5. Sensor design

In the previous chapter, it was shown that if the integrated absorbance of two different spectral lines of water vapour can be measured, then water vapour number density and temperature can be deduced. No guidance was provided for the selection of absorption lines or how such a measurement should proceed. This chapter describes an experimental system which was built to perform this measurement, and provides justification for design decisions made along the way. The design decisions were made with the understanding that measurements would be made in a scramjet combustor operating in a free-piston shock tunnel.

The development of a new sensor can be guided by examining some of the previous examples of diode laser sensors in the literature. Section 5.1 provides a brief review of some of these, section 5.2 outlines the process for selecting which spectral lines to use, section 5.3 describes the physical design of the sensor and section 5.4 describes the data reduction process.

5.1 Other diode laser based sensors

Since their invention in the 60s, diode lasers have been widely used as narrow line-width sources for high resolution spectroscopy. With line-widths significantly narrower than Doppler-broadened line shapes, spectrometers based on semiconductor diode lasers have permitted the experimental study of spectral line shapes [26, 63, 69, 70].

In addition to fundamental spectroscopy, diode laser sensors have found numerous applications for gas-dynamic sensing. Many applications are reviewed by Allen [3], who provides more examples than the brief list given here. In gas-dynamic sensing, the goal is the measurement of bulk gas parameters, rather than molecular spectroscopic parameters. As well as finding the concentration of the absorbing species, sensors can be designed to measure temperature and flow velocity [90]. Flow velocity measurements require the flow to have a component parallel to the probe beam, allowing velocity to be deduced from the Doppler shift of the line centre. With velocity and species concentration known, mass flux can be calculated.

The species chosen for absorption fall into two categories. Either a tracer species can be introduced to the flow in low concentration, or a species can be chosen that is naturally present. Common tracers are rubidium [84, 115] and
potassium [124, 125]. These species absorb strongly near the operation wave-
length of diode lasers used in CD players, which is 780 nm, so suitable lasers
are readily available. The aforementioned references report the use of tracer
species to measure temperature and velocity in pulsed facilities.

While the concentration of tracer species is generally not of interest, the con-
verse is true of naturally present species. In environmental measurements,
species concentration is often the most important parameter, and the use of
diode laser spectroscopy allows in situ measurement from platforms including
balloons [102], aeroplanes [91] and sounding rockets [64]. Measured species
include N₂O, CH₄, CO, HCl, NO₂ [102] with lead salt diodes and CH₄ and H₂O
[31] with telecommunications diodes. Telecommunications diodes operate at
room temperature, which makes them easier to work with than lead salt diodes
which operate at cryogenic temperatures and require liquid N₂ or He cooling.

Species measurements are also important in combustion studies, which has
motivated the development of numerous sensors. Species measured at high
temperature include H₂O [129], O₂ [7], OH [2], CO and CO₂ [120].

In general, diode laser spectroscopy produces results that are related to the
variation of properties along the line of sight. If experimental conditions allow,
tomographic reconstruction can be used to determine gas properties in a 2–
dimensional plane [105]. An alternative approach is to probe many absorption
lines, which all have a different dependence on temperature, and then fit an
assumed line-of-sight function to the experimental data [101].

Examples of diode laser spectroscopy applied to scramjet measurements are
few. One example was reported by Upschulte et al. [118, 119]. This sensor
targeted water vapour near 1310 nm which was present in the Mach 2.1 flow in
a model scramjet combustor. The sensor was configured to measure water con-
centration, temperature and velocity. Temperature in the free-stream ranged
from 540 to 740 K. The measurement was challenging, partially due to the low
strength of the absorption lines that were used, but also because of the turbu-
lent flow. The present work is similar to the work of Upschulte et al. [118, 119].
Notable differences were that, in this work:

- Stronger absorption lines were used, as recommended by Upschulte et al.
  [118, 119];
- Measurements were in a pulsed facility; and
- Water vapour was present only as a product of combustion in the scramjet
  duct. Upschulte et al. [118, 119] measured water vapour present due to
  the burner used to heat the inlet air.

The development of a sensor for scramjet measurements in pulsed facilities has
also been of interest. Tsai [116] reports on a two-line water vapour absorp-
tion sensor intended for scramjet measurements in a pulsed facility. According
to Tsai, the sensor is a refinement of a single-line sensor previously used in
scramjet tests. While Tsai evaluates the performance of the sensor in a flame,
5.2. Selection of spectral lines

The choice of which spectral lines are to be probed by the system has implications for the sensing abilities of the system. As has been seen in equation (4.8) on page 35 the ratio, $R_{ls}$, of the strength of two spectral lines is a function of temperature with relative sensitivity, repeating equation (4.9),

$$\left|\frac{dR_{ls}}{R_{ls}}\right| = c_2 \frac{|E''_1 - E''_2|}{T}.$$

This suggests that choosing two lines with a maximum lower-state energy difference is advisable to achieve the best sensitivity. This requirement is contradicted by the need to choose two lines whose lower-states are sufficiently populated at the intended measurement temperature, a requirement which places a limit on the actual $|E''_1 - E''_2|$ that can be obtained.

Several spectral databases are available that catalogue parameters of spectral lines, including their location, strength and lower-state energy. A commonly used source is the HITRAN database [98] along with its superset companion, HITEMP. HITEMP includes all of the lines of HITRAN but is intended for high-temperature applications; it includes lines that are too weak to be observed at room temperature but become important at flame temperatures.

Over twelve thousand water vapour lines are listed in the HITRAN database between $1 - 2 \mu m$, a part of the spectrum where laser sources are easily available. A systematic approach is required to find the best candidate lines and Zhou et al. [129] present such an approach. They use a similar methodology to that previously taken by other researchers, but report it in a clear and systematic manner. The approach is applicable to the development of other diode-laser spectroscopy systems. Zhou et al. applied their rules to the database in the order:

1. Lines must have sufficient strength over the intended temperature range;

2. Line pairs should be close enough to be traversed in a single laser scan (spacing $\lesssim 1 \text{ cm}^{-1}$) but remain distinct at atmospheric pressure;

3. Line pairs should have similar strength to maximise signal to noise and reduce overlap, Zhou et al. imposed $0.2 \leq R_{ls} \leq 5$;

4. Line pairs require sufficient relative sensitivity, or change in line ratio with temperature; and
5. Lines should be free from interference from neighbouring transitions.

Using this analysis, Zhou et al. found 10 prospective line-pairs in the 1–2 µm region of the water vapour spectrum, all near 1.8 µm. These line pairs were not used here, however, for the reasons outlined below.

For this work, rule (2) can be modified since Zhou et al. required their sensor to operate with a single diode laser and the use of two lasers has the advantage of a wider possible separation between the transition wavelengths of the two lines. It remains advantageous to choose close spectral lines because custom-made diode lasers are priced on the basis of the number ordered: it is much cheaper to buy two diode lasers at the same wavelength and then use the temperature tunability of the lasers to access different spectral lines than it is to order two diodes with different specifications. With this in mind, a separation of up to approximately 15 cm\(^{-1}\) is possible which has the further advantage of reducing the overlap between the two lines, reducing the importance of rule (3).

A further constraint on the choice of spectral lines was due to the physical configuration of the experiment. As explained in section 7.1, the laser output was delivered to the combustor model which was located inside a vacuum-sealed dump tank. This was achieved by using single mode fibre-optic cables and therefore it was desirable to choose a laser wavelength that was compatible with telecommunications fibre optic cables and components which operate best near 1.3 and 1.5 µm.

If we are to follow the approach of identifying candidate line pairs from HITRAN/HITEMP, the line strength variation with temperature needs to be verified in a controlled environment. For temperatures up to around 1000 K a heated test cell can be used, while a burner is required above these temperatures. This step is necessary because:

- Line strengths in HITRAN can have significant errors, above 20% when compared with experiment [114];
- The line strength variation with temperature of lines in HITRAN and HITEMP is not well verified at high temperatures;
- Spectral lines are listed in the databases that do not appear in observations; and
- Spectral lines are observed when they have not been listed in the database, especially at elevated temperatures.

Because of the requirement to verify transitions predicted by HITRAN, and the cost and six-month lead time associated with buying diode lasers, it was decided for this work to use line pairs that have been used previously for water vapour spectroscopy. The lines were to be the same as those used by Allen et al. in previous unpublished work [4]. Allen et al. had identified three spectral lines near 1.39 µm—a location where off-the-shelf telecommunications fibre-optics can be used—suitable for thermometry over the range 300 – 3000 K. Of the three lines,
Table 5.1: Transitions probed in this study

<table>
<thead>
<tr>
<th>Index</th>
<th>Line position [cm(^{-1})]</th>
<th>Quantum Numbers</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Toth[114]</td>
<td>HITRAN[97]</td>
</tr>
<tr>
<td>1</td>
<td>7181.15570</td>
<td>7181.1720</td>
</tr>
<tr>
<td>2</td>
<td>7179.7519</td>
<td>7179.7521</td>
</tr>
</tbody>
</table>

\(^1\) The index is used within this thesis, typically as a subscript

\(^2\) Vibrational quantum number: \((\nu_1, \nu_2, \nu_3)\)

\(^3\) Rotational quantum number: \(J_{K_aK_c}\)

one was used over the entire temperature range, one was used over a ‘low temperature’ range and the other was used over a ‘high temperature’ range with a turnover point at around 1600 K.

The high temperature line was not visible in measurements until temperatures reached 1400 K and was not catalogued in either of the HITRAN or HITEMP databases. This was a further justification for not selecting line-pairs from the HITRAN database since it seemed less reliable at high temperatures.

Preliminary experiments showed that the experimental configuration used here was not sensitive enough to make measurements using the high temperature line used by Allen et al. in shock tunnel experiments. As a result, only two of the three lines were used in this study, and their parameters are shown in table 5.1. Both of these lines are catalogued in HITRAN with the following caveats\(^1\):

- The strength of the line near 7181 cm\(^{-1}\), line 1, is over-predicted by HITRAN when compared with Toth’s measurements [114]. Furthermore, as shown by measurements presented later, at elevated temperatures and atmospheric pressure, a spectral line that is not predicted by HITRAN becomes visible and overlaps the 7181 cm\(^{-1}\) line.

- The line near 7179 cm\(^{-1}\), line 2, was marked as an unresolved doublet by Toth with the quantum number assignments being taken from the

\(^1\)After this thesis had been submitted for examination, the 2004 edition of HITRAN [99] was released. This latest edition is in much better agreement with Toth’s measurements [114] than the 2000 edition of HITRAN [98] used here. For the lines considered in this work, whereas HITRAN 2000 differs from Toth’s measurements by up to 20\%, the difference between HITRAN 2004 and Toth’s measurements is below 5\%.

While it seems reasonable to use HITRAN 2004 in the future, the effect of using Toth’s measurements is small in the present case. If we assume that HITRAN 2004 represents the correct line strengths, then using the line strengths reported by Toth results in the sensor systematically reporting a temperature that is low, by 2.1 K at 296 K (0.7\%) or by 52 K at 1500 K (3.5\%). The only calibration results taken with sufficient reliability to reveal such an offset are shown on page 85. These indicate that the sensor does report a systematically low temperature of this magnitude, at least at room temperature.

Because of the improvements in HITRAN with the 2004 release, systematically searching the database for candidate line pairs should now yield better results.
The strategy used to predict line strength at an arbitrary temperature was to use the reference line strengths reported by Toth and then the lower-state energies, \( E'' \), provided by HITRAN in conjunction with equation (4.6). The result of this prediction for line strength and line ratio is shown in figure 5.1. This shows that line 1 is much stronger at room temperature than at elevated temperatures while line 2 peaks in strength near 900 K. The line strength ratio decreases monotonically as a function of temperature and drops rapidly near room temperature, where line 1 is 75 times stronger than line 2.

The sensitivity of this transition-pair to temperature is shown in figure 5.2. This shows the \( 1/T \) dependence of the sensitivity, which is characteristic of this method of thermometry. At 1550 K the sensitivity crosses 1 and reaches 0.8 at 2000 K. Higher sensitivity to temperature is better, however this analysis shows that it is reasonable to expect temperature measurements up to 2000 K, depending on signal to noise ratio.
5.2. Selection of spectral lines

If we can measure the integrated absorbances $A_1$ and $A_2$ with an uncertainty of 5%, the corresponding relative uncertainty in $R_{ls}$, $\frac{\sigma_{R_{ls}}}{R_{ls}}$, can be found from the relation for the propagation of errors \[ \sigma^2_{R_{ls}} = \frac{\partial R_{ls}}{\partial A_1} \sigma^2_{A_1} + \frac{\partial R_{ls}}{\partial A_2} \sigma^2_{A_2} \] (5.2)

and is given by

\[ \left( \frac{\sigma_{R_{ls}}}{R_{ls}} \right)^2 = \left( \frac{\sigma_{S_1}}{S_1} \right)^2 + \left( \frac{\sigma_{S_2}}{S_2} \right)^2. \] (5.3)

The uncertainty in $R_{ls}$ can be propagated through to $T$ by dividing equation (5.3) by the sensitivity given in equation (5.1), i.e.

\[ \frac{\sigma_T}{T} = \frac{\sigma_{R_{ls}}}{R_{ls}} \left/ \left| \frac{dR_{ls}}{dT} / R_{ls} \right| \right. \] (5.4)

resulting in a maximum relative uncertainty in $T$ of 9% at 2000 K when using the spectral lines given in table 5.1.

Similarly, an analysis can be carried out to determine how well the water vapour concentration is known, given uncertainties in temperature and measured absorbance, signified by $\sigma_T/T$ and $\sigma_A/A$ respectively.

If we neglect uncertainty in the beam path length, and define the integrated absorbance of the two spectral lines as $A_1$ and $A_2$ then the species concentration $N$ is given by

\[ N = \frac{A_1}{(S_1 l)} \] (5.5)

or

\[ N = \frac{A_2}{(S_2 l)}. \] (5.6)

where $S_i$ is the strength of the absorption line, and is a known function of temperature, and $l$ is the path length which we assume to know exactly. In practice,
5. Sensor design

Figure 5.3: Uncertainty in water concentration as a function of temperature, assuming relative uncertainties of 5% in the integrated absorbance of each of the spectral lines.

$N$ has the same numerical value if evaluated from either $A_1$ or $A_2$ when temperature is calculated from the line ratio.

If we find the temperature from the line ratio, $R_{ls} = A_1 / A_2$ and calculate $N$ from the absorption line $A_1$ then $N$ is a function of $A_1$ and $A_2$ and the uncertainty in $N$ is related to the uncertainty in $A_1$ and $A_2$ according to

$$
\sigma_N^2 = \left( \frac{\partial N}{\partial A_1} \sigma_{A_1} \right)^2 + \left( \frac{\partial N}{\partial A_2} \sigma_{A_2} \right)^2.
$$

If we calculate $N$ from $N = A_1 / \{ S_1(T)l \}$ where $T = f(R_{ls}) = f(A_1/A_2)$ we can evaluate $\frac{\partial N}{\partial S_1}$ and $\frac{\partial N}{\partial A_2}$ and find, after some algebra, that

$$
\left( \frac{\sigma_N}{N} \right)^2 = \left( 1 - \frac{dS_1}{dT} / \frac{dR_{ls}}{dT} \right)^2 \left( \frac{\sigma_{A_1}}{A_1} \right)^2 + \left( \frac{dS_1}{dT} / \frac{dR_{ls}}{dT} \right)^2 \left( \frac{\sigma_{A_2}}{A_2} \right)^2.
$$

(5.7)

If we again assume that both $A_1$ and $A_2$ have uncertainties of 5% we can plot equation (5.7). As shown in figure 5.3, this uncertainty has a minimum near 600 K which is below 5%. However, this increases rapidly with increasing temperature.

This analysis shows that for a measured $A_1$ and $A_2$ not only can the temperature and water vapour density be calculated, but we also have a means of predicting the uncertainty in these measurements from equation (5.4) and (5.7) respectively, if we assume a particular uncertainty in $A_1$ and $A_2$. 

\[\text{Figure 5.3: Uncertainty in water concentration as a function of temperature, assuming relative uncertainties of 5% in the integrated absorbance of each of the spectral lines.}\]
5.3 Physical sensor design

The components of the TDLAS system were configured as shown in figure 5.4. Two diode lasers (Laser Components SPECDILAS DFB diodes) were driven with ILX Lightwave Laser Diode Controllers (LDC 3700B) in a time-multiplexed mode of operation. The two lasers scanned approximately 0.5 cm$^{-1}$ across two different absorption lines at a repetition rate of up to 20 kHz, although 10 kHz was more typically used during experiments.

The output from the lasers was coupled into optical fibres which delivered the beam to the test gas location and to a fibre-based interferometer. The interferometer measured the relative frequency of the lasers as they scanned across the absorption lines and was constructed from connectorised optical fibre and commercially available fused-fibre couplers (Newport F-CPL-L12355).

A linear fibre-coupled detector was used to detect the output from the interferometer. However, a more sophisticated detector was used to measure the absorption signal in the test gas. This detector, described in more detail later in this chapter, produced an output related to the log–ratio of two input channels. These channels were labelled the ‘reference channel’ and ‘signal channel’ where the signal channel beam had passed through the test gas.

The signal generator and laser controllers were controlled over the GPIB bus through a custom written LabVIEW [74] interface. Data were acquired from the interferometer and log–ratio detector via a data acquisition card based in the same computer (NI-PCI6110E). While in free-running operation the outputs from the data acquisition channels were continuously displayed, and an example of the control program while in this mode is shown in figure 5.5.

During experiments, data acquisition would be initiated by an external trigger and would run for a predetermined number of scans. These were then post-processed using functions implemented as MATLAB [112] M-files. This automated process converted the raw data from the acquisition system into time-resolved measurements of temperature and water vapour concentration.

A more detailed description of the diode lasers, optical components and detectors follows.
5. Sensor design

Diode lasers

When compared with other lasers, diode lasers are high efficiency and inexpensive devices [53], whose development has been accelerated by their applications in consumer electronics, such as CD and DVD players, and telecommunications. These devices are highly reliable, small and rugged and the TDLAS technique owes a lot of its practical advantages to the characteristics of diode lasers.

As discussed in detail by Saleh and Teich [100], diode lasers are semiconductor devices that convert an injected electrical current into light as it passes through a forward biased p-n junction. The general arrangement of the diode is shown in figure 5.6. This is similar to the structure of light emitting diodes (LEDs), with the addition of reflecting surfaces on either end of the cavity. Photons produced in a diode laser junction, therefore, are the result of stimulated emission, rather than the spontaneous emission that characterises LEDs.

The control of the diode wavelength depends on the reflection properties of the cavity as well as the effective refractive index within the active medium [68]. In general, it is desirable to select a specific wavelength which is reflected back into the cavity to generate a spectrally narrow output. Schemes such as an external cavity, distributed Bragg reflector (DBR) or distributed feedback (DFB) can be employed. These three configurations are shown in figure 5.7. DFB lasers were used in this work.

The effective refractive index within the active region of the laser is dependent on temperature and injection current, providing a convenient means of tuning the diode laser output. The two effects are complimentary, tuning the diode by changing its temperature means a slow temporal response but allows relatively large tuning ranges. Injection current tuning provides a small range but
5.3. Physical sensor design

Figure 5.6: Simplified schematic of a laser diode (after Saleh and Teich [100]). The cleaved faces of the active regions act as mirrors creating a cavity in the active region. More commonly, laser diodes have a more complex structure with multiple layers of semiconductor material. These are known as heterostructure diode lasers and are designed this way to reduce the band gap and therefore threshold current.

Figure 5.7: Different types of edge-emitting diode lasers, showing methods of ensuring single-mode operation. Distributed feedback (DFB) lasers were used in this work.
5. Sensor design

Table 5.2: Characteristics of the DFB laser diodes used in this work.

<table>
<thead>
<tr>
<th>Characteristic</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peak optical power at 25°C</td>
<td>2 mW</td>
</tr>
<tr>
<td>Side mode suppression ratio</td>
<td>−25 dB</td>
</tr>
<tr>
<td>Line width</td>
<td>10 MHz</td>
</tr>
<tr>
<td>Material</td>
<td>InGaAsP</td>
</tr>
<tr>
<td>Temperature tuning coefficient</td>
<td>0.5 cm⁻¹/K</td>
</tr>
<tr>
<td>DC current tuning coefficient</td>
<td>0.07 cm⁻¹/mA</td>
</tr>
<tr>
<td>Beam divergence (FWHM)</td>
<td>25° × 50°</td>
</tr>
<tr>
<td>Supplier</td>
<td>Laser Components GmbH</td>
</tr>
</tbody>
</table>

fast response. In an InGaAsP laser, as used here, increasing either current or temperature increases the wavelength of radiation emitted by the laser.

When applied to a TDLAS system, the most important properties of a diode laser are:

- Wavelength tunability should be rapid and over a large range, compared with the spectral features that need to be resolved;
- The output wavelength should be free of mode hops, i.e. frequency discontinuities, over the tuning range; and
- The laser spectrum should be narrow when compared with the width of the target spectral line.

Laser diodes with these characteristics were purchased from Laser Components \[62\] and their nominal specifications are shown in table 5.2. These were custom-made diodes designed specifically for spectroscopy and their most noticeable disadvantages are high cost and long delivery time. An alternative to using custom made diodes is to use standard telecommunications diodes at around 1310 nm, accessing much weaker water vapour transitions than those near 1390 nm. Reference \[119\] is an example of a sensor that targets these transitions. Two such diodes, Mitsubishi ML776H11F, were purchased to test the remainder of the TDLAS system while waiting on delivery of the spectroscopic diodes.

The operation of laser diodes is complicated by their propensity to be destroyed by relatively weak electrostatic discharges. Furthermore, for spectroscopy, the temperature of the diode needs to be precisely controlled. A block diagram of the control electronics is shown in figure 5.8.

Each laser is housed in an ILX LDM4412 laser diode mount which includes collimating optics. This mount has an integrated thermoelectric cooler and thermistor which form an active feedback loop with the temperature control component of an ILX LDC3724B laser diode controller.

The two laser diode controllers also control the injection current applied to the lasers. The current control electronics can deliver highly stable current supply
5.3. Physical sensor design

with less than 4 µA noise and contain spike protection electronics to prevent diode damage. The controller also accepts an external modulation input which converts an input voltage to an output current with an amplitude of 20 mA/V between DC and 1 MHz.

The signal delivered to the modulation input is designed to time-multiplex the diode lasers, alternately scanning them across the two absorption lines. This was achieved with a single function generator and a circuit shown in figure 5.9. This circuit is a combination of two active half-wave rectifiers, an inverting amplifier and a buffer and was based on circuit fragments given by Horowitz and Hill [56]. Its effect on the input waveform is shown in figure 5.10. The negative half-cycle of the function generator output would drive laser one, and the positive half-cycle would drive laser two. This was most effective when used with a specially crafted input signal so that the output from the multiplexing circuit would scan each laser from low injection current to high injection current. If the injection current was applied high-to-low the output wavelength would first
scan up as the laser turned on and then reverse scanning direction after about a third of the scan, wasting much of the scan time. The more effective mode of operation is shown in figure 5.10.

Optical components

In addition to the laser diodes, there are several optical components necessary for the TDLAS system. These will be considered roughly in the order that they are encountered by the laser beam exiting the laser diodes and the optical components of the system are shown in figure 5.11.

As mentioned above, a method of controlling the wavelength of laser diode emission is to provide feedback into the diode from an external cavity. While the lasers used here are not intended for this mode of operation, an unintentional stray reflection has a similar effect to an external cavity. Therefore, it is important to suppress reflections somehow.

Because of this, TDLAS systems often employ an optical isolator, preferably as soon as possible downstream of the diode itself. In this system, an optical isolator, whose operation is described in textbooks [53, 100], is mounted in the beam path directly after the collimating optics. These are necessarily close to the diode because of the strong divergence of the beam. The optical isolator, an OFR IO-4-1360-VLP was used here, consists of a high-quality polariser followed by a Faraday rotator and then another polariser which is aligned at $45^\circ$ to the first one. The net effect on the forward-propagating beam is to rotate the polarisation state by $45^\circ$. A counter-propagating beam, however, is unable to pass through the isolator since the Faraday effect is non-reciprocal and the beam is blocked as it is rotated the wrong way to be able to exit through the second polariser.
5.3. Physical sensor design

The important feature of the isolator is its suppression ratio. The isolator used here was rated to a suppression ratio of $-44.3$ dB and had a transmission of 95.5%.

After passing through the isolator, the beam was coupled into a fibre optic cable via a F-92-C1 Newport gradient-index (GRIN) lens coupler. This coupler allowed the $x$, $y$ and $z$ location of the fibre optic to be adjusted relative to a stationary GRIN lens. The process of maximising the power transmitted into the fibre was tedious due to the small entrance to the single mode fibre that was used. As is typical for coupling free-space beams into single-mode fibre, there was considerable power loss at this stage. Coupling efficiency was typically around $20 - 30\%$, but this was acceptable since the final measurement was not limited primarily by laser power.

Single mode optical fibre was used to avoid intensity fluctuations from modal interference. To maintain flexibility in the system, connectorised fibre was used with FC/APC connectors. In contrast with other end preparations, the end of the fibre is cleaved at an angle of $8^\circ$ which significantly reduces back-reflections that could otherwise result in étalon effects within the fibre.

Fibre optic cables were linked together in a network via broadband fused-fibre couplers from Newport Corporation. These are analogous in function to beam-splitters in a free-space optical layout, but operate on a different principle. Two fibre-optic cables are arranged within the device so that the cores of the fibres are close enough for the mode fields to overlap, allowing coupling of light from one cable to the other. The devices are designed to a specified splitting ra-
tio, 50/50 and 90/10 were used in this system. They are intrinsically 2-input, 2-output devices, but can be supplied with only three of the four ports connectorised.

In the TDLAS system, fused-fibre couplers were used first to combine the output from the two lasers and then to deliver components of the light to where it was required. One half of the combined laser output was split again into a ‘signal’ and ‘reference’ channel which represented the probe beam and the reference input on a log-ratio detector. The other half was sent to an interferometer, which was itself constructed from fused fibre couplers. The interferometer is functionally equivalent to a Mach–Zehnder interferometer with a fixed path-length-difference. This interferometer provided a measure of the wavelength scanning rate of the laser, as described in section 5.4.

During tunnel experiments, the signal and reference beams were transmitted to the interior of the test section through receptacle-style, vacuum feedthroughs (Oz Optics). These were unavailable with FC/APC end connectors, instead having FC/PC connectors. FC/PC connectors do not have the angled finish and therefore are more susceptible to back-reflections. The configuration of the TDLAS system for tunnel experiments is described further in section 7.1 on page 99.

Returning attention to the probe beam in the system, the guided beam inside the fibre was coupled to a free-space beam by a fibre collimator, a Newport pigtailed GRIN lens (F-COL-9-13) for the tunnel experiments and a Thorlabs connectorised collimator (F230FC-C) in the case of flame and absorption cell measurements. The probe beam was detected and compared to the signal beam on a log–ratio detector, which is described next.

Signal detection

A detector invented by Hobbs [52] and previously used for TDLAS by Allen et al. [5] was used to measure the absorption signal. The method of signal detection is a major consideration in the design of diode laser absorption experiments due to the desire to detect small absorbances against a large intensity modulation imposed by scanning the injection current of the diode laser. As the injection current is scanned to vary the laser wavelength, the power output varies enormously and a small absorption signal can be lost against a large, sloping background.

Various means can be employed to extract the absorption signal from the background. The simplest method, which works quite effectively in many situations [21, 83, 124], is to accept the presence of the background and use a linear detector. This strategy, referred to as direct absorption within this thesis, has the benefit that all analysis of the signal is done in software and, provided that the detector is operating in a linear regime, it is easy to have confidence in the integrity of the measurement being made. One of the significant disadvantages, however, is that the dynamic range of the analogue–digital converter is wasted if absorption signals are small. In such a case, the analogue–digital converter uses up its dynamic range on the sloping background and on the offset of the signal from zero. The measurement also requires interpolation of the background
5.3. Physical sensor design

across the absorption line, making this technique especially vulnerable to stray absorption somewhere else in the optical system. Despite its disadvantages, a small number of direct absorption measurements were made during this work for comparison against results obtained with the log–ratio detector.

A technique that was not used in this work, but is highly effective and popular for high sensitivity TDLAS, are the various forms of wavelength modulation, frequency modulation and phase modulation spectroscopy [13, 82, 64]. These different approaches can be regarded as different versions of the same basic technique, according to Silver [104] who reviews their relative merits. As an example of the sensitivity that has been achieved, two-tone frequency modulation spectroscopy has been used to make measurements of H$_2$O to 1.6 parts in $10^9$ [32].

In general, this class of techniques involves superimposing a high-frequency modulation on the probe beam in addition to the current ramp. The modulation frequency needs to be significantly higher than the scanning rate. This puts sidebands on the probe signal and, after passing through the test gas, a lock-in amplifier can be used to demodulate the signal at some harmonic of the modulation frequency. This is often at $2f$, or twice the modulation frequency, which results in a raw signal that is a function of the modulation parameters but has the same form as a derivative of the absorption signal—the second derivative in the case of $2f$ demodulation.

This process rejects the DC offset and sloping baseline of the laser intensity as well as having low sensitivity to noise from beam steering and background luminosity [123].

In light of its benefits, it is worth explaining why frequency modulation spectroscopy was not used in the present investigation.

For a shock tunnel measurement, a high scanning rate is desirable so that sufficient measurements can be made in the short test time. This requirement is all the more important in the present system where time-division multiplexing is used—effectively halving the potential data rate.

For a given modulation amplitude, diode lasers scan across a wider wavelength range when operating at lower frequencies. Additional modulation of the drive current, as required by frequency modulation techniques, further decreases the scanning range of the laser. The required wavelength scan range is set by the width of the transition under study, so a reduction in the scan range results in a reduction of the possible repetition rate.

A high scanning rate implies the need for a correspondingly high modulation frequency, in the megahertz range. This requires a relatively fast, and therefore small, detector with the result that the system may have an increased sensitivity to beam steering.

Frequency modulation techniques increase the complexity of the system and also the complexity of the analysis process. Depending on the analysis process used, frequency modulation techniques can result in measurements that are sensitive to temperature and pressure as well as the concentration of the target species. In all cases, the signal is a function of the modulation parameters of
5. Sensor design

Despite its benefits, frequency modulation spectroscopy remains sensitive to optical interference. In the present system, optical interference was contributed from a narrow-band filter. The interference induced by this filter depended on the incident angle of the beam, so that beam steering noise resulted in varying optical interference from this filter.

Finally, it was anticipated that the system could be refined in the future for incorporation into a flight test. If the measurement could work without recourse to frequency modulation techniques then, presumably, the potential sensor for a flight test would be easier to implement.

In light of the reasoning outlined above, an electronic noise suppression method was used with steps being taken in the optical design to minimise beam steering and interference from luminosity. While this seems a reasonable choice, it is possible that a frequency modulation scheme would be an interesting avenue of exploration in the future.

In the present system, the probe beam was split into two components, a signal beam and a reference beam. The signal beam passed through the measurement gas and the absorbance measurement was extracted electronically. This was performed using a log–ratio detector invented by Hobbs [52]. The shape of the signal produced by this detector is shown in figure 5.12, compared against direct absorption and $2f$ wavelength-modulation techniques. The circuit schematic is shown in figure 5.13. The log–ratio detector produces a signal that has the expected appearance for an absorption line, without any further processing.

For this work, the ‘ratio-only’ variation of the circuit given by Hobbs was used. The alternative design, which included a linear output as well as a log–ratio output, was not used as Hobbs advised that the ratio-only version of the circuit had better noise suppression on the log output as well as a wider bandwidth. In order to further improve bandwidth, $C_f$ was reduced from 390 pF to 10 pF and high speed versions of the recommended Op-Amps, OP27 instead of OP270, were used.

The detector operation is based around a feedback loop that strives to keep zero current flowing into the inverting input of $A1$. In figure 5.13, the transistors $Q_1$ and $Q_2$ are a matched bipolar transistor pair, so that the signal photocurrent is

![Figure 5.12: The shape of the signal produced by the detector for: (a) direct absorption, (b) $2f$ lock-in wavelength-modulation spectroscopy and (c) electronic log–ratio detector.](image-url)
Figure 5.13: Circuit diagram of the log–ratio detector [52] excluding temperature stabilisation and power supply details. Also known as a balanced ratiometric detector [5] or laser noise canceller [53].
split with a ratio that is dependent on the voltage applied to the base of $Q_1$ but not on the magnitude of $i_{\text{sig}}$. Provided that $i_{\text{ref}} > i_{\text{sig}}$, this voltage is adjusted by a feedback loop that ensures that the current leaving the collector of $Q_5$ matches the current flowing into the collector of $Q_2$.

The output of the circuit is taken from the voltage in the feedback loop and is given by

$$V_{\text{out}} = -G \log \left( \frac{i_{\text{ref}}}{i_{\text{sig}}} - 1 \right)$$

(5.8)

where $G$ is the temperature-dependant gain of the circuit. According to Hobbs [52], $G = kT/e$, where $k$ is Boltzmann’s constant, $T$ is the temperature of the transistor pair and $e$ is the electronic charge, assuming the Ebers–Moll model of the $Q_1$–$Q_2$ pair. Rather than calculate $G$ from equation (5.8), the value for $G$ was measured experimentally and the temperature of the transistor pair was kept constant with an additional temperature control circuit, described later.

The configuration of the circuit means that additive noise, such as the sloping background across the laser scan, is cancelled directly by the $Q_1$–$Q_2$ pair. This suppression is effective out to the bandwidth of the transistor pair, which is generally hundreds of megahertz. In contrast, the reduction in $i_{\text{sig}}$ due to absorption is dependant on the absolute value of $i_{\text{sig}}$ and this multiplicative noise is suppressed only by the feedback loop [54]. This implies that as the bandwidth of the loop is exceeded the observed baseline will remain flat, however absorption features will become distorted and eventually disappear altogether.

The bandwidth of the feedback loop is given by [52]

$$f_c = \frac{1}{2\pi G} \left( \frac{i_{\text{sig}}}{1 + \exp \left( \frac{V_{\text{out}}}{G} \right)} \right) \frac{R_1/(R_1 + R_2)}{C_f},$$

(5.9)

where the meanings of $R_1$, $R_2$ and $C_f$ are given in figure 5.13. Therefore, the loop bandwidth can be maximised by:

- Adjusting $i_{\text{ref}}$ and $i_{\text{sig}}$ so that $V_{\text{out}} \approx 0$;
- Adjusting the splitting ratio of the $R_1/R_2$ voltage divider;
- Maximising $i_{\text{sig}}$; and
- Reducing $C_f$.

With this in mind, $i_{\text{ref}}$ and $i_{\text{sig}}$ were adjusted so that $i_{\text{ref}} \approx 2i_{\text{sig}}$, $C_f$ was reduced to 10 pF and the laser current ramp and optics were optimised to maximise power output. The splitting ratio of the voltage divider was left as-is because a large current passed through this voltage divider when the output was at saturation. This was already causing problems due to local heating of the circuit board, and changing the splitting ratio would have exacerbated this problem.

As shown in equation (5.8), the gain of the detector is dependent on temperature. Hobbs suggested a temperature stabilisation scheme for this detector, and this was included on the detector built for these experiments. This addition to
5.4 Data reduction

The basic detector is shown in figure 5.14. It uses the two spare transistors in the MAT-04 package, one as a temperature sensor and one as a heater, to control the temperature of $Q_1$ and $Q_2$. This was seen to effectively stabilise the gain of the detector after a warm up period of around 20 min.

The output from this detector was then digitised with a data acquisition board and this, combined with the signal from the interferometer, was then analysed to find the temperature and water vapour concentration.

5.4 Data reduction

The process of converting the raw output signals produced by the system into temperature and water vapour concentration is shown in figure 5.15. The system delivers time-resolved voltage measurements, shown in figure 5.16, from:

- The linear detector monitoring the interferometer output; and
- The log–ratio detector or a linear detector measuring the beam power after traversing the test gas.

These need to be converted into absorbance as a function of frequency, which implies two operations:

- Conversion from time in the laser scan to frequency; and
- Conversion of detected signal to absorbance.

These steps are discussed below.
5. Sensor design

Figure 5.15: Data processing steps during data reduction.

Figure 5.16: Raw signals obtained from the TDLAS system when operating in a flame. The vertical lines show user-specified extents of the scan to take to the next processing stage.
5.4. Data reduction

Time-to-frequency conversion

The output of a fixed-beam-path-difference interferometer, such as the fibre-optic interferometer in this system, oscillates between maximum and minimum as the input beam is scanned in frequency. At the output of the interferometer the re-combined beams exhibit some level of constructive or destructive interference. The condition for constructive interference requires that the path length difference, \( \Delta l \), be an integral multiple of the wavelength, \( \lambda \), i.e.

\[
\Delta l = i \lambda
\]

where \( i \) is a positive integer. Alternatively, in frequency space, this equation is expressed as

\[
\Delta l = \frac{ic}{n\nu}
\]

where \( c \) is the vacuum speed of light, \( n \) is the refractive index of the medium and \( \nu \) is the frequency.

Since we have a fixed \( \Delta l \), we can consider the spacing of the maxima in frequency space, \( \Delta \nu \). This is given by

\[
\Delta \nu = \left( i + \frac{1}{n} \right) \frac{c}{n\Delta l} - i \frac{c}{n\Delta l} = \frac{c}{n\Delta l}
\]

and, therefore, is not dependent on \( i \). Importantly for this application, the frequency spacing between maxima is a constant, and is termed the free spectral range of the interferometer. Equation (5.12) also shows that the free spectral range can be reduced by increasing the path length difference to provide sufficient resolution over the small scanning range of DFB diode lasers.

The free spectral range needs to be known in order to determine species concentration, although not for temperature. The free spectral range of the interferometer used in this work was found by measuring the spacing between water vapour absorption lines and comparing these to the locations reported by Toth [114]. It was determined to be

\[
\nu_{FSR} = (0.01032 \pm 0.00005) \text{ cm}^{-1}
\]

where the error was based on the estimated uncertainty in determining the peak locations in the absorption measurement. Since the uncertainty in the free spectral range was low, the error introduced in the conversion from time to frequency was neglected in the calculation of the final measurement uncertainty. Errors introduced by changing path-length difference, e.g. from thermal expansion of the optical fibre, were also ignored.

The algorithm for the conversion smoothed the output of the interferometer with a running mean, removed the linear trend due to the variation in laser power over the laser scan and located zero crossings in this signal, referred to as the de-trended signal, as shown in figure 5.17a.

With the knowledge of interferometer free spectral range, the peak locations can be used to plot a curve of relative frequency versus time, shown in figure
5.17b. Provided that the start of the laser scan is excluded from analysis, the frequency tuning rate is close to linear under a linear modulation of the injection current.

The frequency tuning relationship is highly repeatable for a particular setting for the injection current modulation. So, it is not necessary for the interferometer to be an integral part of the TDLAS system, provided that laser settings remain constant. This was not the case for this work since the system was always under heavy development, so the interferometer output was always recorded and each set of data used its own measurement of laser tuning.

Absorbance measurement

Absorbance in the gas sample was typically measured with a log–ratio detector, which has been described above, however some measurements were also made with a linear detector for comparison. Since these detectors are quite different, the calculation of absorbance from the raw signals differs.

Log–ratio detector

In order to convert the log–ratio detector signal to absorbance, equation (5.8) indicates that we must know the gain, \( G \), of the detector. This gain, while constant after a warm-up time, is not known precisely \( a \ priori \), and must be measured.

In principle, this is easily achieved by applying a known ratio of photocurrents, \( i_{\text{ref}}/i_{\text{sig}} \), to the detector and measuring the output. Rearranging equation (5.8),
In this configuration, the output of laser 1 was held constant and the output of laser 2 was swept with a current ramp at a repetition rate of 11 Hz. The low repetition rate allowed a fraction of the power of laser 2 to be measured with a commercial, highly linear power meter (Newport 840-C) via the 10% output of a 90/10 fused fibre coupler. While this measurement changed as the laser power was varied, it varied linearly with the laser power. Laser 1 was then coupled to the signal channel of the log–ratio detector and laser 2, minus the 10% tap, was coupled to the reference channel of the detector. The output of both the power meter and the log–ratio detector were recorded simultaneously.

The signal measured from the commercial power meter is linearly related to the signal photocurrent, and can be denoted as

\[ V_1(t) = \alpha i_{\text{sig}}(t) \] (5.15)

where \( \alpha \) is a positive scalar and \( t \) is the time since the start of the laser scan.

Since we have also recorded the output of the log–ratio detector, we also have

\[ V(t) = -G \log \left\{ \frac{i_{\text{ref}}}{i_{\text{sig}}(t)} - 1 \right\} . \] (5.16)

This can be re-written as

\[ V(t) = -G \log \left\{ \alpha i_{\text{ref}}/\alpha i_{\text{sig}}(t) - 1 \right\} \] (5.17)
or, from equation (5.15),

\[ V(t) = -G \log \{\alpha_i_{\text{ref}}/V_1(t) - 1\}. \]  (5.18)

This results in two unknown constants, \( G \) and \( \alpha_i_{\text{ref}} \). These can be found by plotting \( V \) against \( V_1 \) and then regression-fitting a curve, in the form of (5.18), to these data. More simply, but less precisely, we can observe the value of \( V_1 \) for which \( V = 0 \). From (5.18), \( \alpha_i_{\text{ref}} = 2V_1 \) at this point. With \( \alpha_i_{\text{ref}} \) known, \( G \) can be found from any other point on the curve. Regression fitting was used to find the gain of the detector where it is presented in this work.

To test the short term stability of the circuit, this process was carried out every ten seconds for a period of one hour. The results of this test are shown in figure 5.19 and show that the detector is remarkably stable after a warm up period of about 20 minutes, as well as showing the effectiveness of this method of determining the detector gain. The long term stability of the circuit was also verified by measuring the gain of the detector at the start and end of the major experimental campaign. Additional measurements were made at other times, particularly when line-strength calibration experiments were being carried out. All of these tests found the detector gain to be stable.

If we denote the measured absorbance as

\[ A_m = \log (i_{\text{ref}}/i_{\text{sig}}), \]  (5.19)

then, rearranging equation (5.8), this is related to the output voltage of the detector by

\[ A_m = \log (\exp (-V/G) - 1). \]  (5.20)
In truth, $A_m$ is not really an absorbance—the log–ratio of two beam intensities—it is simply the log–ratio of two photocurrent outputs. Nevertheless, $A_m$ can be treated as an absorbance measure, based on the following reasoning.

The log–ratio detector uses InGaAs photodiodes, which are extremely linear when operated with a large reverse-bias voltage. 15 V reverse-bias is applied in this detector design, so the ratio of photocurrents should match the ratio of beam intensities to a good approximation, provided that the responsivities of the photodiodes matches. If not, we are actually measuring

$$A_m = \log \left( \frac{\alpha I_{\text{ref}}}{\beta I_{\text{sig}}} \right)$$

where $\alpha$ and $\beta$ are the responsivities of the reference and signal photodiodes respectively and $I_{\text{ref}}$ and $I_{\text{sig}}$ are the two beam intensities. This can also be written as

$$A_m = \log \left( \frac{I_{\text{ref}}}{I_{\text{sig}}} \right) + \log \left( \frac{\alpha}{\beta} \right)$$

so that using mismatched photodiodes results in a constant offset in the measured absorption. A similar argument follows for the case of any fractional losses due to misalignment of the beam onto detectors, dirty windows or other effects that do not depend on beam intensity or frequency. Therefore, this measurement does not provide us with an absolute measure of absorbance since there are uncharacterised broadband losses in the system which superimpose an offset on the absorbance signal. Instead, absorbance is measured relative to a background level. Since we usually set $I_{\text{ref}} \approx 2I_{\text{sig}}$ this background absorbance is usually $\log 2 \approx 0.7$ and absorption lines are seen as additional absorbance on top of this background.

Effect of luminosity

The interpretation of the output from the log–ratio detector also depends on the assumption that the signal beam, $I_{\text{sig}}$, is composed of monochromatic diode laser radiation. In some environments, $I_{\text{sig}}$ will also be composed of a fraction of broadband luminosity, $L$. Since the contribution of broadband luminosity to $I_{\text{sig}}$ is unrelated to the operation of the laser, its presence could be expected to systematically affect the absorption measurement.

The effect of luminosity on the signal can be expressed by considering $I_{\text{sig}}$ to be

$$I_{\text{sig}} = I'_{\text{sig}} + L,$$

where $L$ is a constant and $I'_{\text{sig}}$ is the intensity of the monochromatic laser radiation. From equation (5.19) and (5.23), the measured absorbance will then be given by

$$A_m = \log \left( \frac{I_{\text{ref}}}{I'_{\text{sig}}} \right) - \log \left( 1 + \frac{L}{I'_{\text{sig}}} \right).$$

The effect of luminosity on the measured absorption is depicted in figure 5.20. The effect of luminosity changes across the scan due to the change in laser output power. Luminosity is problematic because of the distortion it causes in the baseline; if the baseline is fit from the shape either side of the absorption line, the integrated absorbance would be underestimated.
5. Sensor design

It is possible to correct for luminosity by measuring a fraction of the laser power across a scan and then examining the offset caused by luminosity in parts of the scan well away from the absorption line. This was not feasible in shock tunnel experiments because the baseline was not stable enough. Instead, additions were made to the design of the system to minimise luminosity entering the detector.

Linear detector

The conversion process from raw signal to absorbance is quite different when a linear detector is used. In this case, there is no comparison beam so the estimation of background is taken from the parts of the scan either side of the absorption features where there is little absorption present. When using a linear detector, there is the possibility of a direct measure of luminosity if the laser is switched off for some part of the scan.

The procedure used in this work is similar to several previous investigator’s [124, e.g.] and is illustrated in figure 5.21. The process relies on the laser being scanned a sufficient distance so that a significant amount of signal is present on either side of the absorption line. Furthermore, if the laser is switched off for part of the scan then the component of the signal arriving at the detector from background luminosity, say \( L \), can be deduced. If we fit a curve to the background either side of the absorption line, say \( B(t) \) which can be a line or higher-order polynomial, then the absorbance at a particular time during the laser scan is given by

\[
A(t) = \log \frac{S(t) - L}{B(t) - L}. \tag{5.25}
\]

Regardless of the detector used, the absorbance measured as a function of
5.4. Data reduction

The analysis technique for direct-absorption measurements.

At this stage of the analysis we have two measurements of absorbance as a function of relative frequency for the two absorption lines and we need to convert this to the integrated absorbance over each of the absorption lines. However, there are several factors that hinder this conversion, including:

- Baseline slope—due to different photodiodes on the two channels, vibration, frequency-dependent losses, luminosity, etc.;
- General noise;
- Line shapes that change with pressure and temperature; and
- Spectral lines overlapping with the target absorption line.

There are two competing methods that can be used to perform the conversion. Either one can take a direct numerical integral of the absorption feature or a line shape model can be fit to the absorption line. In the latter case, the integrated absorption is one of the fitting parameters.

For this work it was necessary to fit absorption lines to the data since there is an additional spectral line overlapping the targeted spectral line near 7181 cm$^{-1}$, at high temperature. Furthermore, since calibration and measurements were carried out at quite different pressures, the chosen technique needed to be insensitive to pressure. As shown later, using a fixed width integral means accepting results that change with pressure because of the relatively large absorption that is transferred to the wings as the line profile becomes wider and a Lorentzian profile begins to dominate. Fitting curves to absorption lines does not even require that a background region is present in the scan, as shown by

Figure 5.21: The analysis technique for direct-absorption measurements.
Nagali and Hanson [71] who made high pressure measurements using TDLAS and extracted data by fitting curves to the broad peaks of absorption features.

Fitting also has the advantage of returning information of the quality of the fit, which can be used to estimate measurement uncertainty. Line shape information is also produced from fits.

The simplicity of taking a direct integral is in favour of this method, which can be a major consideration in embedded systems. Fitting requires substantial, and non-constant, processing time and more human intervention than a direct integral. Since the sensor in this work was employed for measurements in a pulsed facility, it was just as convenient to record the full line shapes during an experiment, and then run the fitting routine afterwards.

The fitting routine assumes a Voigt line shape since more sophisticated line shapes were not required to match shock tunnel data. The model fit to data was

\[
A_{\text{model}} = \sum_{i=1}^{n} \left[ S_i g(\nu; \nu_0, \gamma_{d,i}, \gamma_{l,i}) \right] + (a \nu + b),
\]

where the modelled absorption depended on the relative frequency, \( \nu \), and the fitted parameters were the frequency offset of the strongest line centre, \( \nu_0 \), the Doppler half-width, Lorentz half-widths and strength of each absorption line, \( \gamma_{d,i}, \gamma_{l,i} \) and \( S_i \), as well as \( a \) and \( b \) to allow for a sloping, offset background. In this expression, \( g \) represents the Voigt line shape.

A MATLAB [112] non-linear least-squares fitting routine, \texttt{lsqnonlin}, employing a modified Gauss–Newton search was used to perform the fits. The Voigt line profile was computed by Wells’ method [127] implemented as part of the Genspect [94] spectral model.

Error estimation

Through use of a curve-fitting methodology, the uncertainty in the measured absorption can be estimated for each curve fit performed. In this work, this was achieved by Monte Carlo simulation using the bootstrap method. This method of determining uncertainty is described by Press et. al. [92, section 15.6] who note that the method’s advantages include its:

- Simplicity of implementation;
- Applicability to non-normally distributed data; and
- Ability to produce non-symmetric upper and lower bounds.

The bootstrap method was used to find error bounds of integrated absorbance at 90% confidence intervals and, for this application, proceeds as follows.

After a curve is fit to one data scan, we are in possession of:
A vector of parameter values, $p$, which include the area under the curve, the position and slope of the baseline, the centre wavelength of the transition, the Lorentz half-width and the Gaussian half-width; and

$N$ data points which consist of discrete $(\nu, A)$ pairs. These are the data which we fit the curve to; $\nu$ is wavenumber and $A$ absorbance. The number of data points, $N$, is set by the sampling rate of the data acquisition system and the scanning rate of the laser.

In order to estimate the error in the parameter values, we want to generate many synthetic data sets. We fit curves to each of these synthetic data sets and use the spread in fitted parameter values to estimate the uncertainty in the parameter values, $p$, which were fit to the real data.

This can be achieved by generating $M$ new data sets which are each comprised of $N$ data points by randomly drawing points from our original data set—i.e. the measurement—but allowing for points to be repeated. Therefore, each of the $(\nu, A)$ points in the original data set will appear zero, one, or more times in each of the $M$ new data sets and each of the $M$ data sets will be different.

We can then apply the original curve fitting process to each of the $M$ data sets, thereby obtaining a set of parameter values $p_1, \ldots, p_M$. If we consider the distribution of one of the parameter values, say the integrated absorbance, then we can find a range that includes 90% of the integrated absorbance values by discarding the largest 5% and smallest 5% of values and examining the range of the resulting data set.

If we were in a position to perform the measurement repeatedly under known conditions, we would also obtain a distribution of measured $p$ around the known true value of $p$. With the bootstrap method, we assume that the distribution that we obtain from our synthetic data sets is similar to the distribution in this hypothetical case, although we expect that our measured value of $p$ will be different from the true value of $p$.

Under this assumption, the interval we found above represents the interval which includes the true $p$, with 90% probability and can be used to estimate the error in the measured parameters.

The bootstrap method assumes that the measured data points are independent and identically distributed, and this may be a problem since wavenumber is sampled at approximately evenly-spaced intervals. According to Press et. al. [92, p 692] then in this case

\[ \text{\ldots you can usually get away with pretending that these are \textit{"iid"}} \text{\ldots} \]

It is possible to verify that we can get away with this assumption in the present case by using synthetic data. 1000 data sets were generated by generating 1000 identical Voigt profiles and adding normally distributed noise to each one. Curves were then fit to each of these and the integrated absorbance of each was found. After the width of the interval containing 90% of the realisations was
computed, this was then compared against a bootstrap estimation of the 90% confidence interval. The bootstrap estimate was calculated from only one of the synthetic data sets. The agreement, as shown by figure 5.22, shows that the method provides reasonable estimates of the error in line fits with up to 35% uncertainty.

In results presented later, the number of new data sets created, $M$, was chosen as 100. This was a compromise between large $M$ and available computing power and tests on synthetic data showed that it was sufficiently large to give reasonably consistent error estimates. The requirement for $M$ to be relatively large means that this method of determining uncertainty is computationally intensive.

Nevertheless, the results justify the investment, since measurement uncertainty can be estimated from a single scan. This is useful since averaging consecutive measurements to estimate uncertainty is impossible in many situations.

**Determination of temperature and number density**

The determination of temperature and number density can be thought of as solving two simultaneous equations,

\[
A_1 = S_1(T)N_{\text{H}_2\text{O}}l \\
A_2 = S_2(T)N_{\text{H}_2\text{O}}l
\]  

(5.27)  

(5.28)
for temperature, $T$, and water vapour concentration $N_{\text{H}_2\text{O}}$. In these equations $A_1$ and $A_2$ are the integrated absorbance due to line 1 and line 2, $S_1$ and $S_2$ are the line strengths of line 1 and line 2 and $l$ is the beam path-length.

Dividing equation (5.27) by equation (5.28), we can eliminate $N_{\text{H}_2\text{O}}$ and $l$ and re-write the equations in terms of the line strength ratio $R_{ls}(T)$. We now have

$$\frac{A_1}{A_2} = R_{ls}(T) \quad (5.29)$$

which can be solved for temperature by using the relationship given in equation (4.8) on page 35.

In principle, temperature can also be found from the Gaussian component of the line-shape and determined from a single absorption line. This was not performed for this work, in tunnel measurements because there was too much noise and in flame measurements because the line profile was distorted by Dicke narrowing so that the fitted Gaussian width no longer corresponded well with temperature.

Having found temperature, the strength of either line 1 or line 2 can be determined from equation (4.6) on page 35 and, since we know $l$, $N_{\text{H}_2\text{O}}$ can be evaluated. As we are solving simultaneous equations, the same result is obtained from using either of the two absorption lines.

Since we built an ensemble of values for both $A_1$ and $A_2$ to determine their uncertainty, the uncertainty in $T$ and $N_{\text{H}_2\text{O}}$ can be determined by finding $T$ and $N_{\text{H}_2\text{O}}$ for each pair of $A_1$ and $A_2$ values in the ensemble. In so doing, we build up a distribution for $T$ and $N_{\text{H}_2\text{O}}$ from which we can extract the 90% confidence interval.

Drawing on the characteristics of other diode laser sensors, a design for a temperature and water vapour sensor has been outlined in this chapter. The theoretical sensitivity of the spectral lines has been considered, with the implication that the sensor operation becomes more difficult at high temperature.

Two possible detection strategies are possible with this sensor. A dual beam approach using a log-ratio detector is better at rejecting noise, but it is influenced by broadband luminosity. In luminous environments, therefore, broadband luminosity needs to be excluded from the detector or accounted for during analysis.

Data produced from either of these detectors can be converted to temperature and water concentration measurements including an estimate of the measurement precision, although calibration experiments are required to determine measurement accuracy.
5. Sensor design