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Development of a sensor for temperature and water concentration in combustion gases using a single tunable diode laser

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Abstract

The water vapour spectrum in the 1–2 μ m near-infrared region is systematically analysed to find the best absorption transitions for sensitive measurement of H₂O concentration and temperature in combustion environments using a single tunable diode laser with typical distributed feedback single-mode scanning range (1 cm^{-1}) . The use of a single laser, even with relatively narrow tuning range, can offer distinct advantages over wavelength-multiplexing techniques. The strategy and spectroscopic criteria for selecting optimum wavelength regions and absorption line combinations are discussed. It should be stressed that no single figure of merit can be derived to simplify the selection process, and the optimum line pair should be chosen case by case. Our investigation reveals that the 1.8 μ m spectral region is especially promising, and we have identified 10 of the best water line pairs in this spectral region for temperature measurements in flames. Based on these findings, a pair of H₂O transitions near 1.8 μ m was targeted for the design and development of an initial single-laser sensor for simultaneously measuring H₂O concentration and temperature in atmospheric-pressure flames. As part of the sensor development effort, fundamental spectroscopic parameters including the line strength, line-centre frequency and lower state energies of the probed transitions were measured experimentally to improve the current databases. We conclude with demonstration results in a steady and a forced atmospheric-pressure laboratory combustor.

Keywords: gas temperature, water mole fraction, diode laser, combustion monitoring and control

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Sensor systems based on absorption spectroscopy techniques offer significant opportunities and advantages for *in situ* measurements of multiple flowfield parameters such as temperature, pressure, velocity and density due to their high sensitivity, high spectral resolution, fast time response, robustness and non-intrusive character [1–7]. Because of

their compact and rugged packaging as well as low cost, compatibility with optical fibre and relative ease of use, tunable semiconductor diode lasers are nearly ideal sources for sensor applications of these spectroscopic techniques. By proper selection and wavelength tuning of a single diode laser, it is feasible to monitor simultaneously both gas concentration and temperature in combustion environments [7–13].



Figure 1. Survey spectra of H_2O at 1000 K in the NIR region based on the HITEMP database.

Water is an attractive combustion species to monitor, as it is one of the primary products and an excellent indicator of overall combustion efficiency, while temperature, as a fundamental parameter of combustion systems, determines the overall thermal efficiency. Simultaneous measurements of H_2O concentration and temperature thus hold high potential for combustion sensing and control.

Although the structure of a water molecule is simple, its absorption spectrum is relatively complicated. Figure 1 graphically depicts the near-infrared (NIR) line strengths of water over a range of wavelengths from 1 to 2 μ m at a temperature of 1000 K. The widespread and strong absorption transitions provide many options for measuring H₂O and temperature in combustion environments. Building upon the concepts of time-division multiplexing (TDM) and wavelength-division multiplexing (WDM) using two-diode lasers, our research group has performed measurements of H2O and temperature for several years using a pair of features near 1.343 and 1.392 μ m [8]. However, these dual-laser methods have some disadvantages with regard to system complexity and cost. Using a single laser would both simplify the sensor system and reduce cost. Arroyo et al [2] developed an H₂O sensor system near 1.385 μ m using the single-laser concept. Unfortunately, the accuracy and the sensitivity of this sensor for temperature measurements are low, limited by the constrained choice of laser wavelengths (and hence absorption transitions) available at that time. Improvements in the performance, reliability and wavelength availability of tunable diode lasers now offer the potential to increase detection sensitivity and accuracy for H₂O concentration and temperature measurements using a single diode laser.

The most important step in the sensor design is the line pair selection. A proper selection of the line pair can improve the accuracy and performance of the sensor. However, it should be pointed out that the line pair selection is complicated by many interrelated factors which determine the final sensor performance of a particular line pair. Among the most important factors that must be considered in the selection of a line pair are: (a) absorption strength, (b) appropriate spectral separation, (c) temperature sensitivity, (d) lack of interference from nearby transitions and (e) effects of boundary layers. It

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should be stressed that the interaction among all these factors has a considerable influence on the line pair selection process, so that no single figure of merit can be derived to simplify this step, and therefore the optimum line pair should be chosen case by case.

The primary goal of this work is to elucidate useful design rules for the selection of the optimum transitions for a robust, single-diode-laser sensor system for real-time measurements of temperature and water vapour mole fraction in combustion gases at elevated temperature. (The temperature range of interest is 1000-2500 K.) By analysing the NIR water spectrum in the 1–2 μ m range using the criteria we develop, the 10 most promising (by our criteria) NIR single-laser water transition pairs are suggested for temperature measurements in flames; all these pairs lie near 1.8 μ m. One of the optimum transition pairs, located near 1.8005 μ m (5554 cm⁻¹), is selected and utilized to develop a prototype single-laser sensor system. Fundamental spectroscopic measurements of the selected H₂O transitions are used to validate the HITRAN/HITEMP databases [14]. The spectroscopic parameters updated (line strengths, line-centre positions and lower state energies) form the theoretical basis for future applications of this diode laser sensor system. Subsequent to the spectroscopic efforts, the utility of this new sensor is demonstrated in a small-scale laboratory combustor. We conclude that this system has the desired flexibility, high speed and accuracy to be a useful tool for fundamental and applied combustion monitoring. It is important to emphasize that this paper will concentrate on the temperature measurement technology based on two-line water vapour absorption. Building on this research, however, temperature strategies based on absorption in more than two lines may then be derived to yield expanded temperature information [16], and therefore enable temperature measurements in non-uniform conditions.

2. Fundamental spectroscopy

The NIR H₂O spectrum has nearly half a million transitions at 1000 K in the range $1-2 \mu m$. Temperature measurement strategies based on absorption spectroscopy techniques require measurements of at least two transitions. There are multiple different spectroscopic criteria one must consider in choosing a line pair. Understanding the definitions of the various spectroscopic parameters and how they affect the sensor performance will greatly simplify the selection process.

As is well known, the transmission, T_{ν} , of narrowlinewidth radiation at frequency ν through a uniform medium of length L (cm) is described by the Beer–Lambert relation

$$T_{\nu} = \left(\frac{I}{I_0}\right)_{\nu} = \exp(-k_{\nu}L) \tag{1}$$

where I and I_0 are the transmitted and incident spectral intensities and the product $k_{\nu}L$ represents the spectral absorbance, α_{ν} .

The spectral absorption coefficient k_{ν} (cm⁻¹) can be expressed as

$$k_{\nu} = P_{\rm abs} S(T, \nu_0) \phi_{\nu} \tag{2}$$

where P_{abs} (atm) is the partial pressure of the absorbing species, $S(T, v_0)$ (cm⁻² atm⁻¹) and v_0 (cm⁻¹) are the line strength and

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Table 1. Coefficients of the polynomial expression for the partition function of H_2O .				
Coefficients	$70 < T < 405 { m K}$	$400 < T < 1500 {\rm ~K}$	1500 < T < 3005 K	
a b c d	$\begin{array}{c} -0.44405\times10^1\\ 0.27678\times10^0\\ 0.12536\times10^{-2}\\ -0.48938\times10^{-6} \end{array}$	$\begin{array}{c} -0.94327\times10^2\\ 0.81903\times10^0\\ 0.74005\times10^{-4}\\ 0.42437\times10^{-6} \end{array}$	$\begin{array}{c} -0.11727\times10^4\\ 0.29261\times10^1\\ -0.13299\times10^{-2}\\ 0.74356\times10^{-6} \end{array}$	

line-centre frequency of the transition, respectively. ϕ_{ν} (cm) is the line-shape function of a particular transition, which is normalized such that $\int \phi_i(\nu) d\nu \equiv 1$. Thus the integrated absorbance of a single transition can be expressed as

$$A_{i} = \int_{-\infty}^{+\infty} \left[-\ln\left(\frac{I}{I_{0}}\right) \right] d\nu = P_{abs}LS_{i}(T).$$
(3)

The relationship that describes the relative line strengths at an arbitrary temperature T and a reference temperature T_0 is given by

$$S_{i}(T) = S_{i}(T_{0}) \frac{Q(T_{0})}{Q(T)} \left(\frac{T_{0}}{T}\right) \exp\left[-\frac{hcE_{i}''}{k} \left(\frac{1}{T} - \frac{1}{T_{0}}\right)\right] \\ \times \frac{1 - \exp(-hc\nu_{0,i}/kT)}{1 - \exp(-hc\nu_{0,i}/kT_{0})}$$
(4)

where Q(T) is the partition function. The partition function of water is determined over a range of temperatures by using the following polynomial, which represents the best fit of a summation over all calculated energy levels:

$$Q(T) = a + bT + cT^2 + dT^3.$$

The coefficients of the polynomial expression for water are tabulated in table 1 [17].

The water temperature may be inferred from the measured ratio of integrated absorbance for two different temperaturedependent transitions. Because the two integrated absorbances are obtained with the same partial pressure of water and same path length, the ratio of these two integrals reduces simply to the ratio of line strengths, which by equation (4) is given by

$$R = \frac{S_1(T)}{S_2(T)}$$

= $\frac{S(T_0, \nu_1)}{S(T_0, \nu_2)} \exp\left[-\left(\frac{hc}{k}\right)(E_1'' - E_2'')\left(\frac{1}{T} - \frac{1}{T_0}\right)\right]$ (5)

where $S(T_0, v_i)$ is the line strength of the transition centred at v_i (cm⁻¹), for the reference temperature T_0 ; *h* is Planck's constant (J s); *c* is the speed of light (cm s⁻¹); *k* is Boltzmann's constant (J K⁻¹); *E''* is the lower state energy (cm⁻¹); and *T* is the gas temperature (K). Note that the two transitions are sufficiently close to each other (within a single laser scan) that the last ratio term of equation (4) may be set to one.

The relative sensitivity of this ratio to temperature can be obtained by differentiating equation (5):

$$\left|\frac{\mathrm{d}R/R}{\mathrm{d}T/T}\right| = \left(\frac{hc}{k}\right)\frac{|(E_1'' - E_2'')|}{T}.$$
(6)

3. Selection of water line pairs

There have been several studies of transition selections for absorption spectroscopy thermometry. Chang [18] investigated candidate line pairs for NO thermometry near 226 nm in the UV region, and Arroyo *et al* [2] identified a useful H₂O line pair near 1.38 μ m for H₂O thermometry. Nagali and Hanson [3] investigated a diode laser sensor for monitoring water vapour in high-pressure combustion gases in the 1.3–1.4 μ m region. However, a systematic analysis of the broader NIR (1–2 μ m) H₂O spectrum aimed at thermometry has not been reported. The design rules discussed here should prove useful to those interested in temperature sensing using absorption spectroscopy.

A primary objective of this study is to discuss the selection of optimum H₂O line pairs for absorption measurements of temperature and water mole fraction in representative combustion environments (1000–2500 K, $P \approx 1$ atm). At present we limit the selection to transitions accessible within the tuning range of single diode lasers currently available. The following selection criteria are developed.

3.1. Both lines need sufficient absorption over the selected temperature range

The peak absorption of the transition is

$$\alpha_{\nu,\text{peak}} = S_i(T) P x_{\text{H}_2\text{O}} L \phi_{\nu,\text{peak}}$$
(7)

where *P* (atm) is the total static pressure, $S_i(T)$ (cm⁻² atm⁻¹) is the line strength, *L* (cm) is the path length, $\phi_{\nu,\text{peak}}$ is the peak value of line-shape function, and $x_{\text{H}_2\text{O}}$ is the mole fraction of water. An empirical approximation to the Voigt profile [19] is used here to calculate the peak value of the line-shape function.

We assume a minimum detectable absorbance of 10^{-4} , which together with a desired signal-to-noise ratio of 10 requires that the peak absorption be greater than 10^{-3} . In addition, the peak absorption must be less than about 0.8 to avoid experimental difficulties associated with 'optically thick' measurements.

For a path length of 5 cm and a combustion product water vapour mole fraction between 0.01 and 0.3 at a pressure of 1 atm,

$$\alpha_{\nu,\text{peak}} = S_i(T) P x_{\text{H}_2\text{O}} L \phi_{\nu,\text{peak}}$$

= $S_i(T) 1 \text{ atm } 1\% 5 \text{ cm } \phi_{\nu,\text{peak}} \ge 10^{-3}$
 $\alpha_{\nu,\text{peak}} = S_i(T) P x_{\text{H}_2\text{O}} L \phi_{\nu,\text{peak}}$
= $S_i(T) 1 \text{ atm } 30\% 5 \text{ cm } \phi_{\nu,\text{peak}} \le 0.8$

so that the constraint on the product of line strength and lineshape function becomes

$$0.53 \text{ cm}^{-1} \text{ atm}^{-1} \ge S_i(T)\phi_{\nu,\text{peak}} \ge 0.02 \text{ cm}^{-1} \text{ atm}^{-1} \quad (8)$$

in the temperature range 1000-2500 K.

A total of 856 transitions in the HITEMP [14] database meet the absorption strength criterion in the 1–2 μm NIR region.

3.2. The absorption lines lie within a single laser scan, and do not overlap significantly at atmosphere pressure

A typical rapid-tuning range of a single-mode distributed feedback (DFB) diode laser is 1 cm^{-1} . Hence we require that the spectral separation of the line pairs must lie between 0.1 and 0.6 cm⁻¹. If line spacing is larger than 0.6 cm⁻¹, ambiguity in the baseline fit will result in unacceptable uncertainty in the measurements. If line spacing is smaller than 0.1 cm⁻¹, the two lines will overlap at atmosphere pressure. This criterion reduces the potential candidates to 339 line pairs.

3.3. The absorption ratio should be single valued with temperature and the line strengths of the two lines should be similar

The absorption ratio is best determined if the measurement uncertainty is similar for the two absorption transitions. In addition, if one transition is much stronger, the wing of the strong transition will have obvious influence on the measurement of the weak transition. A line strength ratio between R = 0.2 and 5 is thus imposed. Although the limits of R are somewhat arbitrary, this criterion ensures that these two transitions have similar signal-to-noise ratio [3]. There are 285 line pairs which satisfy the first three criteria.

3.4. The two lines should have sufficiently different lower state energy E'' to yield an absorption ratio that is sensitive to the probed temperature

From equations (3) and (4), the line strength ratio can be obtained from the ratio of the integrated absorbance area for two transitions.

$$R(T) = \frac{S_1(T)}{S_2(T)} = \frac{A_1}{A_2}.$$
(9)

This ratio is a function of two integrated absorbance areas A_1 and A_2 , which are measured from the best Voigt fit to the line-shape profile. The uncertainty of *R*, represented by the standard deviation σ_R , is then calculated using the error propagation equation [20],

$$\sigma_R^2 \cong \sigma_{A_1}^2 \left(\frac{\partial R}{\partial A_1}\right)^2 + \sigma_{A_2}^2 \left(\frac{\partial R}{\partial A_2}\right)^2 + 2\sigma_{A_1A_2}^2 \left(\frac{\partial R}{\partial A_1}\right) \left(\frac{\partial R}{\partial A_2}\right).$$
(10)

The partial derivatives in equation (10) are represented as follows:

$$\frac{\partial R}{\partial A_1} = \frac{R}{A_1} \qquad \frac{\partial R}{\partial A_2} = -\frac{R}{A_2}.$$
 (11)

Assuming the integrated absorbance areas A_1 and A_2 are uncorrelated, dR/R can be estimated using

$$\left|\frac{\mathrm{d}R}{R}\right| \approx \frac{\sigma_R}{R} \cong \sqrt{\left(\frac{\sigma_{A_1}}{A_1}\right)^2 + \left(\frac{\sigma_{A_2}}{A_2}\right)^2}.$$
 (12)

The sensitivity of line strength ratio to temperature is obtained from equation (6). It is generally desirable that the temperature sensitivity be as high as possible, resulting in a more accurate sensor.

If the integrated absorbance can be determined within 4%, in order to obtain a temperature accuracy of 5% in the

 Table 2.
 Line selection result using the selection criteria in the NIR region based on HITEMP.

Transitions between 1 and 2 μm	447 207
Transitions, satisfying 1	856
Line pairs, satisfying 1, 2	339
Line pairs, satisfying 1, 2, 3	285
Line pairs, satisfying 1, 2, 3, 4	24
Line pairs, satisfying 1, 2, 3, 4, 5	10

temperature range of 1000–2500 K, the constraint on minimum lower state energy difference becomes

$$|\Delta E_i''| = |E_1'' - E_2''| \ge \left|\frac{\mathrm{d}R/R}{\mathrm{d}T/T}\right| T \frac{k}{hc}$$
$$= \frac{0.04\sqrt{2}}{0.05} 2500 \frac{1}{1.4388} = 2000 \text{ cm}^{-1}.$$
(13)

It can also be seen from this equation that a line pair with a high lower state energy difference is desired to have high temperature sensitivity. This criterion is most acute at the highest temperature of interest, i.e. flame temperatures. There are a total of 24 line pairs that satisfy the first four criteria, and they all have good temperature sensitivity in the temperature range 1000–2500 K.

3.5. The two lines should be free of significant interference from nearby transitions

In all, 14 of the promising pairs of transitions are rejected because of the appearance of adjacent interference features. The remaining 10 line pairs are regarded as the most promising water vapour features for temperature measurement in combustion environments using the selection criteria noted above, including a single laser with a 1 cm⁻¹ scan range. Table 2 summarizes the line selection result. It is clear that studies with different criteria may yield other line pair choices, and it is hoped that presentation of the current selection guidelines will facilitate future investigations of other H₂O transitions and other species, particularly as lasers with broader tuning range become available.

Figure 2 shows the calculated candidate H_2O spectra (P = 1 atm, 10% H_2O and 90% air) based on the HITEMP database [14]; spectroscopic constants are listed in table 3. Figure 2 allows visual inspection of these candidate line pairs. First, note that typically one or both transitions absorb strongly at room temperature, which makes these line pairs sensitive to interference from absorption by ambient water vapour in room air. Consequently it may be necessary to purge outside the target measurement zone.

The line pairs are also ranked by their temperature sensitivity in table 3. Figure 3 presents the temperature sensitivities of the line strength ratio of line pairs 2, 5 and 10 as a function of temperature, using equation (6) and data from HITEMP. Line pair 5 has the largest temperature sensitivity because it has the largest lower state energy difference. If the sensitivity is greater than 1.065, and if the integrated absorbance of individual transitions can be determined within an accuracy of 4%, the subsequent error in the temperature is less than 5%.

Real-time temperature measurements generally require a simple data reduction strategy, e.g. using ratios of the peak



Figure 2. Expanded view of absorption spectra for the selected $H_2O(10\%)$ line pairs in the NIR region based on the HITEMP database; evaluated for P = 1 atm, 10% H_2O , 90% air.

absorption to avoid time-consuming fits to the line shape. However, nearly half of our candidate line pairs (5, 6, 7 and 9) suffer significant interference from nearby lines that limit the direct use of peak absorption ratio to determine temperature, introducing the need for various levels of correction to the peak ratios. For this reason, we have excluded these line pairs from further consideration, though it is certainly possible to develop correction algorithms or look-up table strategies that would allow use of these line pairs.

Ideally, the peak absorption ratio should also be insensitive to pressure. Since the HITEMP database does not provide a value of self-broadening coefficient $\gamma_{H_2O-H_2O}$ for most of the transitions in table 3, the sensitivities of the ratio of peak absorption to pressure and mole fraction are not calculated here. Since pressure effects could become important for realtime temperature measurements in practical systems, it is clear that experimental data for line broadening are critically needed in support of accurate temperature sensing.

From the above discussion, figure 2 and table 3, we see that some line pairs have good temperature sensitivity but



Figure 3. Calculated temperature sensitivity of line strength ratio as a function of temperature for line pairs 2, 5 and 10 based on the HITEMP database.

limited line spacing; thus they are unsuitable for high-pressure applications since the pressure-broadening mechanism will

Table 3. Candidate H₂O line intensity pairs for measurements of temperature and water concentration in the NIR region based on HITEMP.

Line pair	λ (nm)	$v (cm^{-1})$	10 ³ s at 1000 K (cm ⁻² atm ⁻¹)	E'' (cm ⁻¹)	delt E'' (cm ⁻¹)	Sensitivity rank	Line spacing (cm ⁻¹)	Notes
1	1881.23	5315.670	2.1058	2552.88	2457.70	3	0.568	A, B, C
	1881.03	5316.238	3.7153	95.18				
2	1863.29	5366.847	1.9957	2433.80	2017.59	10	0.349	B, C, D
	1863.17	5367.196	3.2740	416.21				
3	1839.95	5434.922	42.2922	173.37	2164.31	5	0.228	A, C, D
	1839.88	5435.150	10.0224	2337.67				
4	1822.75	5486.214	10.2280	503.97	2048.89	7	0.466	B, C
	1822.60	5486.680	2.9274	2552.86				
5	1818.83	5498.025	2.8254	3391.17	2781.06	1	0.178	A, C
	1818.78	5498.203	6.4334	610.11				
6	1818.78	5498.203	6.4334	610.11	2020.11	8	0.224	С
	1818.70	5498.427	5.0516	2630.22				
7	1818.70	5498.427	5.0516	2630.22	2019.88	9	0.570	B, C
	1818.51	5498.997	19.2885	610.34				
8	1812.26	5517.987	3.4634	3135.80	2474.25	2	0.304	A, B, C, D
	1812.16	5518.291	8.1060	661.55				
9	1810.62	5522.964	4.6316	2818.42	2060.64	6	0.491	B, C
	1810.46	5523.455	7.3145	757.78				
10	1800.57	5553.797	2.6036	3314.88	2331.97	4	0.378	A, B, C, D, E
	1800.45	5554.175	9.3542	982.91				

Notes: A: good sensitivity; B: large separation, may be used at higher pressure; C: interfering absorption by room air, purge needed; D: isolated from nearby interference; E: verified experimentally.

make them indistinguishable, while others have large line spacing but moderate temperature sensitivity. In addition, interference absorption by ambient water vapour should be minimized. Considering all these factors, more than half of the line pairs in table 3, namely line pairs 1, 2, 3, 4, 8 and 10, should be suitable for use with a single-laser sensor in combustion applications.

Line pairs 8 and 10 are the two most promising choices because of their large temperature range, good temperature sensitivity and relative isolation from other neighbouring transitions. We have selected line pair 10 for detailed investigation here due to laser availability. In order to proceed with the development of this potential temperature sensor, we must first validate the HITRAN/HITEMP databases, as past work has revealed discrepancies in these databases, especially at high temperature.

4. Spectroscopy experiments, results and discussion

Preliminary spectroscopic experiments for line pair 10 $(5553.80 \text{ and } 5554.18 \text{ cm}^{-1})$ were presented previously [21]. The needed fundamental spectroscopic parameters, including line strengths, line-centre frequencies and lower state energies, are measured using low-pressure H₂O in a heated cell. Figure 4 shows the reduced pair of experimental profiles corresponding to the absorption features at 944 K. Based on the HITEMP database, there are altogether four transitions, as shown in figure 5. 'Line 1' and 'line 4' are low-temperature lines, which are included in HITRAN and HITEMP. 'Line 2' and 'line 3' are high-temperature lines, which are included only in HITEMP. The line strengths for these four transitions are plotted versus temperature in figure 6, as calculated using HITEMP and measured in our heated cell. For 'lines 1, 2, 4', the general agreement between measured spectroscopic parameters and those published in the HITEMP database is good, so we recommend adopting the values listed in the



At atmospheric pressure 'line 1' and 'line 4' are blended. The line strength of 'line 4' is about 7% of 'line 1' at 1000 K and 5% at 1500 K. The effect of 'line 4' is included in the data analysis to improve accuracy; therefore the peak ratio in this case is defined as 'line 2' / ('line 1'+ 'line 4').

The ratio of peak absorption is often used to infer temperature for real-time measurements. Unlike the line strength



Figure 4. Reduced H₂O line shape (line pair 10) recorded in a static cell at T = 944 K, $P_{H_2O} = 17.44$ Torr.

HITEMP database for further use. Note that 'line 3' is a weak transition and ignored for this work.

meter. The measured 'line 1' and 'line 4' positions agree

The line positions are also measured using a wavelength

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Table 4. Spectroscopic data for the selected H_2O line pair.					
Line no	Frequency (cm ⁻¹)	Line strength at 296 K $(cm^{-2} atm^{-1})$	Lower state energy (cm^{-1})		
2 3 1 4	5553.86 5554.04 5554.18 5554.21	$7.298 \times 10^{-7} 3.628 \times 10^{-7} 7.662 \times 10^{-3} 9.200 \times 10^{-3} $	3314.883 3139.505 982.912 173.365		



Figure 5. Line strength of the transitions contributing to line pair 10 near 1.8 μ m at 1000 K based on HITEMP parameters.



Figure 6. Calculated and measured line strengths for the components of line pair 10 as a function of temperature. 'Line 2' is the high-temperature transition at 5553.86 cm^{-1} ; 'line 1' is the low-temperature transition at 5554.18 cm^{-1} .

ratio, the peak absorption ratio is also dependent on water mole fraction and pressure via the line-shape function. To illustrate the relative insensitivity of these factors on the peak absorption ratio of the selected line pair, figure 7 shows the peak absorption ratio as a function of temperature for values of water mole fraction in the range 8-12% at a constant pressure of 1 atm. The results show that a 20% change in water mole fraction only leads to a 1% change in the measured gas temperature. Hence, the peak absorption ratio of this line pair is relatively independent of water mole fraction, which enables simplified data reduction for real-time temperature measurements.

Figure 8 presents the line strength ratio and peak absorption ratio for line pair 10 and their corresponding temperature sensitivities as a function of temperature. At temperatures below 960 K, the line strength ratio is less than



Figure 7. The ratio of peak absorbance coefficients, R_{peak} (line pair 10), calculated as a function of temperature for various values of water mole fraction at 1 atm.



Figure 8. The ratio of line strength and peak absorbance coefficients and their sensitivity to temperature versus temperature for line pair 10.

0.2, which makes accurate measurements of line strength ratio difficult. At temperatures above 3300 K, although the sensitivity is still good, the absorption coefficient of the two transitions becomes quite small. Thus, the selected H_2O line pair for temperature measurement is suitable for use in the temperature range 960–3300 K.

5. Combustion demonstration

Figure 9 illustrates the arrangement employed for a combustion demonstration. Light from a DFB InGaAsP diode laser emitting near 1.8 μ m is directed across a flat diffusion flame stabilized on a Hencken burner. The diode laser is temperature and current controlled (ILX Lightwave LDC-3900) and injection current tuned (SRS DS345) across the



Figure 9. Schematic diagram of the measurement system applied to a Hencken burner.

two absorption transitions. The beam path is purged to avoid interference from ambient water vapour. The flow rates of fuel (C_2H_4) and air are measured using calibrated flowmeters. Water vapour absorption is measured 1 cm above the 5 cm \times 5 cm square flame.

The laser is scanned at 500 Hz across the H₂O line pair to record spectrally resolved absorption line shapes. The transmitted signal is sampled at 1 MHz, which corresponds to 2000 points in each laser scan. The initial intensity signal I_0 is determined by fits outside the absorption lines and extrapolated to the line centre to infer peak absorption. Gas temperatures are inferred from the measured line strength ratio, using equation (5), for each scan (2 ms).

Results are shown in figure 10 for an air flow rate of 64 1 min⁻¹ and fuel flow rate of 2.9 1 min⁻¹ (overall equivalence ratio ~ 0.65). The thermocouple measurements (type S thermocouples, 5 mil wires) are corrected for radiation loss [22]. (The typical correction is 50 K.) The thermocouple is traversed forwards and backwards to confirm stability of the flame temperature. Since the boundary layer is not negligible in this case, it is clear that an assumption of uniform temperature, implicit in the absorption ratio method, will lead to systematic error. The temperature of primary interest is typically the temperature in the core region, which is measured to be 1740 K using the thermocouple. Under the assumption of uniform temperature and mole fraction, the temperature inferred from laser absorption data is determined to be 1620 ± 30 K along this path, i.e. 120 K (7.0%) below the true core temperature, and the measured water mole fraction is determined to be 7.9 \pm 0.3%, i.e. 0.8% (9.2%) under the corresponding calculated equilibrium mole fraction (8.7%).

It is of course not necessary to assume uniform conditions along the absorption path as long as some spatial characteristics of the temperature and absorber concentration are prescribed. For example, in the present case it is reasonable to assume a trapezoidal-shaped temperature distribution with a



Figure 10. Measured temperatures in the burned-gas region above a C_2H_4 -air flame in a 5 cm \times 5 cm Hencken burner.

boundary layer thickness estimated from either the observed thermocouple data or simple mixing-layer analyses. A linear mixing model may be assumed for the water mole fraction between the combustion products' value in the core region and room air humidity at the edge of the flame so that the water mole fraction profile along the line of sight is also a 'trapezoid'.

Using such a simple model, the remaining unknowns, to be inferred from the peak ratio absorption data, are the core temperature (T_{core}) and core water mole fraction (X_{core}). We may solve for T_{core} and X_{core} interactively, recognizing that the integrated absorbance is now given by

$$A_{i} = P \int_{0}^{L} X_{\rm H_{2}O} S_{i,\rm H_{2}O}(T) \,\mathrm{d}x.$$
 (14)

We first assume an approximate core temperature from the uniform temperature assumption and solve the integrated absorbance of one transition for the core water mole fraction X_{core} . Using this X_{core} value, we solve the integrated absorbance of the other transition for T_{core} ; this T_{core} value is further used to solve for a new value of the core water mole fraction, and so on. For the flat-flame diffusion burner used here, convergence is obtained in five iterations to $T_{\text{core}} =$ 1760 K, only 20 K (1.2%) from the radiation-corrected thermocouple value, and the water mole fraction in the core region is about 9.0%, merely 0.3% (3.4%) from the theoretical calculated mole fraction.

This demonstration experiment confirms the sensitivity and potential accuracy of absorption-based temperature sensing, while also illustrating the potential problems associated with non-uniform properties along the line of sight. For combustion flows of the type studied here, it may be sufficient to assume an approximate temperature distribution in reducing the data, or to select line pairs immune to the effect of cold edges [15]. Under other conditions where temperature changes significantly along the absorption path and the relative temperature profile is unknown, the two-line absorption temperature technique may not yield useful results. In such cases, it may be attractive to consider use of a larger number of absorption lines, as has been reported for an oxygen sensor by Sanders et al [16]. They demonstrate the use of many absorption lines to determine the extent of the hot (or cold) regions in the optical path.

The laser absorption sensor offers fast time response for line-of-sight measurements making it well suited for control of combustion instabilities. To illustrate the use of the sensor to identify acoustic combustion instabilities, a disturbance was introduced in the flame by modulating the fuel flow with a speaker attached to the bottom of the Hencken burner (see figure 9). The speaker is driven with a 50 Hz sine wave, thus producing an oscillating gas temperature. Figure 11 shows a time series of gas temperature (top panel) and the Fourier transform (lower panel). The dominant and harmonic modes of the temperature fluctuations are clearly shown in the power spectrum. The width of each bar is around 0.33 Hz, which corresponds to the frequency resolution in the determination of the discrete Fourier transform over a 3 s sampling interval. Note the prominent acoustic fluctuation frequency of 50 Hz. These results demonstrate the utility of this sensor for quantitative, accurate identification of acoustic disturbances, as may be utilized for combustion control. The ability of the H₂O sensor to measure concentration and gas temperature and track fluctuations illustrates the potential of this sensor for real-time monitoring and control of combustion.

6. Summary

A single-diode-laser sensor based on absorption spectroscopy techniques is demonstrated to provide rapid and accurate temperature measurements in a combustion environment. The strategies and criteria to select optimum water features in the 1–2 μ m wavelength range have been detailed. The 10 best NIR water transitions for temperature measurements in flames with a single DFB laser were determined by systematically analysing the water spectra in this spectral region. The optimum line pairs are all in the 1.8–1.9 μ m region. The greatest advantage of these water line pairs is the potential to measure both with a single scan for one diode laser. Even though different laser specifications may



Figure 11. Measured temperature and its power spectrum in the burned region above the C_2H_4 -air flame.

enable other (more widely spaced) line pairs, the line selection criteria described here may be applied for a quantitative evaluation of potential transitions. Discrepancies between the experimentally determined spectroscopic parameters and the HITRAN/HITEMP databases are also found in this region. Thus, it is absolutely necessary to verify or experimentally determine the fundamental spectroscopic parameters in the development of a practical sensor.

A specific line pair (number 10) was investigated experimentally, and the pertinent spectroscopic parameters determined from cell experiments, yielding improvements in the spectroscopic database. This line pair should be applicable for temperature measurements in the range from 960 to 3300 K. Demonstration experiments were conducted in a steady and a forced Hencken burner. The presence of cold boundary layers was shown to impact the temperature inferred assuming uniform conditions, but a simple assumption of a trapezoidal temperature distribution was shown to recover very accurate values for the core temperature of the flow. Experiments with forced flames confirmed the utility of the sensor to monitor temperature fluctuations, with potential applications to combustion control.

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