Determination of Temperature Distributions in Air using a Scanning Vertical-Cavity Surface-Emitting Laser

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ABSTRACT
Tunable diode laser absorption spectroscopy (TDLAS) is a very useful technology for making temperature and species concentration measurements in high-temperature flows [1]. In common with most laser-based spectroscopic techniques, its nonintrusive nature and species selectivity have seen it used in atmospheric sensing, combustion studies and compressible flows. TDLAS has been used to measure temperature, velocity and concentration in all these environments.

TDLAS also has advantages that differentiate it from other laser-based techniques. The diode lasers and infrastructure are relatively inexpensive because much of the technology has been developed for the telecommunications market. The small scale and fast scan rates of these devices make them an excellent choice for use as embedded sensors in a variety of industrial applications. The signal from these devices is coherent, allowing spatial filtering in highly luminous environments, and wavelength multiplexing of the devices provides potential for simultaneous multi-species detection.

For all these advantages, TDLAS has a significant limitation that is desirable to overcome: the path-integrated nature of the measurement. If the region through which the beam travels has uniform temperature and mole fraction over the path of the beam and during the scan time, then well-established methods exist that allow measurement of both temperature and species concentration [1]. The current state of the art, however, is insufficient to determine a distribution of temperature or mole fraction along a single line of sight. The distributed feedback (DFB) diode lasers used for most TDLAS temperature and mole fraction measurements can only be current-tuned over a relatively limited range of ±0.1 nm. This is sufficient to scan across one or two transitions in most near-infra-red absorption spectra. Typical temperature measurement systems use the ratio of the area under two transitions to determine the temperature, and usually require two DFB lasers to make one such measurement. If there are temperature variations along the path of the beam, the temperature measured by the diode laser will be an average value, weighted by the response of the ratio of the line strengths to the temperature variations.

If a nonuniform temperature distribution is to be measured, tomographic techniques are usually employed [2]. These techniques can be made to produce good results, but the measurements can be complex to set up, requiring a number of emitters and detectors or a moveable emitter/detector pair. The data analysis is also not trivial.

In many cases of industrial interest there exists a temperature distribution that can be described using a simple analytical form such as a top-hat distribution or a Gaussian distribution, with unknown peak temperature and width parameter. An attempt to measure a temperature using two transitions in such a situation will result in an underestimate of the peak temperature. This paper presents a method for determining peak temperature and width of the temperature distribution along a single line of sight, using a single laser source. For the sake of simplicity, we assume a constant mole fraction along the line of sight and a top-hat spatial temperature distribution. We briefly describe the method and then present the results of some temperature measurements performed using the technique with appropriate analytical descriptions of the absorption behaviour of the top-hat temperature distribution.

Sanders et al. [5] first used the temperature-distribution measurement method employed in this paper. To our knowledge this is the only other use of the technique in the literature. The main difference between this method and that typically used for temperature measurements is the type of laser employed. Sanders et al. used a vertical-cavity surface-emitting laser (VCSEL) [6]. These lasers can produce a circular beam, and the small volume of the lasing material means that their wavelength can be very rapidly current-tuned over ranges exceeding 1 nm. This ‘wavelength agility’ allows several absorption transitions to be covered in a single wavelength scan, a property that is necessary for measuring temperature distributions. Experiments have shown [7] that VCSELS can make close to shot-noise-limited absorption measurements of optical densities as low as 7\times10\textsuperscript{-9}, comparable to the best DFB laser measurements.

If each of the transitions in an absorption scan has a slightly different sensitivity to temperature, the path-integrated absorption signal will be slightly different for each. Using a number of transitions, the measured absorption can in principle be linked to the temperature distribution. This is achieved by nonlinear-least-squares comparison of the experimental absorption spectrum with simulated spectra obtained using initial approximations to the analytic coefficients describing the temperature distribution.

Sanders et al. [5] demonstrated the technique's ability to differentiate between two cells of equal length but at different temperatures and to measure a linear variation in temperature.
over a known distance. In this paper, we extend the technique to measurement of an approximate top-hat temperature distribution in a tube furnace with an important additional variable: distribution width. We are concerned with the implications of introducing this parameter to the technique’s ability to uniquely determine temperature distributions.

2. THEORETICAL BACKGROUND

The A-band of oxygen consists of a series of weak magnetic-dipole electronic transitions. The absorption process is described by the Beer-Lambert law

\[
\ln \left( \frac{I}{I_0} \right) = -\int_{-\infty}^{\infty} S(T) g(v - v_o) \rho \chi dv dl
\]

where \( I \) is the integrated intensity of the laser beam, \( I_0 \) is the integrated laser intensity in the absence of absorption, \( L \) is the total propagation path length, \( p \) is pressure, \( \chi \) is the mole fraction of the absorbing species, \( g \) is the unity-normalised laser lineshape function and \( S \) is the transition lineshaper, defined as [1]

\[
S(T) = S(T_0) \frac{Q(T)}{Q(T_0)} \exp \left[ \frac{hcE^*}{kT} \left( \frac{1}{T} - \frac{1}{T_0} \right) \right]
\]

where \( Q \) denotes the partition function for the molecule, \( E^* \) is the lower-state energy of the transition, and \( T_0 \) is a reference temperature. In this study the Voigt profile is used to describe the lineshape. Transition strengths and energies for the oxygen A-band are tabulated using the HITRAN 2000 database [4] and the simulated fit spectra are calculated using the GENSPECT code library [3], a collection of Matlab scripts that perform line-by-line absorption calculations. An in-house code has been written in Matlab using these routines, to fit the distribution given a reasonable initial approximation for the parameters, using the Gauss-Newton nonlinear-least-squares method. For a computed resolution of 0.01 cm\(^{-1}\), the fitting routine will produce a two-parameter fit to the data within 20 seconds and 12 spectrum evaluations, on a 1 GHz desktop PC.

3. DISTRIBUTION FITTING

As mentioned previously, the temperature distribution we are interested in fitting is the simplest that can be considered practically useful: a top-hat distribution. It has three parameters: peak temperature \( T_1 \), baseline temperature \( T_2 \) and width \( \alpha \). The choice of this distribution fits reasonably well with the furnace we are using to validate the technique, and allows a straightforward integration of Eq. (1) by substituting the lineshaper in Eq. (2). This results in an absorbance for each of the \( i \) transitions scanned across, given by

\[
\ln \left( \frac{I}{I_0} \right) = -S(T_0) \frac{Q(T)}{Q(T_0)} \rho \chi \times \left[ \alpha \exp \left( \frac{hcE^*}{k} \left( \frac{1}{T_1} - \frac{1}{T_0} \right) \right) \right] \exp \left( L - \alpha \right) \exp \left( \frac{hcE^*}{k} \left( \frac{1}{T_2} - \frac{1}{T_0} \right) \right)
\]

An indication of the sensitivity of the relation to each of the three parameters can be found using the partial derivatives with respect to \( \alpha \), \( T_1 \) and \( T_2 \). From Eq. 3, the absorbance varies linearly with \( \alpha \), but in a more complex manner with the two temperature parameters. For the appropriate temperature values, there is sure to be an optimal value for the distribution width. The form of the temperature sensitivity is more complex, but Eq. 3 indicates that the existence of a unique optimum pair \( T_1 \) and \( T_2 \) is difficult to prove in general.

![Figure 1: Change in the integrated absorbance across a 1-nm wavelength range between 760.5 and 761.5 nm with a 10-K change in temperature.](image)

The sensitivity of this distribution-fitting method is illustrated in Fig. 1. The plot is obtained by evaluating spectra 10 K above and below each set temperature, summing the squared difference between the two spectra. This technique was used to determine the most sensitive region of the spectrum for temperature measurements between 290 K and 1800 K. The temperature decreases by more than three orders of magnitude between these values, showing that the transition used in this study are significantly more sensitive to lower temperatures than high temperatures. This fact has important implications for measurements in flowfields where there is a small, hot region embedded in a larger room-temperature flow path.

Tests of the fitting capabilities of the method were performed using simulated data generated using GENSPECT, allowing us to test the method without the added complication of experimental uncertainty. These tests provide insight into the complex interactions that generate the sensitivity to the three fit parameters, and they help determine whether a unique converged solution can be achieved for the top-hat temperature distribution. Results are presented here for \( T_1 = 800 \) K, \( T_2 = 290 \) K and \( \alpha = 0.6 \) m over a 1-m path length. The results of these computational tests can be summarised as follows:

- The solver did not converge to a unique solution when attempting to fit to all three parameters. The solver would converge to any of several solutions, a few of which are shown in Fig. 2. The spectra for these fitted values are nearly identical, despite the large differences in peak temperatures and widths between the different distributions. The plots show that the optimisation will fit to either a thinner region of higher temperature or a thicker region of lower temperature.
- If the width was set constant and not equal to half the total path length, the solution would converge to one of two values, depending on the initial guesses for the two temperatures. Initial guesses for which \( T_1 > T_2 \) would converge to the correct values. If \( T_2 > T_1 \), the solver would converge to a local minimum for which \( T_2 > T_1 \). If the width is half the path length, the two solutions are degenerate.
4. APPARATUS AND METHOD

Figure 3 shows the apparatus used in the experiment. An Avalon Photonics VCSEL laser (AVAP-760SM) produces up to 500 µW of single-mode radiation, with a quoted spectral width of < 30 MHz. The laser temperature is controlled using a Thorlabs TED 200 temperature controller, and the current is controlled using a Thorlabs LCD200 VCSEL laser diode controller. The current controller is modulated using a 100-Hz sawtooth waveform from an Agilent 3320A function generator. The current is modulated from the 3 mA threshold until multimode behaviour starts to be produced, at a drive current of approximately 7 mA. This tunes the laser over a sufficiently large wavelength range to capture eight isolated transitions. The wavelength region between 760.5 and 761.5 nm was chosen for this investigation after 1-nm regions across the entire $\lambda$-band were investigated and this region was shown through simulations to have the highest temperature sensitivity over the temperature range of interest.

The beam is collimated using a 12-mm focal length antireflection-coated lens and split into two beams of equal intensity, one of which passes through a periscope and traverses the 38-mm-diameter tubular furnace (Carbolite MTF 12/38/250) twice. The furnace is open-ended with spun quartz plugs at each end, leaving a 10-mm-diameter aperture for optical access. The path length difference between the two beams is chosen to be equal to twice the distance between the mirrors on either side of the furnace. This allows the detection system to cancel the effect of the room-temperature path travelled by both beams. The beam splitter is wedged, the collimating lens tilted slightly, and the detector windows removed to prevent the formation of interference fringes in the detected signal.

The detection system uses a log-ratio detection circuit — a log102AID integrated circuit and two high-speed silicon PIN photodiodes (Thorlabs FDS100). Balanced ratiometric detection was chosen for this experiment because it cancels common-mode noise in the laser, removes the ramp offset that occurs in direct absorption measurements and produces an output that is directly related to the absorbance used in the fitting routine [1]. Use of ratiometric detection also removes the need to purge the surrounding gas of oxygen, because the effects of absorption over the common paths cancel at the detector. The log102AID has a built-in operational amplifier that is used to amplify the signal for acquisition by a National Instruments PCI-6115 data acquisition system. Using this system, a signal-to-noise ratio of 100 was achieved for single-scan spectra over the 1.13-m path length. The smallest significant scale over which temperature variations could be measured is 10–15 mm.

Figure 4 shows a sample spectrum fit to the furnace distribution for 1273 K. The amplification factor was used for all the furnace measurements.

The laser wavelength was calibrated against diode injection current using an Ando 6315 optical spectrum analyser. Because the system current-tuned over eight transitions, the wavelength had to be more finely calibrated using a polynomial to fit the experimental peak locations to the theoretical peak locations. Additionally, although the ratiometric detector removes the offset from the signal, the nonlinear behaviour of the current response at currents above 6 mA required a polynomial fit for the spectrum's baseline. The transitions were spaced sufficiently far apart for this to be feasible. The measurements were sufficiently repeatable that a single pair of these calibrations sufficed for all the analysed spectra at each condition.

Fifty spectra were acquired for each of two furnace set temperatures: 773 K and 1273 K. The temperature in the furnace was measured using a type K thermocouple. A tube furnace has two advantages for this study over a laminar flame: variations due to changes in oxygen mole fraction across the path length are removed, and the thermocouple measurement does not need to be corrected for radiation losses.

A room-temperature spectrum was compared with a computed spectrum at the same conditions. The amplification factor of the circuit was determined by scaling the experiment until the spectrum best fitted that of the calculation. This amplification factor was used for all the furnace measurements.

5. EXPERIMENTAL RESULTS

Figure 4 shows a sample spectrum fit to the furnace distribution for 1273 K. Experiment and computation are consistently well matched between individual scans at the
same nominal furnace conditions. There is a discernible decrease in fit quality towards the high-wavenumber end of the scan range, mostly because of the nonlinearity of the baseline signal at higher injection currents.

Fitting a top-hat distribution to the measured spectra produced parameter values of $T_1 = 769 \pm 11$ K and $\alpha = 0.542 \pm 0.005$ m for the lower temperature and $T_1 = 1283 \pm 41$ K and $\alpha = 0.597 \pm 0.005$ m for the higher temperature, as shown in Fig. 5. Despite the thermocouple measurements showing a more rounded distribution with a noticeable slope that cannot be replicated using the top-hat functional form, the assumed distribution agrees with the peak thermocouple measurement at both temperatures to within the standard deviation of the measurements. The greater width of the distribution at the higher temperature is also captured by the fitting technique.

Tests were also performed to investigate the sensitivity of the measurements to the assumed background temperature. Overestimating the background temperature of the higher temperature distribution by only 10 K generated a systematic error in the peak temperature of 12 % and reduced the fitted width by 5 %.

6. CONCLUSIONS

These experiments have shown that both the peak temperature and width of a simple temperature distribution can be precisely determined along a line of sight for a temperature distribution using two free parameters, where the mole fraction of the absorbing species is constant. Better than 3.5 % agreement with thermocouple measurement was achieved in both cases. Careful measurement of the fixed background temperature was required to avoid large systematic errors in the measured peak temperature.

Care needs to be exercised when the width of the distribution is fixed and the two temperatures are treated as free variables. When the two path lengths differ, the fitting routine would fit to a local minimum different from the correct solution depending on the initial guess. If all three parameters were allowed to vary, the routine could not find the correct distribution, a result supported by fitting simulated spectra. These problems are caused by the lack of sensitivity of the A-band transitions at high temperatures. Similar spectra can be produced using significantly different temperature distributions, so the method as used here requires high signal-to-noise ratios in experimental measurements. More complex molecules with a greater variety of rotational energies within the scan range of the laser would produce more sensitive measurements. The technique would also better capture the distribution using a function that allows a gradient between the two temperatures, and this is the focus of current work. The existence of local minima suggests that a population-based optimisation method may be more successful for fitting any two-parameter combinations, but the differences between spectra appear to be too subtle to allow a three-parameter fit to this distribution regardless of the optimisation method used.

REFERENCES


