DIODE LASER ABSORPTION SPECTROSCOPY FOR TEMPERATURE MEASUREAMENTS

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Abstract. The application of absorption spectroscopy, using diode lasers, for thermometry and species measurements has been well established previously for environmental measurements, combustion studies and gasdynamic measurements. The theoretic basis of the technique is also well established. As a monochromatic beam from a diode laser passes through an absorbing medium, the transmitted intensity of the beam is related to the initial intensity by the Beer-Lambert relation. Gas temperature can be determined from the ratio of absorbance for two different absorption transitions of the same species with different energy values. The aim of this work is to verify the possibility of applying diode laser spectroscopy using just one diode laser to obtain water vapor temperatures and concentrations in a scramjet combustor (**S**upersonic **C**ombustion **R**amjet) that was constructed in the lab of CTA-IEAv. To validate the method a 22 cm pathlength furnace was used. The laser beam was pitched through the furnace cell by a fiber-optic collimator and the signal was collected on a photodiode detector. The laser was tuned to the water vapor absorption lines at 7179.75 cm^{-1} and 7181.15 cm^{-1}. For spectra simulation the software ReadHi and the HITRAN and HITEMP database were employed. The obtained temperature was near 560 K and agrees with the thermocouple measured temperature

Keywords: *diode- laser sensor, absorption spectroscopy, combustion, tunable diode laser absorption.*

1. INTRODUCTION

The precise measurement of the temperature in flames is crucial in any quantitative flame study. This is due to the high sensitivity of chemical reaction rates with the temperature, and the consequent necessity for temperature profile measurements as input data for chemical modeling. Precision better than 5% (~100 K) is frequently needed (Rensberger et al, 1989). Infrared absorption spectroscopy has become an important tool used by researchers to determine properties such as temperature and species concentration in high speed and high enthalpy flows. The wide availability of room temperature infrared diode lasers makes infrared laser spectroscopy particularly attractive and this technique has been used in many research and industrial applications (Baer et al, 1994). Moreover, considerable research has been performed in the determination of spectroscopic parameters such as strength and position of absorption features for many species including water vapor (Arroyo et al, 1993). Parameters used in high resolution spectroscopy can be found in the HITRAN (Rothman et al, 2005) database. In This work we used the software ReadHi (Reacognition of Experimental Absorption Data for HITRAN species) written in the C++ Builder Language for Windows (R. J. Ribeiro, 2006). The spectral constants necessary for this simulation (such as line positions, integrated intensities at 296 K, air-broadened and self-broadened halfwidths) can be found in HITRAN and HITEMP databases (Rothman et al, 1998, Rothman et al, 2001, Rothman et al, 2005). The spectra are simulated considering a Voigt line shape, resulting from the convolution of the Lorentzian profile (collision broadening due to pressure effects) with the Gaussian function (Doppler line shape due to temperature effects). The software allows the simulation of the spectra for various experimental conditions and it is possible to change the total and partial pressures of the molecules, the pathlength and the temperature.

The selected lines in this work were chosen due to their favorable temperature dependence and their accessibility with the particular laser diode used in the measurements. One application of infrared laser absorption spectroscopy is the determination of species concentration in combustion flows in air-breathing engines such as gas turbines and scramjets. This technique is readily applied to supersonic combustion in a hydrogen fueled scramjet engine, where the main combustion product is water vapor.

2. SPECTROSCOPY THEORY

The absorption of electromagnetic radiation near infrared by water vapor is described by Beer-Lambert Law, Eq. (1). The ratio of the transmitted intensity I to the incident intensity I_0 of laser radiation at frequency ν is exponentially related to the transition linestrength S [cm^{-2} atm^{-1}], lineshape function g [cm], partial pressure of the absorbing species P_i [atm], and the pathlength l [cm] through the absorbing medium.

$$\left(\frac{I}{I_0}\right) = \exp(-S(T)g(\nu)P_i l) \tag{1}$$

It is convenient to convert the laser intensities to absorbance $\alpha(\nu)$, which is related to the transition parameters by

$$\alpha(\nu) = -\ln\left(\frac{I}{I_0}\right) = S(T)g(\nu)P_i l \tag{2}$$

The lineshape function g is defined so that its integrated value over frequency is unity,

$$\int_{-\infty}^{+\infty} g(\nu)d\nu = 1 \tag{3}$$

The lineshape function reflects the broadening mechanisms in the medium by thermal motion (Doppler broadening) and intermolecular collisions (collisional or pressure broadening). Doppler broadening is described by the Doppler width $\Delta\nu_D$, which is the Full-Width at Half-Maximum (FWHM) of the absorption line in the Doppler limit:

$$\Delta\nu_D = \nu_0(7.1623\times10^{-7})\left(\frac{T}{M}\right)^{1/2} \tag{4}$$

where ν_0 is the center line frequency, T is the temperature [K], and M is the molecular weight [g/mol] of the absorbing species. Similarly, collisional broadening is described by the FWHM as a result of collisions, $\Delta\nu_c$. At a given temperature, the collisional width is directly proportional to the system pressure P and the sum of the mole fraction , X_A, for each perturbing species A multiplied by its broadening coefficient $2\gamma_{B-A}$:

$$\Delta\nu_c = P\sum_A X_A 2\gamma_{B-A} \tag{5}$$

Here, B is the absorbing molecule and A represents the possible collision partners. The broadening coefficient varies with temperature according to the following expression

$$2\gamma(T) = 2\gamma(T_0)\left(\frac{T_0}{T}\right)^N \tag{6}$$

where T_0 is a reference temperature [K], $2\gamma(T_0)$ is the broadening coefficient at the reference temperature, and N is the temperature coefficient, which is typically in the range 0.5 to 1. For cases in which neither Doppler nor collision broadening can be neglected, the true lineshape is a combination of the two distributions, resulting in a Voigt profile. The Doppler and collisional widths are related by the Voigt a parameter as following:

$$a = \frac{\sqrt{\ln 2\Delta \nu_c}}{\Delta \nu_D} \tag{7}$$

Diode laser absorption measurements of water vapor temperature use a two-line technique. Temperature is inferred from the ratio of the integrated absorbance of two molecular transitions of the same species (H_2O). The use of the integrated absorbance ratio eliminates the H_2O partial pressure dependence, and temperature can then be calculated by employing the temperature dependencies of each transition. Thus, the temperature is

$$T = \frac{c_2(E_1^" - E_2^")}{\ln R + \ln \frac{S_1(T_0)}{S_2(T_0)} + c_2 \frac{(E_1^" - E_2^")}{T_0}} \tag{8}$$

where E_1", E_2", $S_1(T_0)$ and $S_2(T_0)$ are the lower-state energies and line strengths at a reference temperature T_0, respectively, for the two transitions, $c_2 = hc/k$ where, h is the Planck's constant (6.626 x10^{-34} J-s), c is the speed of light in vacuum (3x10^{10} cm/s), k is the Boltzmann's constant (1.38x10^{-23} J/K) and R is the ratio of the measured integrated absorbance areas. From equation 8, if two lines of different E" which are spectrally close are chosen, then the R_{ls} ratio of line strengths (Arroyo et al., 1994) given by

$$R_{ls}(T) = \frac{S_1(T)}{S_2(T)} = \frac{S_1(T_0)}{S_2(T_0)} \exp\left[-c_2(E_1^" - E_2^")\left(\frac{1}{T} - \frac{1}{T_0}\right)\right] \tag{9}$$

is a unique function of T.

2.1. Selection of Spectral Lines

The choice of the spectral lines to be probed by the system has implications in the sensibility of the measurement system. According to equation 9, the ratio R_{ls} of the strength of two lines is function of temperature and suggests that to choose two lines with the highest possible energy difference and is necessary to achieve the best sensitivity (Arroyo et al., 1994). In this work the ReadHi software (Reacognition of Experimental Absorption Data for HITRAN species) (Ribeiro R. J., 2006) was used to simulate the spectra at various experimental conditions as, for example, the total and partial pressures of the molecules, the path length and the temperature. The simulated spectrum is shown on the screen and it is possible to store the data (wave number versus the absorbance) in ASCII. The software supplies the position and the intensity of the resultant peaks in the spectrum. It is useful to obtain the data of intensity ratio between absorption peaks as function of the temperature, important in flame temperature determination using diode laser spectroscopy. Figure 1 shows the simulated (ReadHi software) absorption spectrum of the water molecule at several temperatures. The choice of the line pairs for this work was 7179.75 cm^{-1} and 7181.15 cm^{-1} using a single laser with emission in the 1.39 μm region. The simulated conditions were: pathlength = 22 cm, total pressure = 1 atm, partial pressure$_{H2O}$ = 0,019 atm and temperature ranging from 250 K to 1600 K.

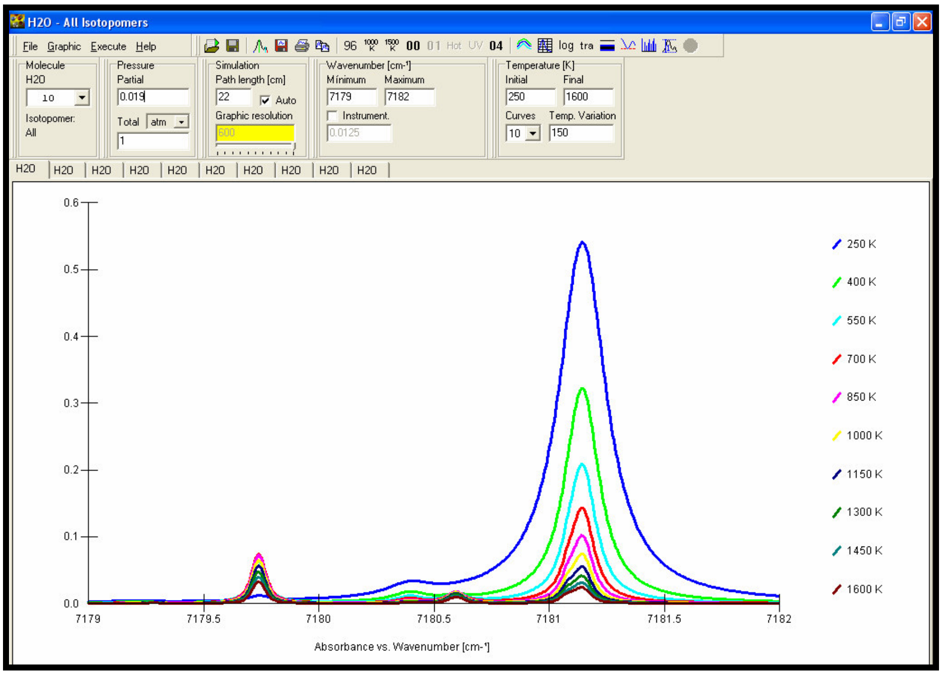

Figure 1. ReadHi simulation of water vapor absorption spectra in 7179,75 cm^{-1} and 7181,15 cm^{-1}. The simulated conditions: pathlenght = 22 cm, P = 1 atm, P_{H2O} = 0,019 atm.

3. Experimental Procedure

Two H_2O transitions at 7179.75 cm^{-1} and 7181.15 cm^{-1} were selected based on the desired absorption and temperature sensitivity of the pair. The system includes one fiber pigtailed InGaAsP DFB semiconductor diode laser (Laser Components) at 1.39 μm modulated at 10-kHz frequency by an injection current modulation ramp (Newport modular controller series 8000). The laser outputs were connected using appropriate single-mode fiber and couplers 50/50 (Optkink). Part of the radiation is collimated and crosses a 22 cm panthlength of the burner flame. The laser beam is then collected by a photodiode detector Newport 818-BB-30A. The other part of the radiation was directly collimated by the detector (reference signal). The signals detected were sent to an oscilloscope (Tektronix 7D20) from where the average signals were sent to the computer through an GPIB/USB interface (Agilent). The program for the data acquisition was made using the HP-VEE software. The flame studied in this work was obtained burning LPG (Liquefied Petroleum Gas) with an equivalence ratio ϕ = 3.0. Figure 2 shows the general arrangement of this combustion experiment.

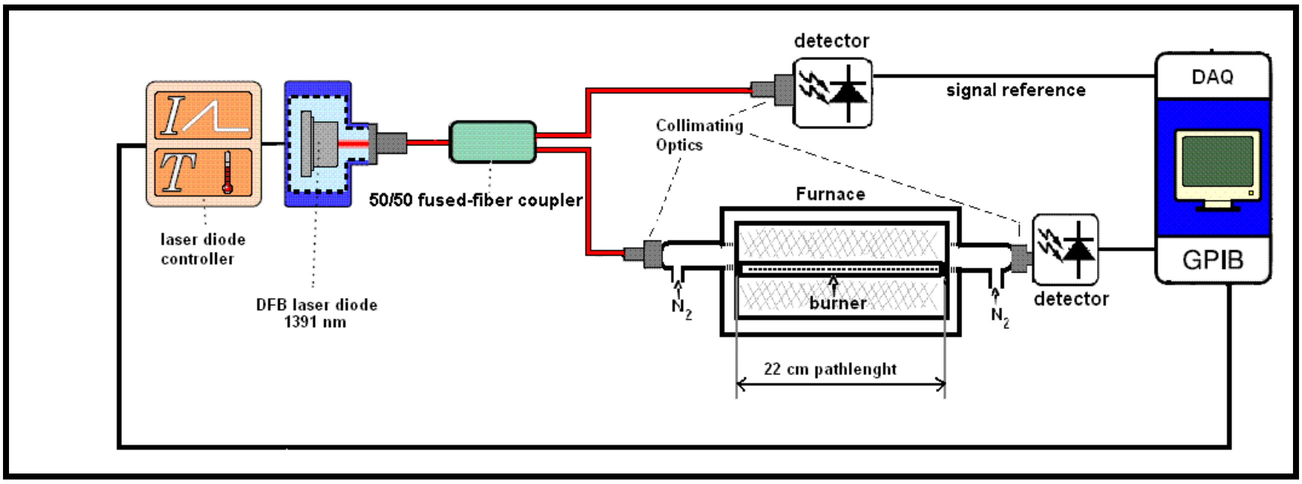

Figure 2. Layout of the Tunable Diode Laser Absorption Spectroscopy System.

Around of the burner, a cell purged with nitrogen gas was placed. This protects the main flow from the external environment, reducing the absorption of the ambient water vapor at 7181.15 cm^{-1}. Figure 3(a) shows a photograph of the system and Figure 3(b) the cell purged with nitrogen coupled to the furnace.

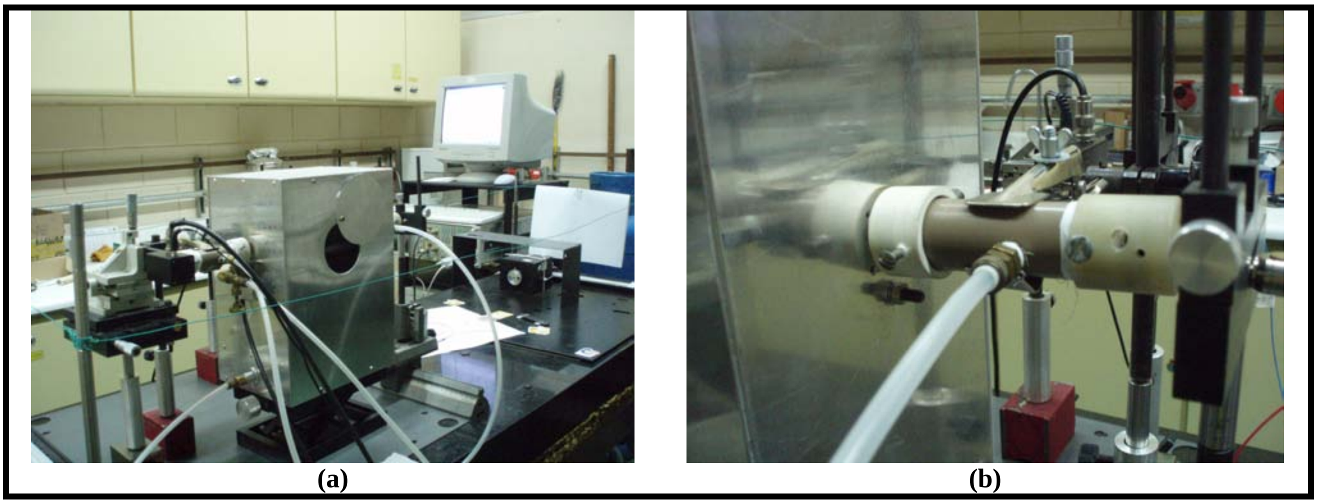

Figure 3. (a) Photograph of the system and (b) the cell purged with nitrogen.

The measurements of the relative intensity were carried out only for lines that absorb above of 5% of the incident laser radiation in this temperature range. Figure 4 (a) presents the graphs of absorbance in 7179.75 cm^{-1} and 7181.15 cm^{-1}, Figure 4 (b) shows the relative intensity ratio between these two lines. It is important to notice that the absorption line must show a minimum absorbance of the 0.01 in order to be detectable using this technique.

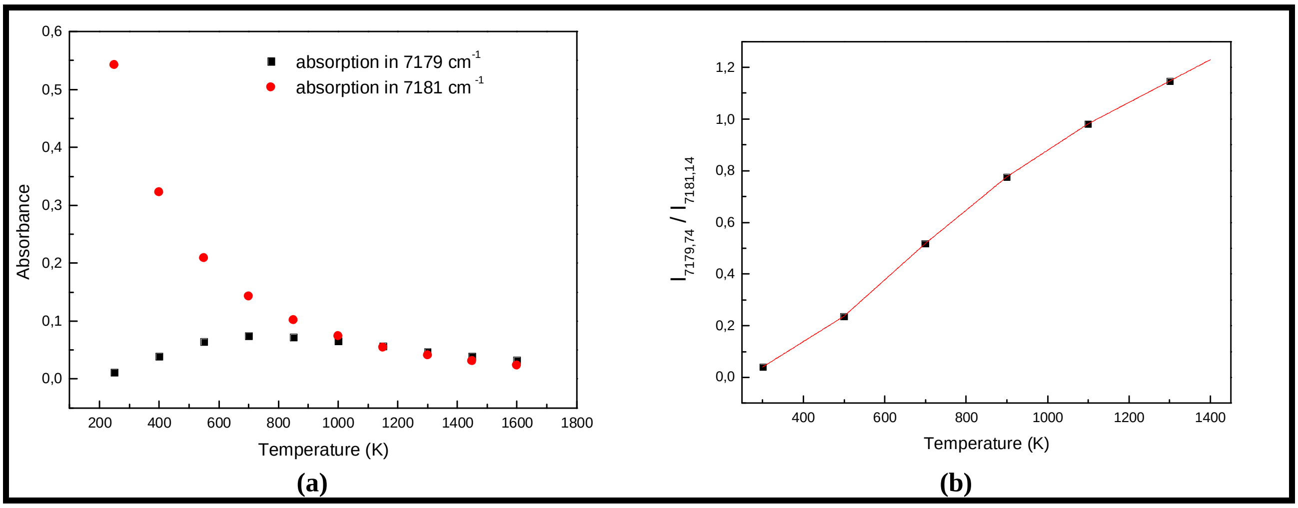

Figure 4. Absorbance of the chosen absorption lines: in 7179.75 cm^{-1}, and 7181.15 cm^{-1} (a) and lines strength ratio variation with temperature (b). Calculated using the ReadHi software.

4. Results

Absorption measurements were made by two different methods: obtaining the absorption spectra for each chosen line separately or the spectra with two lines of absorption in a single scan. The laser is scanned by varying the injection current and maintaining the diode temperature constant. In this way, it was possible to observe if a variation of the temperature occurs in the two different ways of spectrum acquisition using a single diode laser. The experimental spectra for both analyses are presented in Figure 5 (separated scan line absorption) and Figure 6 (two lines absorption in the same scan). From the absorption intensities, and using the relationship given by equation 9, the temperatures were obtained. The results showed a good agreement between the two forms of calculation and are the following: 573 K for the line intensity obtained from the separate spectra and 558 K for line intensity obtained from the single scan. The temperature was also measured directly with a K-type thermocouple (chromel-alumel junction). The obtained temperature for the same conditions of flame was 550 K, which means a good agreement.

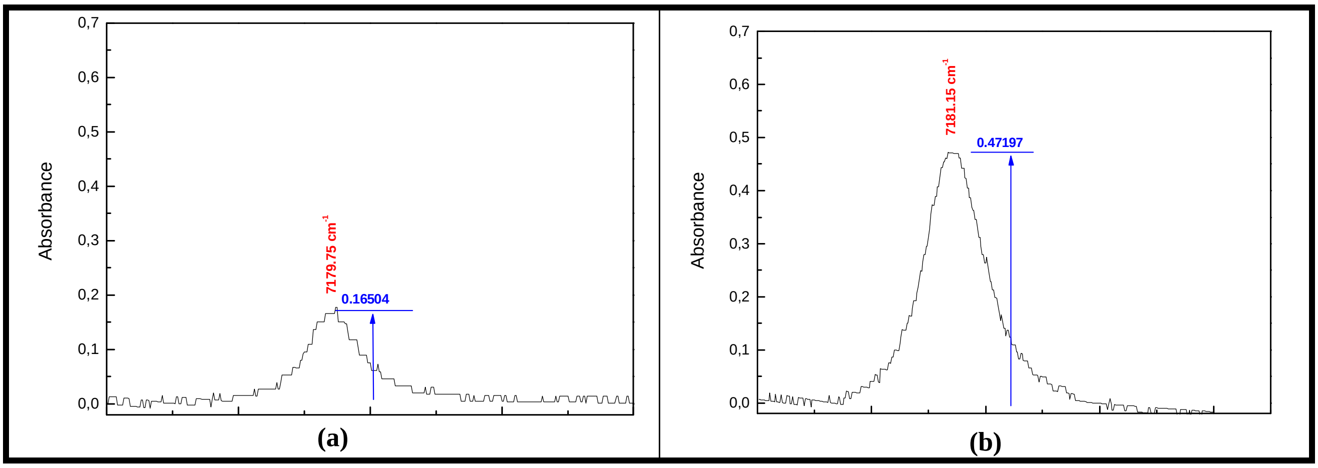

Figure 5. Experimental absorption line spectra obtained with separate scans. (a) 7179.75 cm^{-1} and (b) 7181.15 cm^{-1}. The ratio of line strengths indicated a temperature of 573 K.

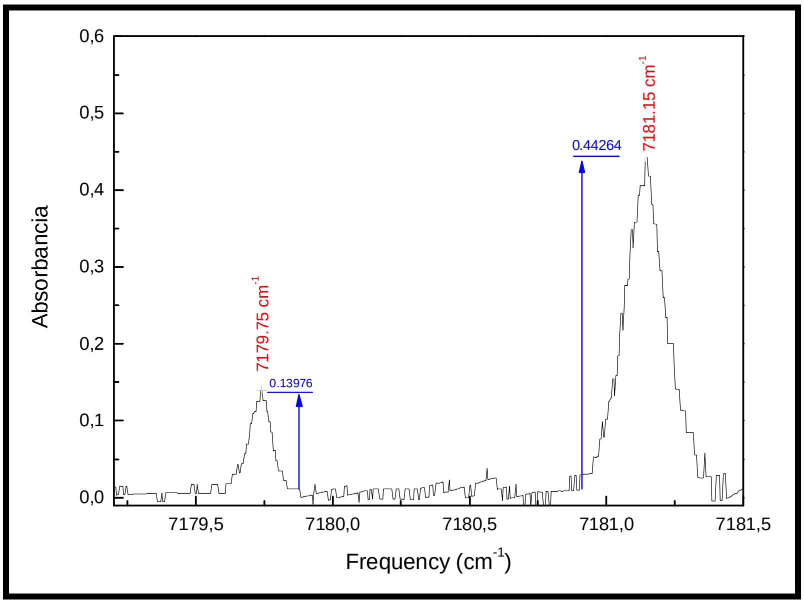

Figure 6. Experimental absorption line spectra obtained in a single scan. The ratio of line strengths indicated a temperature of 558 K.

5. Conclusion

A sensor system using diode laser absorption spectroscopy at 1.39 μm tuned at a 10-kHz modulation rate was developed for temperature measurements of water vapor in a furnace. The non intrusive line-of-sight absorption technique using the sensor system was tested in the laboratory. In this work the ReadHi software was used in the spectra simulation at the experimental conditions. It is useful to obtain data for intensity ratios between absorption lines in function of the temperature, important in flame temperatures determination using diode laser spectroscopy. The preliminary study presented in this paper shows that for two methods of analyses used for the determination of the temperature in a LPG (Liquefied Petroleum Gas) flame with equivalence ratio $\phi = 3.0$ is adequate and the results show good agreement with thermocouple measurements. The obtained temperature from the line intensity using separate spectra was 573 K and from line intensity obtained a single scan was 558 K, close to the measurement with thermocouple (550 K). These experiments indicate the possibility to apply diode laser spectroscopy to obtain water vapor temperature in a scramjet combustor (Supersonic Combustion Ramjet).

6. REFERENCES

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