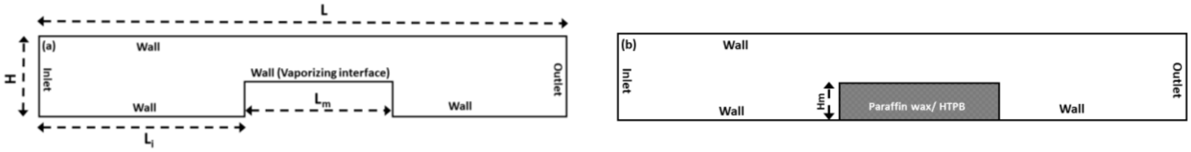


Figure 5. Computational domain for the simulation (a) Single phase domain (b) Multiphase domain

Three essential physics of Multiphase hybrid combustion simulations are- flow turbulence, phase change and combustion model. Considering the potential computational load and the pursued combustion flow field, two equation SST k-w model is preferred over detailed Large Eddy Simulation (LES) and Direct Numerical Simulation (DNS). The Volume of Fluid (VOF) method is employed to handle the phase mass transport, in which the velocity field of the liquid-gas mixture is used to advect the volume fraction of individual phases (α_p). The mass transport by vaporization and pyrolysis (thermal decomposition) is included in the framework of VOF, by adding volumetric source terms, like the previous works of Schlottke et. al [5] and Tanguy et. al [6]. The Enthalpy Porosity technique is employed for melting, due to its ability to handle non-isothermal melting of alloys in Eulerian framework. For the tested flow conditions in the present work, the rate of combustion is expected to be limited by the mixing time scale (Damkohler number Da >>1). So, turbulent mixing-timescale-based Eddy Dissipation Model (EDM), developed in the work of Magnussen [7], is employed for combustion modelling. In EDM, a turbulent time scale is defined, using local turbulent kinetic energy and dissipation rate. The formulation includes a problem specific reaction rate parameter, which is generally set based on validations with pertinent experiments. The detailed combustion reaction is represented by a single equilibrium reaction step and the relative mass fraction of final combustion products were evaluated using NASA CEA code. The details of the simulation set up are listed in Table 1.

Numerical aspect	Solution method
PV coupling	PISO
Gradient	Green Gauss Node based
Pressure	Body force weighted
Momentum, Species, Energy (convective)	Second order upwind
Multiphase	VOF (Compressive)
Turbulence	SST k-w
Melting	Enthalpy Porosity technique
Radiation	Discrete Ordinate Method (DOM)

Table 1. Summary of Simulation set up.

A representative computational domain to simulate Multiphase hybrid combustion is shown in Fig.7 (b). The dimensions of the computational domain and operating conditions were adopted from the lab-scale experiment conducted in the work of Dunn et. al [8] and are provided in Table 2. The domain and operating conditions of Dunn et al. are similar to those planned in future work on the setup described in Section 2.2. Complementary single-phase simulations (Fig. (a)) were conducted, to set the turbulent reaction rate parameter and to provide a reference for Multiphase combustion. In single phase combustion, the fuel surface is represented by a wall (top surface) and the vaporization rate is imposed as mass source term at the cell adjacent to the wall.

PARAMETER	INPUT VALUES
Domain Dimension [mm]	$L_i = 217.5, L = 400, H = 25.4$
INITIAL CONDITIONS	
Dimensions (Fuel Slab) [mm]	$L_m = 73$ & $H_m = 9$
Subcool [K]	≈ 42 $(Paraffin\ wax)$
BOUNDARY CONDITIONS	
Oxidizer mass flux $\left[\frac{kg}{m^2 s}\right]$	$G_o = 16$&40
Pressure [Pa]	101325
Inlet temperature [K]	300

Table 2. Computational domain dimension and operating conditions.

The paraffin wax fuel (mixture of hydrocarbons) is represented by $C_{32}H_{66}$ hydrocarbon [9]. Based on the work of Leccese et. al [9], $C_{32}H_{66}$ hydrocarbon is assumed to thermally crack into Ethylene (C_2H_6) and the combustion is modeled as single step equilibrium reaction of Ethylene (NASA CEA). The details of the reaction are given below:

$$C_{32}H_{66} \rightarrow 16\ C_2H_6 + H_2$$

$$C_2H_4 + 2.025O_2 \rightarrow 1.24\ CO + 0.76\ CO_2 + 1.29H_2O + 0.71H_2$$

3. Results and Discussion

3.1 Cantera simulation of flat flame with fixed temperature profile

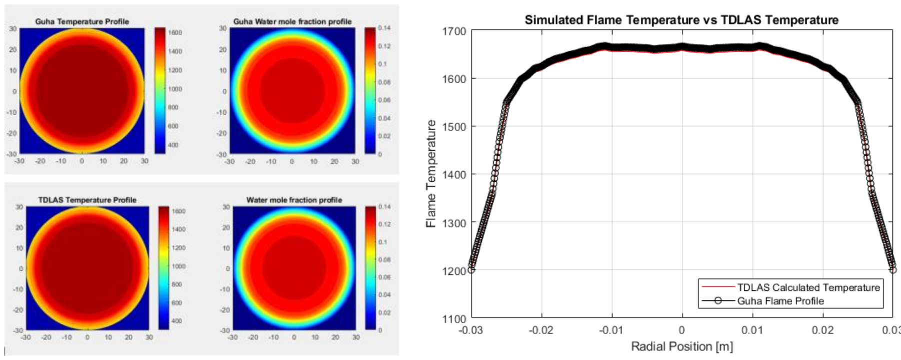


Figure 6. Preliminary testing of TDLAS code with a flat flame simulation using Cantera.

To test the validity of the TDLAS post processing code, the code was tested on a temperature profile found in Guha [10]. This allows for a simulated TDLAS dataset at each of these temperature values by pulling the absorption coefficient from HAPI at each point. To test this set of data in a single sweep, a line pair was chosen that exhibits good temperature sensitivity throughout most of the range of temperature within the flame. This allows for a single transition pair to provide data for every point in the flame. Note at higher temperatures, this line pair deviates from the correct temperature profile due to the increased sensitivity of the absorption transition near 1650K. This can make consistent temperature calculations difficult to achieve unless a more ideal absorption pair is selected for this area.

3.2 Flat flame burner temperature profile results

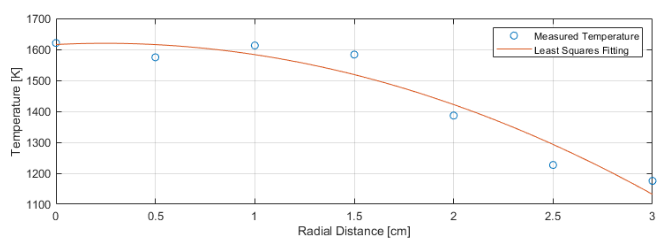


Figure 7. Preliminary temperature measurements of a flat flame methane-air burner at a HAB of 7mm.

A total of seven data points were collected on the flat flame burner to demonstrate the capabilities of the TDLAS system after the code was tested on the flame data previous mentioned. The adiabatic flame temperature for methane and air at an equivalence ratio of 1 was calculated to be around 2225K with a one-dimensional simulation being created using Cantera. All the data points in the region scanned by the TDLAS were far below the adiabatic flame temperature. The center of the burner (radial distance of zero) saw the highest temperature with the value decreasing outward as expected. The “flat-flame” nature can be seen up to about 1.5cm but more data points will be necessary to track this. As expected, the data points closer to the center of the flame were more sensitive to noise in the datasets when compared to the cooler edge. A least squares fit was added to the graph to help visualize the temperature trend.

3.3 Hybrid combustion simulation results with TDLAS

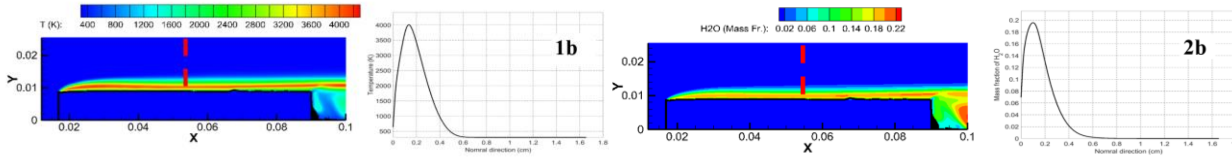


Figure 8. Multiphase combustion simulation 1a) Temperature contour 1b) Centerline temperature 2a) H2O mass fraction contour 2b) Centerline H_2O mass fraction

The zero point in the line plot identifies the liquid-gas fuel interface. The liquid fuel-gas interface is marked in black in the contour plots.

4. Conclusions

The preliminary data from the TDLAS system on the burner shows that it has the capacity to measure appropriate absorption responses within a flame and that the laser characteristics are within specification. There are some concerns with the high temperature sensitivity of the absorption transitions near the center of the flame and a more stable pair of transitions may be chosen in the future to promote consistent measurements. Data points in this region were noted to have a high sensitivity to the Voigt fit, absorption transition pair selected, lower energy level values and line strength magnitudes. Overall, additional tuning will be required before moving to the hybrid combustor system. Some key areas of interest just above paraffin fuel slab have also identified when transitioning to the combustor.

5. Acknowledgements

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6. References

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