

Design and Validation of a Single-Head Laser Absorption Spectroscopy Probe using a Fiber Optic Circulator

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ABSTRACT

A compact laser absorption spectroscopy probe has been designed for single-head, two-wavelength-scanning direct absorption temperature measurement. A fiber-optic circulator is used for both the pitch and catch components with a reflector. Cramér-Rao lower bound analysis and Monte Carlo simulations have been conducted to investigate the minimum variance and efficiency of the temperature estimator based on the presented absorption measurement technique using the selected H₂O line pairs. A lab flame has been used to validate the designed probe with a reference thermocouple. The measured temperature by the prototype LAS probe and thermocouple agrees well within ± 1 % up to 1470 K.

1. Introduction

Tunable Diode Laser Absorption Spectroscopy (TDLAS) has been used as a proven and unique method for diagnosing and characterizing high-temperature gases in harsh wind tunnels and combustion environments. Bolshov et al. [1] and Goldenstein et al. [2] reviewed its applications for measuring temperature, pressure, species concentration, and velocity in laboratory flames, combustors, and IC engines. Although the principles and measurement techniques of TDLAS are well understood and have been applied in various aerothermal and combustion conditions, LAS has fundamental limitations in spatial resolution and in the influence of temperature non-uniformity due to its laser-path-averaged/line-of-sight-integrated measurements. Generally, it also requires multiple access windows to pitch and catch laser beams. While tomographic techniques have been leveraged to reconstruct LAS measurements spatially, there are many efforts in developing compact single-ended optical probes for LAS to avoid the influence of temperature non-uniformity and the requirement of multiple access windows, such as fiber-coupled LAS sensors with reflectors [3, 4, 5] and sapphire rods and beam steering mirrors [6, 7, 8]. Recently, Hansemann et al.[9] introduced a spatially resolved single-ended TDLAS system using time-of-flight light detection, requiring a GHz sampling and an equivalent detector. Although these sensors pitch and catch the beam on the same side by using beam reflectors, they still use separate fiber optics or fiber bundles to pitch the

transmitted light (single-mode fiber) and catch the reflected light (multi-mode fiber). In this paper, a new fiber-coupled LAS probe with a fiber-optic circulator is introduced to achieve the design goals of a compact, single-head LAS probe with minimal optical components, thereby enabling TDLAS for in situ measurements of combustion gases.

2. Laser Absorption Spectroscopy

The principle of LAS is given by Beer's law, which describes the light absorption (α) through a uniform gas as shown in equation (1),

$$\frac{I_{IN}}{I_{OUT}} = \exp(k_v L) \quad (1)$$

where, k_v is the absorbance coefficient per unit length [cm^{-1}], I_{IN} is the input intensity, I_{OUT} is the transmitted intensity, and L is the path length [cm], respectively. The absorption (α) is related to gas properties by $\alpha(v) = k_v L = S(T)\phi(v - v_0)pcL$ where $S(T)$ is the line strength (integral intensity) [$\text{cm}^{-2}\text{atm}^{-1}$], ϕ is the line shape [cm], v_0 is the center frequency [cm^{-1}], p is the pressure [atm], and χ is the mole fraction of the absorption species. The line shape depends on temperature, pressure, and broadening (Doppler and collisional). Note that for most combustion gases, the line shape is usually modeled by the Voigt profile, and the integrated absorbance (A) can be measured by integrating the area of the transition lines, as shown in Figure 1 and equation (2).

$$A = S(T)pcL \quad \text{with} \quad \int_{-\infty}^{\infty} \phi(v - v_0)dv = 1 \quad (2)$$

Therefore, the absorbing species mole fraction (χ) is obtainable if the line strength $S(T)$ is known, and the line strength is a function of temperature as shown in equation (3).

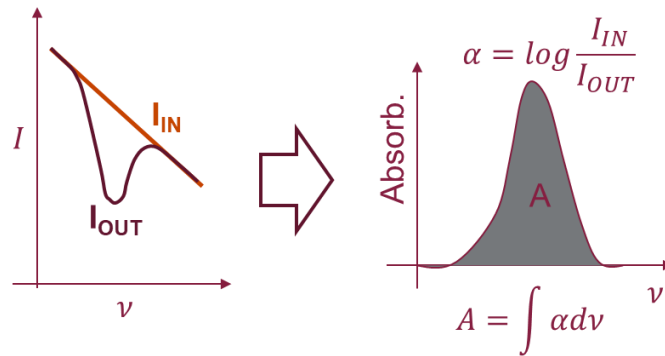


Figure 1. Measurement process of integrated absorbance.

$$S(T) = S(T_0) \frac{Q(T_0)}{Q(T)} \exp \left[-\frac{hcE''}{k} \left(\frac{1}{T} - \frac{1}{T_0} \right) \right] \left[\frac{1 - \exp \left(\frac{hcv}{kT} \right)}{1 - \exp \left(\frac{hcv}{kT_0} \right)} \right] \quad (3)$$

where $Q(T)$ is the partition function, E'' is the low state energy of transition [cm^{-1}], h is Planck's constant [erg s], c is the speed of light [cm/s], k is the Boltzmann constant [erg/K], and T_0 is the reference temperature (296 K). By using two different transitions, the ratio of line strengths at two different center frequencies is given as

$$R(T) = \frac{S_1(T)}{S_2(T)} = \frac{S_1(T_0)}{S_2(T_0)} \exp \left[\frac{hc\Delta E}{k} \left(\frac{1}{T} - \frac{1}{T_0} \right) \right] \quad (4)$$

where ΔE is the difference of the lower state energy (E'') between two transitions, in the scanned-wavelength absorption technique, the ratio of integrated areas (integrated absorbance, A in Figure 1) of the transition lines is the ratio of line strengths, since they were measured simultaneously at the same pressure, mole fraction, and path length, which is only a function of temperature. Therefore, the temperature can be calculated by

$$T = \frac{\frac{hc}{k}(E_2'' - E_1'')}{\frac{hc}{kT_0}(E_2'' - E_1'') + \log R + \log \frac{S_2(T_0)}{S_1(T_0)}} \quad (5)$$

where $R = A_1/A_2$ and the subscripts 1 and 2 refer to the values at two different center frequencies.

3. Compact single-head TDLAS probe with fiber optic circulator

As shown in Figure 2, a conventional LAS requires two access windows to pitch and catch the laser light, which was previously identified as an application limit of conventional LAS. In contrast, the single-head LAS probe presented in this paper requires only one access window to pitch and catch the laser light using an optical circulator. Note that an optical circulator is a three-port device that allows light to travel in only one direction, as shown in Figure 2(c). Therefore, laser light can be directed and captured for LAS using a single fiber optic with a reflector. Note that this reflector is not limited to only mirrors and retroreflectors, and a polished metal surface in the target environment could also serve as the reflector.

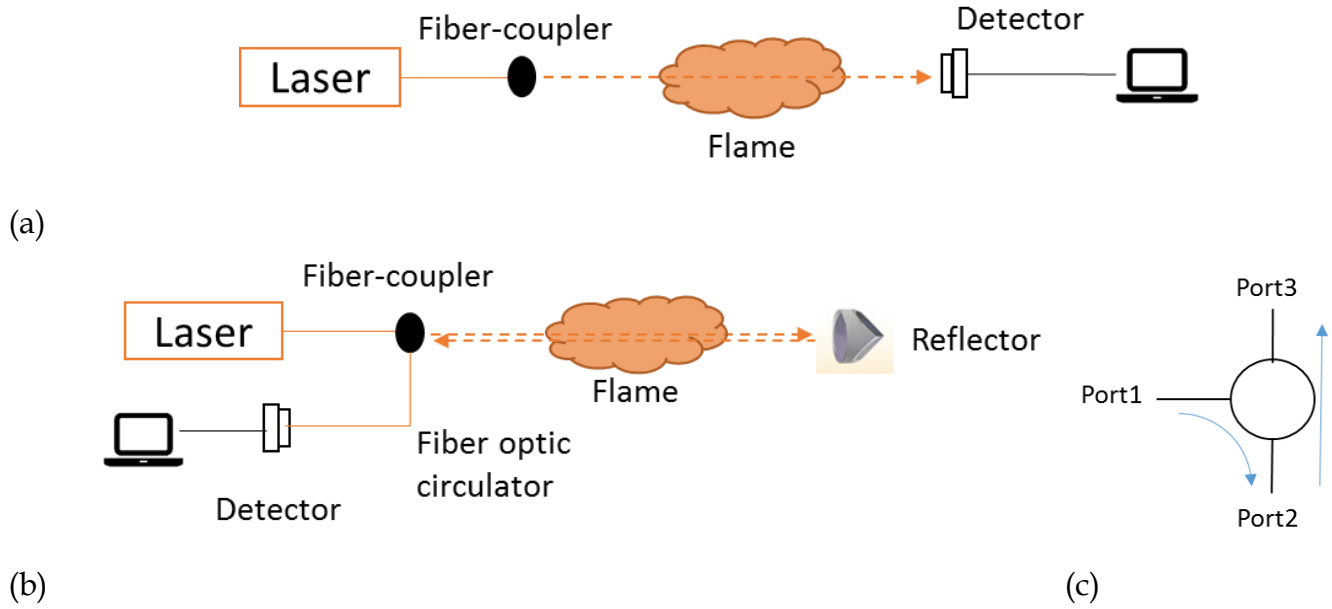


Figure 2. Conventional fiber-coupled LAS (a) and single-head fiber-coupled LAS concept (b) using a fiber optic circulator (c).

The schematic of the proposed single-head LAS probe head is presented in Figure 3. It consists of a 4-axis adjustment (linear and angular), a beam collimator, and a light pipe. Similar to the sapphire rods used in previous works [6, 7, 8], this light pipe is a fused silica rod that avoids heat damage to probe optics and minimizes absorption by ambient air along the beam path. Therefore, this minimally invasive LAS probe is capable of in situ temperature measurements while mitigating measurement biases arising from local temperature non-uniformity. The beam alignment complexity for pitch and catch, and the required number of optical components/fiber optics, are also reduced by its single-head optical probe design with a fiber-optic circulator.

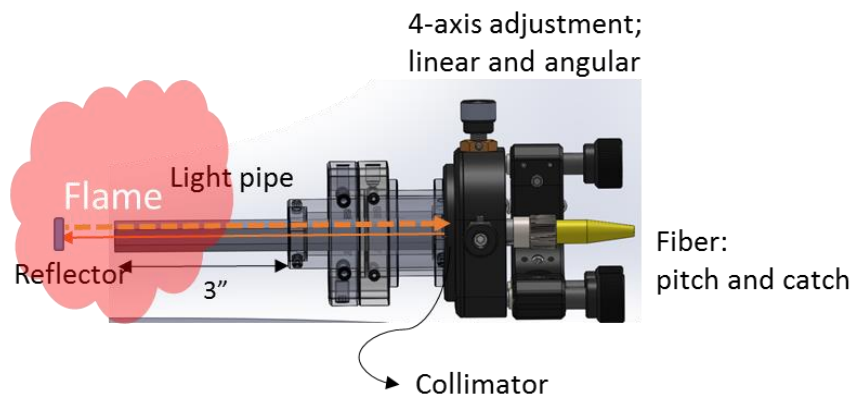


Figure 3. Schematic prototype single-head LAS probe.

Figure 4 shows the schematic of the TDLAS setup using the fiber-optic circulator LAS probe. Two wavelengths are used for the scanned-wavelength direct absorption technique.

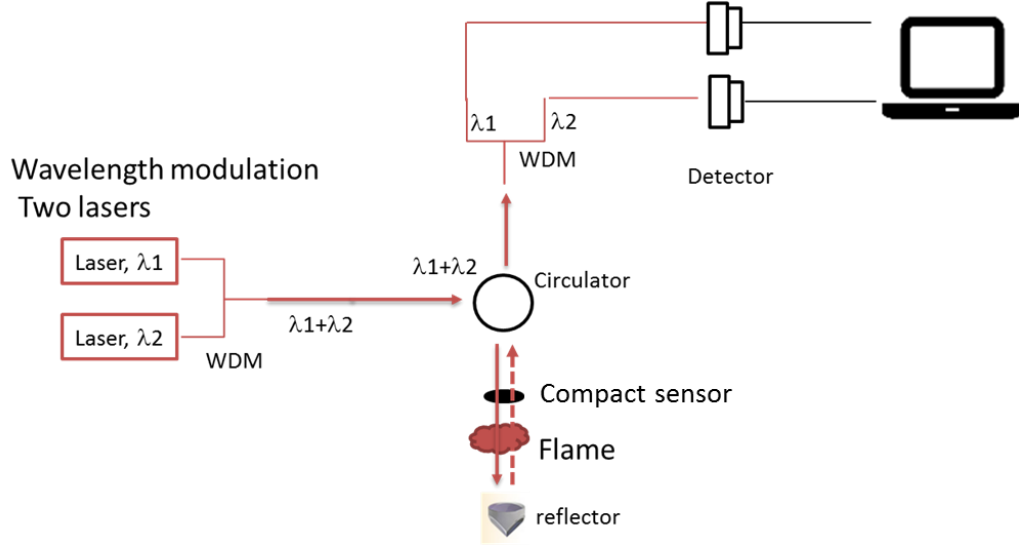


Figure 4. TDLAS layout with optical circulator. WDM: wavelength-division multiplexing.

4. Cramér-Rao lower bound (CRLB) and Monte Carlo simulation (MCS)

To investigate a theoretical lower bound on the variance of the temperature estimator and the efficiency of the presented method, CRLB and MCS have been performed and compared. CRLB(T) can be derived from Eq (4) for a random noise case [10],

$$CRLB(T) = \frac{\sigma_R^2}{\left(\frac{dR}{dT}\right)^2} = \left(\frac{T^2 k}{hc \Delta E}\right)^2 \left(\left(\frac{\sigma_{A_1}}{A_1}\right)^2 + \left(\frac{\sigma_{A_2}}{A_2}\right)^2 \right) \quad (6)$$

where, $\sigma_{A_i}^2$ is the variance of A_i for each line. Therefore, $\frac{\sigma_{A_i}}{A_i}$ is simply to be $\frac{1}{SNR_{A_i}}$. As shown in Eq (6), the lower bound of the temperature variance increases with T^4 and decreases with ΔE^2 and $SNR_{A_i}^2$. Three pairs of H₂O lines have been considered, and their spectroscopic data and absorption cross-sections are presented in Table 1 and Figure 5, respectively. $\frac{\sqrt{CRLB(T)}}{T}$ is presented in Figure 6 with the effect of ΔE ($\propto 1/\Delta E$) and temperature ($\propto T$). These pairs are very common for H₂O detections, and line pair 1 is used for the MCS and the validation tests, as it shows the highest CRLB of temperature.

Table 1. Spectroscopic data for H₂O lines.

Line pair	ν, cm^{-1}	E'', cm^{-1}	$S(T_0), \text{cm}^{-2} \text{atm}^{-1}$
1[11]	7185.58	1045.06	0.0147
	7444.37	1806.67	0.000462
2[12]	7476.95	1899.01	0.000133
	7477.37	3319.45	1.29×10^{-7}
3[13]	7185.58	1045.06	0.0147
	7454.45	1962.51	0.000173

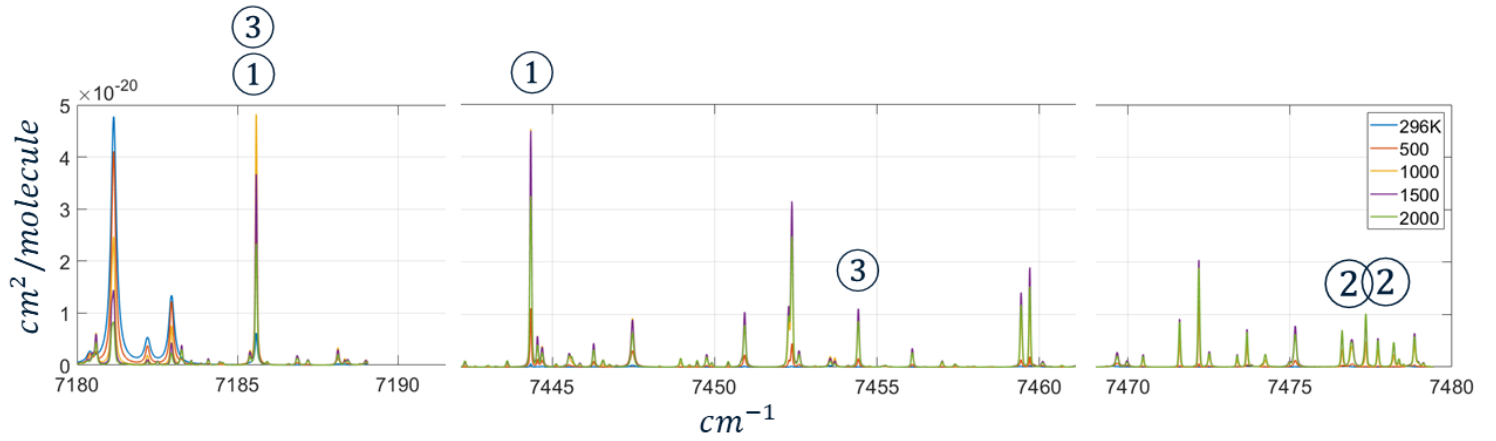


Figure 5. Absorption cross-section for the selected three pairs at 1 atm [10].

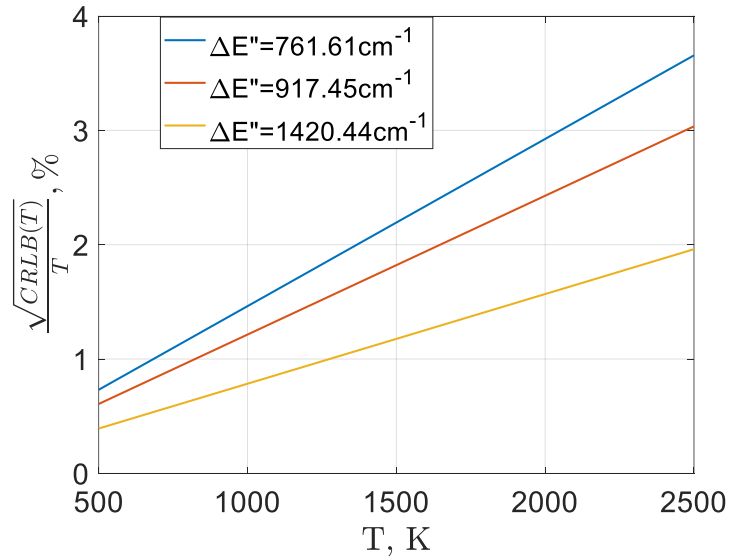


Figure 6. CRLB of measured temperature at SNR = 25dB.

The MCS has been performed for a range of SNRs (10~35 dB) and a temperature (1,000~2,500 K). The simulated absorption signals are shown in Figure 7, and the simulation results from 3,000 iterations are shown in Figure 8, with a comparison to the CRLB of temperature. For $\text{SNR} \geq 20$ dB, the MCS results approach CRLB(T), and the temperature bias is less than 0.5 %. The estimating method based on the measured absorption ratio appears very efficient within the range of consideration.

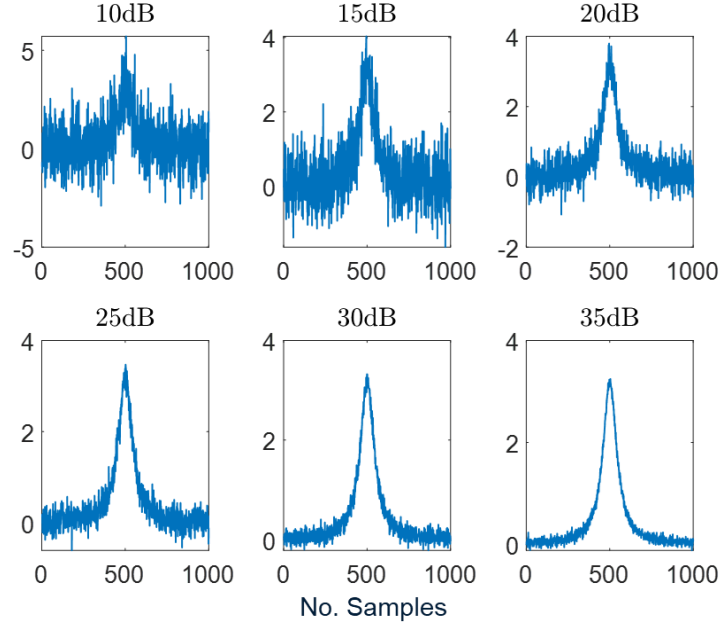


Figure 7. Simulated TDLAS signals for MCS.

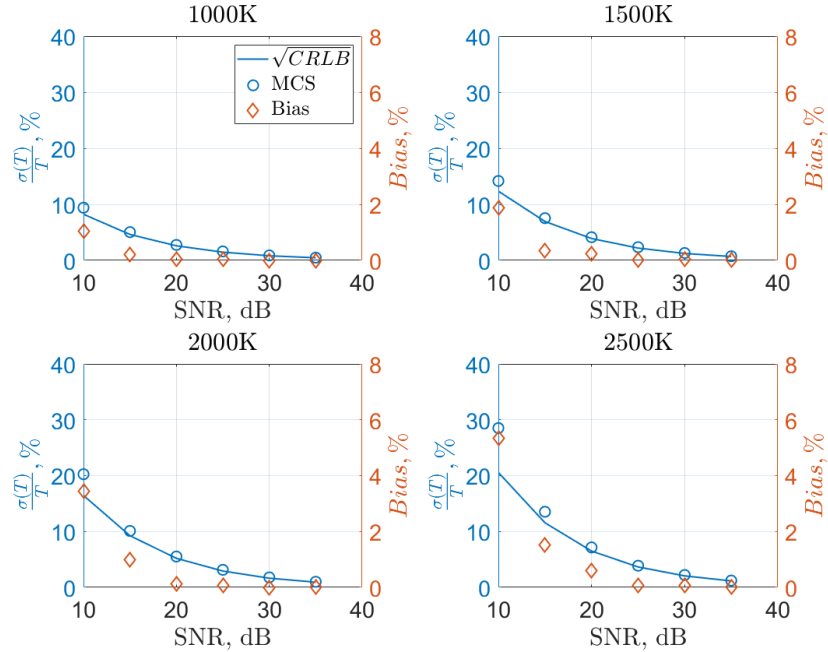


Figure 8. CRLB and MCS for line pair 1, $\Delta E'' = 761.61 \text{ cm}^{-1}$.

5. Validation experiments and Results

To validate the concept of a single-head fiber-optic circulator LAS probe, the prototype shown in Figure 3 has been built and used to measure flame temperature, with a Type-B thermocouple (0.8 mm diameter) simultaneously for comparison. The flame was generated by burning an air/Methane mixture as shown in Figure 9. The light from two tunable diode lasers of 7185.5 cm^{-1} and 7444.3 cm^{-1} was transmitted into the flame through the circulator probe. A fused silica mirror was used as a reflector, and the light was directed to the probe, where a photo detector recorded the absorption of each light pulse. Note that two wavelengths were combined before the circulator and separated after the circulator by WDMs. Both lasers scanned approximately $\pm 0.5\text{ cm}^{-1}$ band at the rate of 100 Hz for the scanned-wavelength direct absorption technique. The simultaneous absorption signals are presented in Figure 10 with the reference thermocouple measurements.

The flame temperatures measured by the single-head LAS probe and the thermocouple are presented in Figure 11. Both measurements agree well, with a difference of less than 1% cross the overall temperature range, demonstrating that the proposed LAS probe can measure temperature even in high-temperature environments. Note that the LAS probe and the thermocouple measured 293.5K and 295K at room temperature, respectively. It is worthwhile to mention that the LAS probe captured a much higher standard deviation (σ) for the flame temperature ($\sigma/\bar{T}$ up to 17%) than the room temperature ($\sigma/\bar{T} \approx 2\%$). The higher standard deviation appears mainly due to flame fluctuations caused by a low gas-mixture flow rate and the intrusiveness of the optical setup (light pipe and mirror in the flame).

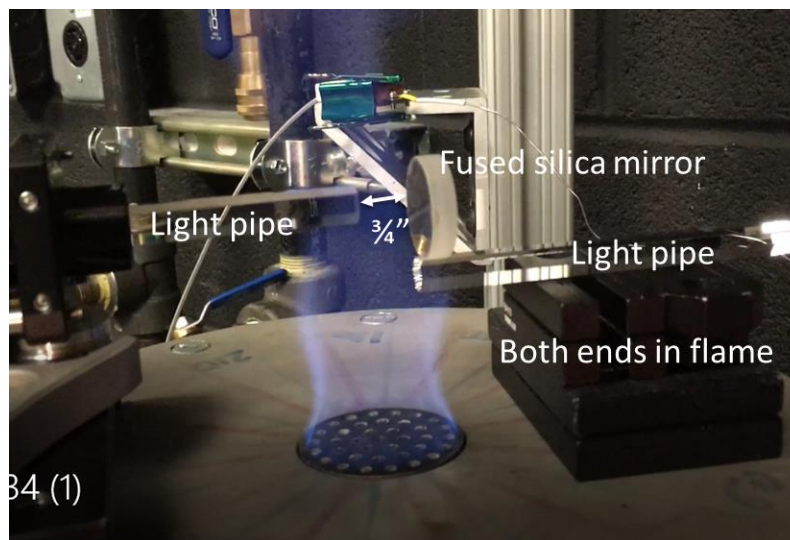


Figure 9. Benchtop setup for flame temperature measurements with a single-head TDLAS probe.

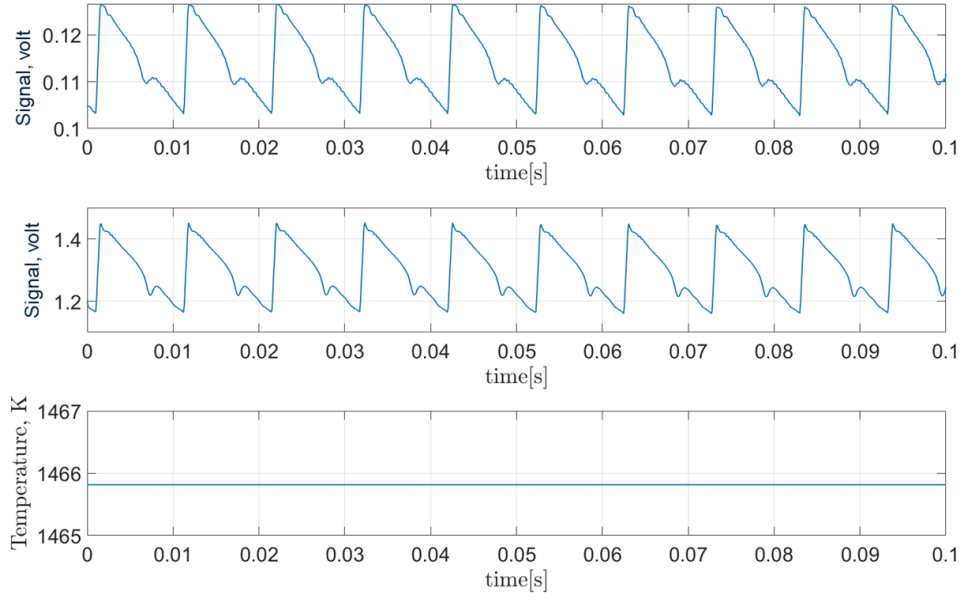


Figure 10. Simultaneous two absorption signals, 7185.58 cm^{-1} and 7444.37 cm^{-1} with a reference thermocouple reading from top to bottom.

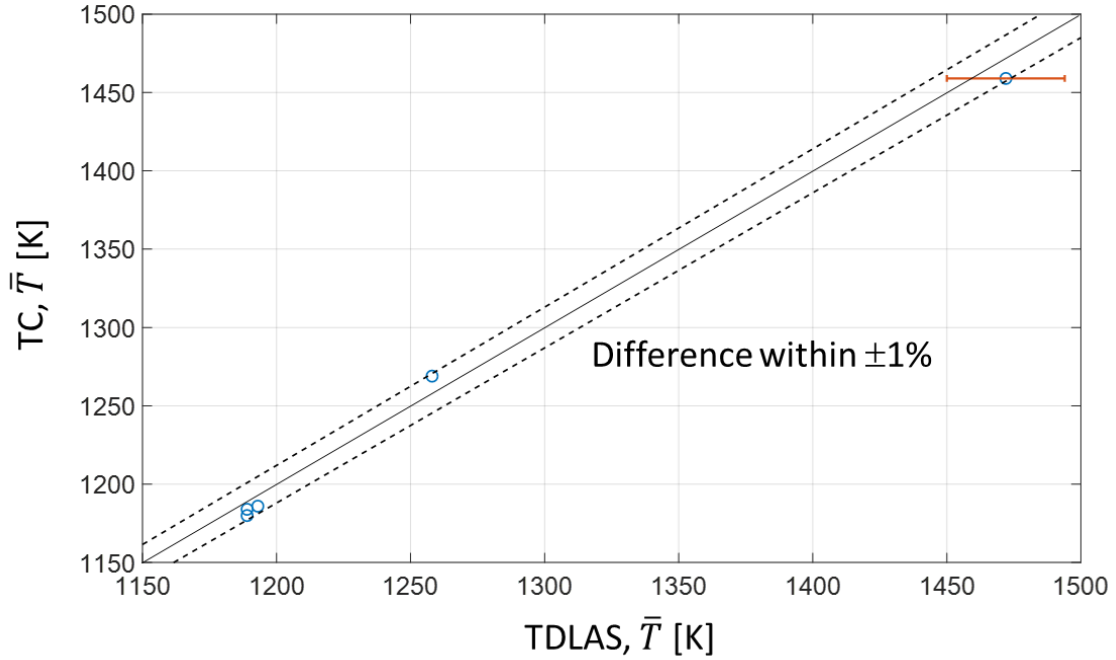


Figure 11. Flame temperature comparison measured by single-head LAS probe (TDLAS) and thermocouple (TC).

6. Conclusions

This paper describes the design and validation of a single-head TDLAS probe using a fiber-optic circulator, which minimizes the required optics and form factor for pitch-and-catch line-of-sight

measurements. The temperature estimator based on wavelength scanning direct absorption measurements of two H₂O lines has been considered for the CRLB and MCS. The MCS results show that the variance of temperature is very similar to CRLB, and the temperature bias is less than 0.5 % for SNR $\geq$ 20 dB. Validation measurements have also been conducted to determine the flame temperature, and these have been compared with thermocouple measurements. The temperature measured by two methods agrees well, within ± 1 %. Therefore, the proposed single-head compact TDLAS probe can expand the TDLAS application space in a significantly limited space, with minimal optical access, and for general line-of-sight measurements. For practical applications, further development and effort will be required to address pitch-catch beam interference, lower SNRs caused by reflectors, and high-pressure environment operations.

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