Development and demonstration of a diode laser sensor for a scramjet combustor

A thesis submitted for the degree of Doctor of Philosophy of the Australian National University

Alan David Griffiths

December 2004, revised September 2005
This thesis contains no material which has been accepted for the award of any other degree or diploma in any university. To the best of the author’s knowledge and belief, it contains no material previously published or written by another person, except where due reference is made in the text.

Alan Griffiths
December 2004
Summary of Thesis

Hypersonic vehicles, based on scramjet engines, have the potential to deliver inexpensive access to space when compared with rocket propulsion. The technology, however, is in its infancy and there is still much to be learned from fundamental studies.

Flows that represent the conditions inside a scramjet engine can be generated in ground tests using a free-piston shock tunnel and a combustor model. These facilities provide a convenient location for fundamental studies and principles learned during ground tests can be applied to the design of a full-scale vehicle.

A wide range of diagnostics have been used for studying scramjet flows, including surface measurements and optical visualisation techniques.

The aim of this work is to test the effectiveness of tunable diode laser absorption spectroscopy (TDLAS) as a scramjet diagnostic.

TDLAS utilises the spectrally narrow emission from a diode laser to probe individual absorption lines of a target species. By varying the diode laser injection current, the laser emission wavelength can be scanned to rapidly obtain a profile of the spectral line. TDLAS has been used previously for gas-dynamic sensing applications and, in the configuration used in this work, is sensitive to temperature and water vapour concentration.

The design of the sensor was guided by previous work. It incorporated aspects of designs that were considered to be well suited to the present application. Aspects of the design which were guided by the literature included the laser emission wavelength, the use of fibre optics and the detector used. The laser emission wavelength was near 1390 nm to coincide with relatively strong water vapour transitions. This wavelength allowed the use of telecommunications optical fibre and components for light delivery. Detection used a dual-beam, noise cancelling detector.

The sensor was validated before deployment in a low-pressure test cell and a hydrogen–air flame. Temperature and water concentration measurements were verified to within 5% up to 1550 K. Verification accuracy was limited by non-uniformity along the beam path during flame measurements.

Measurements were made in a scramjet combustor operating in a flow generated by the T3 shock tunnel at the Australian National University. Within the scramjet combustor, hydrogen was injected into a flame-holding cavity and the
sensor was operated downstream in the expanded, supersonic, post-combustion flow. The sensor was operated at a maximum repetition rate of 20 kHz and could resolve variation in temperature and water concentration over the 3 ms running time of the facility.

Results were repeatable and the measurement uncertainty was smaller than the turbulent fluctuations in the flow. The scramjet was operated at two fuel-lean equivalence ratios and the sensor was able to show differences between the two operating conditions. In addition, vertical traversal of the sensor revealed variation in flow conditions across the scramjet duct.

The effectiveness of the diagnostic was tested by comparing results with those from other measurement techniques, in particular pressure and OH fluorescence measurements, as well as comparison with computational simulation. Combustion was noted at both of the tested operating conditions in data from all three measurement techniques.

Computation simulation of the scramjet flow significantly under-predicted the water vapour concentration. The discrepancy between experiments and simulation was not apparent in either the pressure measurements or the OH fluorescence, but was clear in the diode laser results.

The diode laser sensor, therefore, was able to produce quantitative results which were useful for comparison with a CFD model of the scramjet and were complimentary to information provided by other diagnostics.
Acknowledgements

Over the last few years, I have been fortunate to receive assistance from many, many people. My supervisor, Frank Houwing, provided much-needed encouragement and advice. The contribution of my advisers, John Close and Neil Mudford is also much appreciated. Paul Walsh was responsible for all things related to the scramjet model and T3, and was astounding with his technical abilities. Paul also provided support which was probably more valuable than his extensive technical skills.

Other members of the research group have also provided advice and assistance. In particular, Andrew Neely, Russell Boyce, Sean O'Byrne and Jeff McGuire provided advice with experiments and CFD, while Ingo Stotz found the time to run additional calculations for my conditions.

Phil Hobbs and Mark Allen were generous in their responses to my emails and they both supplied information that was extremely helpful for my work.

Electronics advice and fabrication was provided by Shane Grieves and Sharon López saved me from administrative chaos on many occasions.

Thanks to the other students and staff within the physics department who have helped make this experience fun. Also to all of my friends, who have, against all predictions, made living in Canberra loads o fun.

Thanks finally to my family, Jill and her family.

Thanks to you all.
4 Absorption spectroscopy theory
  4.1 Molecular ro-vibrational energy levels and absorption lines .. .. 31
  4.2 The relationship between line and gas properties ............ 33
    Strength of absorption lines .................................. 35
    Shape of absorption lines ...................................... 36
      Natural broadening ............................................ 37
      Pressure broadening .......................................... 37
      Doppler broadening .......................................... 37
      Combined pressure and Doppler broadening .................... 38
      More advanced line shapes ................................... 38
  4.3 Spectral model of water vapour ............................. 39

5 Sensor design
  5.1 Other diode laser based sensors ............................. 43
  5.2 Selection of spectral lines .................................. 45
  5.3 Physical sensor design ...................................... 51
      Diode lasers .................................................. 52
      Optical components .......................................... 56
      Signal detection ............................................. 58
  5.4 Data reduction ............................................... 63
      Time-to-frequency conversion ............................... 65
      Absorbance measurement .................................... 66
      Log-ratio detector .......................................... 66
      Effect of luminosity ....................................... 69
      Linear detector ............................................. 70
      Integrated absorbance from spectral absorbance ............ 71
      Error estimation ............................................ 72
      Determination of temperature and number density ......... 74

6 Sensor verification
  6.1 Measurements at room temperature ........................ 77
    Experiment configuration ..................................... 78
    Applicability of Voigt profile ............................... 79
    Comparison with literature .................................. 81
    Sensitivity to pressure ..................................... 82
<table>
<thead>
<tr>
<th>Contents</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature measurement in room air ........................................... 83</td>
</tr>
<tr>
<td>6.2 Flame measurements ................................................................. 85</td>
</tr>
<tr>
<td>Experimental configuration .............................................................. 86</td>
</tr>
<tr>
<td>Independent measurement of flame properties ........................................ 88</td>
</tr>
<tr>
<td>Determining temperature with a bare thermocouple ................................ 88</td>
</tr>
<tr>
<td>Determining water vapour number density ............................................. 91</td>
</tr>
<tr>
<td>Spectroscopic measurements of flame properties .................................... 91</td>
</tr>
<tr>
<td>Radial temperature and concentration profiles ....................................... 92</td>
</tr>
<tr>
<td>Calibration results .............................................................................. 93</td>
</tr>
<tr>
<td>Time-resolved measurements .................................................................. 95</td>
</tr>
<tr>
<td>7 Scramjet-based measurements ............................................................ 99</td>
</tr>
<tr>
<td>7.1 Test outline and sensor configuration ............................................... 99</td>
</tr>
<tr>
<td>7.2 Absorbance before processing .......................................................... 104</td>
</tr>
<tr>
<td>7.3 Luminosity check ............................................................................ 107</td>
</tr>
<tr>
<td>7.4 Integrated absorbance ................................................................. 108</td>
</tr>
<tr>
<td>7.5 Temperature and water vapour time series ....................................... 112</td>
</tr>
<tr>
<td>7.6 Traverse across duct ....................................................................... 113</td>
</tr>
<tr>
<td>7.7 Measurements in ethylene-fueled combustor ..................................... 115</td>
</tr>
<tr>
<td>8 Interpretation of results ................................................................. 119</td>
</tr>
<tr>
<td>8.1 Confirmation of combustion ........................................................... 119</td>
</tr>
<tr>
<td>8.2 The source of measurement uncertainty .......................................... 122</td>
</tr>
<tr>
<td>8.3 Water vapour mixture fraction ........................................................ 123</td>
</tr>
<tr>
<td>8.4 Comparison with CFD .................................................................... 126</td>
</tr>
<tr>
<td>9 Conclusions ....................................................................................... 135</td>
</tr>
<tr>
<td>References ......................................................................................... 137</td>
</tr>
<tr>
<td>Glossary of symbols ........................................................................... 147</td>
</tr>
</tbody>
</table>
List of Figures

1.1 Comparison of rocket and aircraft take-off mass fractions. . . . . 2

2.1 Scramjet-powered vehicle concept. .......................... . . . . . . . . 6
2.2 The rocket-boost stage of two scramjet flight tests. . . . . . . . . . 9
2.3 A piezoelectric pressure transducer. .......................... 12

3.1 Side elevation of T3 . ............................................. 16
3.2 Operation of the T3 shock tunnel. ............................. 17
3.3 Stagnation pressure trace. ................................. 18
3.4 Scramjet duct geometry. ................................ 23
3.5 Scramjet inlet. ............................................. 24
3.6 Scramjet inlet luminosity. ................................ 24
3.7 Important components of the fuel injection system. ............... 26
3.8 Details of the pressure transducer mounts. ................... 26
3.9 Hydrogen mass flow. ........................................ 30
3.10 Equivalence ratio during tunnel runs. ........................ 30

4.1 Vibrational quantum number assignments for H$_2$O. ........... 32
4.2 Ro-vibrational energy levels in H$_2$O. .......................... 33
4.3 An idealised spectroscopy experiment. ........................ 33
4.4 Pressure and Doppler broadening effects on line shape. ........ 36
4.5 Voigt profile fitted to a Galatry profile. ........................ 39
4.6 Water vapour spectrum between 1 and 2 $\mu$m. .................. 41
4.7 Water vapour absorption at 500, 1000, 1500 K. .................. 41

5.1 Line strength and ratio variation with temperature. .......... 48
5.2 Line ratio sensitivity as a function of temperature. ........... 49
### List of Figures

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.3</td>
<td>Uncertainty in water concentration as a function of temperature.</td>
<td>50</td>
</tr>
<tr>
<td>5.4</td>
<td>Layout of the TDLAS system.</td>
<td>51</td>
</tr>
<tr>
<td>5.5</td>
<td>The LabVIEW-based acquisition and control system.</td>
<td>52</td>
</tr>
<tr>
<td>5.6</td>
<td>Schematic of a diode laser.</td>
<td>53</td>
</tr>
<tr>
<td>5.7</td>
<td>Types of single-mode diode lasers.</td>
<td>53</td>
</tr>
<tr>
<td>5.8</td>
<td>Laser diode control subsystem.</td>
<td>55</td>
</tr>
<tr>
<td>5.9</td>
<td>Multiplexing circuit schematic</td>
<td>55</td>
</tr>
<tr>
<td>5.10</td>
<td>Waveforms from the multiplexing box.</td>
<td>56</td>
</tr>
<tr>
<td>5.11</td>
<td>Optical components of the sensor.</td>
<td>57</td>
</tr>
<tr>
<td>5.12</td>
<td>The shape of detector signals.</td>
<td>60</td>
</tr>
<tr>
<td>5.13</td>
<td>Circuit diagram of the log–ratio detector.</td>
<td>61</td>
</tr>
<tr>
<td>5.14</td>
<td>Circuit diagram of temperature stabilisation electronics.</td>
<td>63</td>
</tr>
<tr>
<td>5.15</td>
<td>Data processing steps during data reduction.</td>
<td>64</td>
</tr>
<tr>
<td>5.16</td>
<td>Raw TDLAS signals from a flame.</td>
<td>64</td>
</tr>
<tr>
<td>5.17</td>
<td>Conversion from time to frequency over the laser scan.</td>
<td>66</td>
</tr>
<tr>
<td>5.18</td>
<td>Equipment configuration for log–ratio detector calibration.</td>
<td>67</td>
</tr>
<tr>
<td>5.19</td>
<td>Detector stability.</td>
<td>68</td>
</tr>
<tr>
<td>5.20</td>
<td>Effect of luminosity on detector signal.</td>
<td>70</td>
</tr>
<tr>
<td>5.21</td>
<td>The analysis technique for direct-absorption measurements.</td>
<td>71</td>
</tr>
<tr>
<td>5.22</td>
<td>The analysis technique for direct-absorption measurements.</td>
<td>74</td>
</tr>
<tr>
<td>6.1</td>
<td>Test cell measurement configuration.</td>
<td>78</td>
</tr>
<tr>
<td>6.2</td>
<td>Voigt and Galatry fits to test cell absorption data.</td>
<td>80</td>
</tr>
<tr>
<td>6.3</td>
<td>Comparison of observed and predicted spectra in test cell.</td>
<td>82</td>
</tr>
<tr>
<td>6.4</td>
<td>Comparison of measured, HITRAN and Toth line strengths.</td>
<td>84</td>
</tr>
<tr>
<td>6.5</td>
<td>Sensitivity of integrated absorbance determination to pressure.</td>
<td>84</td>
</tr>
<tr>
<td>6.6</td>
<td>Histogram of temperature measured in room air.</td>
<td>85</td>
</tr>
<tr>
<td>6.7</td>
<td>McKenna Products flat-flame burner.</td>
<td>86</td>
</tr>
<tr>
<td>6.8</td>
<td>Experimental arrangement for flame measurements.</td>
<td>87</td>
</tr>
<tr>
<td>6.9</td>
<td>Model of the thermocouple used for radiation correction.</td>
<td>89</td>
</tr>
<tr>
<td>6.10</td>
<td>Flame temperature profile and fitted trapezoid profile.</td>
<td>92</td>
</tr>
<tr>
<td>6.11</td>
<td>Temperature from thermocouple and TDLAS in a burner.</td>
<td>94</td>
</tr>
<tr>
<td>6.12</td>
<td>Ratio of measured to predicted water vapour concentration.</td>
<td>95</td>
</tr>
<tr>
<td>6.13</td>
<td>Temperature measured in an unsteady flame.</td>
<td>96</td>
</tr>
<tr>
<td>6.14</td>
<td>Histogram of measurement uncertainty in a flame.</td>
<td>97</td>
</tr>
</tbody>
</table>
List of Figures

7.1 Fibre-optic launch module. ................................. 102
7.2 Detector module. ........................................ 103
7.3 Launcher module installed in duct. ...................... 104
7.4 Scramjet with covers in place. ............................. 105
7.5 Unprocessed absorbance signal. .......................... 105
7.6 Raw signal from standard detector. ..................... 107
7.7 Flow luminosity. ........................................ 108
7.8 Curve fits to high equivalence ratio data. ............. 110
7.9 Curve fits to low equivalence ratio data. ............... 110
7.10 Absorbance as a function of run time, high $\phi$. .......... 111
7.11 Absorbance as a function of run time, low $\phi$. .......... 111
7.12 Temperature time-series. ................................ 112
7.13 Temperature time-series from multiple shots. ......... 113
7.14 Number density time-series from multiple shots. ...... 114
7.15 Temperature across the duct. ............................ 115
7.16 Water vapour concentration across the duct. ......... 116
7.17 Temperature for ethylene test. .......................... 117
7.18 Water vapour concentration for ethylene test. ....... 117

8.1 Pressure along scramjet floor. ........................... 120
8.2 Pressure rise due to combustion. .......................... 121
8.3 OH–PLIF for high $\phi$. .................................. 122
8.4 OH–PLIF for low $\phi$. .................................. 123
8.5 Pressure at duct floor .................................... 124
8.6 Water partial pressure normalised by wall pressure. ...... 125
8.7 Measured and CFD-predicted pressure. .................... 127
8.8 Temperature predicted by CFD. ............................ 128
8.9 Water mole fraction predicted by CFD. ................... 129
8.10 Temperature and water vapour in the measurement plane. 130
8.11 CFD-predicted, simulated TDLAS and measured temperature. 130
8.12 CFD-predicted and simulated TDLAS $H_2O$ concentration. 131
1. Introduction

In order to reach low earth orbit, a vehicle must travel at a speed in excess of Mach 25. The present method of obtaining such a speed is to use a rocket engine for propulsion. This has the disadvantage, however, that most of the vehicle’s take-off mass is comprised of oxygen, or some other oxidiser, leaving little allowance for payload and vehicle structure. This is despite the fact that the majority of the rocket’s energy is expended during flight through the earth’s oxygen-rich atmosphere.

In contrast to rockets, aeroplanes powered by jet engines need not carry oxidiser, so that a vehicle with the same take-off mass as a rocket can transport a larger payload. Furthermore, take-off mass can be distributed to the vehicle structure, which can allow the vehicle to be re-usable and safer to operate. This is compared graphically in figure 1.1.

The problem with using aeroplanes to enter orbit is speed: the fastest piloted air-breathing vehicle, the SR-71 Blackbird, has a maximum flight Mach number of 3.2 and its engine technology, the ramjet, has a theoretical maximum Mach number of around 6 [50]. This implies that another engine concept is required for an airbreathing vehicle to enter orbit.

An airbreathing engine with the ability to operate in this flight regime is the supersonic-combustion ramjet or scramjet. As suggested by the name, a scramjet is a ramjet engine where the airflow, and hence combustion, remains supersonic through the engine rather than being slowed to below Mach 1, which is the case in a conventional ramjet. This concept is far from new and, at first glance, represents an evolutionary step up from an existing engine technology.

In practice, this step has shown itself to be non-trivial with the first successful flight testing of a scramjet-powered vehicle occurring in 2004. Part of the reason for this lag between the idea and demonstration is due to incomplete understanding of the physical processes that occur in the complex supersonic, turbulent and combusting flow found in a scramjet combustor.

Development of such an understanding requires experiments to be carried out at conditions which simulate the conditions inside a scramjet engine in flight, a formidable task in itself, and then use some diagnostic to work out what is actually happening in the test combustor. These results can then be used directly, or used as part of a computer model, to assist with the development of a new scramjet design.

Tunable diode laser absorption spectroscopy (TDLAS) is one such diagnostic technique and has been applied to environmental measurements, combustion
measurements, shock tube measurements and measurements in hypersonic flows. Examples of its use in scramjets, however, are few. This thesis documents the development of a sensor based on tunable diode laser absorption spectroscopy, and its application to a model scramjet combustor.

Specifically, the aim of this research project was to test the effectiveness of tunable diode laser absorption spectroscopy as a diagnostic, when applied to the measurement of water vapour concentration and temperature in a scramjet combustor.

The scope of this research was limited as follows:

- Testing was limited to a generic scramjet combustor which had been designed for use in a free-piston shock tunnel—the T3 shock tunnel located at the Australian National University; and
- Although tuned for the particular measurement environment, the TDLAS sensor would be based on proven techniques and existing designs.

These limits were chosen so as to maximise useful results produced by the research while accepting the limited time and resources available to the project.

In order to fulfil this aim, it is useful to have an understanding of the field of supersonic combustion research to help judge what is required of a new diagnostic. Chapter 2 provides a brief background of this research effort including the principles of scramjet operation, ways of testing scramjets and an overview of some diagnostics that are used with scramjet flows. Following this, chapter 3 describes the particular facility and scramjet model used for this work.

The theory underlying TDLAS follows in chapter 4. This is included to explain the processes that make the measurement possible and give some insight into the strengths and limitations of the technique. Chapter 5 builds on this theory with more practical discussion of how a sensor can be designed, and describes
the sensor built for this work. This chapter also includes some discussion of previous applications of TDLAS. The operation of the sensor is verified in chapter 6 and measurements in the combustor are reported in chapter 7.

In chapter 8, results obtained with other techniques are collated and compared with those from the sensor developed in this work. This provides a means to judge the effectiveness of the TDLAS sensor. Conclusions based on this comparison are presented in chapter 9.
1. Introduction
2. Supersonic combustion research

In chapter 1, it was noted that the problem of designing a practical scramjet-powered vehicle remains unsolved, despite decades of research. The purpose of this chapter is to provide a brief background of this research effort in order to demonstrate how the research presented here fits into a much larger field. Three components of this research effort are considered: the principles of scramjet operation; the mechanics of testing a scramjet design and the methods by which information can be extracted from the flow during a test.

Each of these components are presented in order to justify the development of tunable diode laser absorption spectroscopy, TDLAS, as a scramjet diagnostic. An understanding of the operating principles of a scramjet, for instance, is beneficial in order to decide what measurements should be made to improve its performance, thus influencing the development of a sensor.

Also important for the development of a sensor is the way in which scramjets are tested. Scramjets are designed for flight at extremely high speeds, up to Mach 25 for a vehicle designed to access earth orbit, and generating an airflow to match such flight speeds is difficult. All present methods of generating such airflows require various compromises in their design that a sensor must be able to accommodate—for instance flight tests require sensors to be compact and rugged while pulsed facilities, such as shock tunnels, require sensors to have a temporal response of significantly less than the milliseconds-long test time.

Furthermore, knowledge of existing diagnostic techniques, several of which are already available to our research group, is important to determine the worth of developing a new technique. The final part of this chapter discusses some of these techniques in terms of the information that they can produce and the effort required to get this information. A new sensor, then, should compliment the features of present diagnostic techniques.

2.1 Principles of Scramjet operation

Shown diagrammatically in figure 2.1, a scramjet is similar in concept to a ramjet engine. In contrast with turbojet or turbofan engines, there are no turbines to compress the incoming airflow. Instead, the shape of the intake and the vehicle’s forward motion combine to compress the incoming airflow. Since this is a supersonic airflow, this happens through a series of shocks.
Within the engine, fuel is injected into a supersonic airflow. This is in contrast to a ramjet engine where the airflow in the combustion chamber is subsonic. The design of the combustion chamber may incorporate features such as cavities in the sidewalls, to induce recirculation zones and act as flame-holders, or numerous other design attributes to improve the mixing of fuel and air while minimising drag.

Finally, the flow out the rear of the engine is expanded through a diverging nozzle analogous to the nozzle at the exit of rocket engines. The forward thrust generated by the engine can be considered to be due to the pressure on the thrust surface which is part of the diverging nozzle.

There are a number of effects that complicate the process of generating forward thrust. The fuel and air must mix and combust within the residence time of the combustor, which is typically on the order of a millisecond [28, e.g.]. Therefore, design of a combustor requires detailed knowledge of the fuel–air mixing mechanism and the combustion mechanism. Furthermore, in order to minimise drag, the engine needs to be integrated with the vehicle airframe. These effects are expanded upon below.

**Fuel-air mixing**

In order to produce thrust in a scramjet engine, fuel and air must react in the combustor segment of the engine, which requires thorough mixing over a short time period. Unfortunately, mechanisms that enhance mixing often have the side-effect of increasing drag. This is of particular concern in a scramjet engine, when compared to a ramjet engine design, since mixing is inherently more difficult in a supersonic airflow where disturbances are unable to propagate upstream. Consideration of the drag produced in the combustor is particularly important because of the disproportionate contribution that drag here can make to the total drag experienced by the vehicle [87].
Mechanisms for increasing mixing are often situated in the vicinity of the injector ports. The consideration of where fuel will be injected and in which direction opens up numerous possibilities for mixing enhancement. One approach is to inject fuel from a central strut, shaping the strut so as to induce vorticity in the flow. Designing the strut to increase mixing, however, has a tendency to increase total pressure loss [42], reducing net thrust.

A competing method is to inject fuel from combustor walls, where the design objective to increase mixing while minimizing drag still holds. Apart from strut injection, multiple configurations for introducing the fuel into the combustor are possible. Some of these include:

- Injection from a flat wall into the combustor at various injection angles [10];
- Inclusion of a cavity in the combustor wall, thereby inducing a recirculation region, with fuel injection upstream of the cavity or directly into the cavity [9, 48, 49]; and
- Injection upstream of the combustor into the cold airstream which allows the fuel and air to mix before combustion is initiated by the increase in temperature as the mixture enters the combustor [81].

While the combination of many of these design features is possible in a practical combustor, in fundamental studies these injection methods are usually studied in isolation in a research combustor. This was the approach taken in this work where the combustor was configured with injection into a single cavity.

Supersonic combustion

While it is necessary for the fuel to mix with air within the combustor, this is not enough for the generation of thrust—the mixture must also react. Because the time-scale of the chemical reactions involved are similar to the residence-time of the mixture in the combustor, a high degree of fidelity is required in the modelling of fuel-air chemistry and, because heat release affects the flow, this needs to be coupled with simulation of the airflow itself. This requirement is reflected in the complexity of reaction models that are employed in the simulation of scramjet combustors. As an example, Drummond et al. [29] present a model of hydrogen–air chemistry that includes 9 chemical species and 18 reactions for a reaction which, to a first approximation, is simply

$$\text{2H}_2 + \text{O}_2 \rightarrow \text{2H}_2\text{O}.$$  

This model treats nitrogen as inert, so that if we want to include the effects of NOx formation we need to add even more reactions and species to the model. Evans and Schexnayder include nitrogen chemistry, with a model including 12 species and 25 reactions [33].

Neglecting heat transfer and materials consideration, the fuel–air chemistry sets the ideal temperature inside the combustor. Low temperatures, close to
the fuel’s ignition limit, increase the delay between fuel-air mixing and combustion. Extremely high temperatures are also undesirable, causing dissociation of O\textsubscript{2} and N\textsubscript{2} and a reduction in heat release. These considerations set an appropriate temperature range of approximately 1440 K to 1670 K \cite{50} for the static temperature of air entering a scramjet combustor, although some recent work indicates that these temperatures need only be attained in certain ‘hot pockets’ in the flow rather than across the entire intake \cite{81}.

Airframe–engine integration

Another consideration for scramjet design is the necessity to integrate the engine with the vehicle’s airframe. At hypersonic flight speeds, drag considerations preclude the use of podded engines on struts and, as shown in figure 2.1, the entire length of the vehicle contributes to the flow through the engine.

As a consequence of this, the ultimate design of a scramjet engine needs to be highly integrated with the design of the vehicle that it powers. For practical reasons, simplicity of the flow and simplicity of the experimental apparatus, it is often desirable to build a model only of the combustor segment of a scramjet. In this case, the facility providing the flow would be configured to produce a flow analogous to the conditions after the intake of a vehicle in flight.

Experiments which model only the scramjet combustor, although carried out with the end goal of scramjet flight in mind, are better considered as fundamental studies of supersonic combustion. The research presented in this report falls into this category.

2.2 Scramjet testing

In order to run an experiment to simulate supersonic combustion in a scramjet, a high velocity, high enthalpy airflow is required. The way this test flow is generated has implications for the design of sensors used for the study of supersonic combustion and three possible methods of generating such an airflow are discussed below.

Flight testing

A guaranteed way of duplicating the conditions of a scramjet in flight is to run experiments in flight. This is a step that is certainly necessary near the end of a design cycle where a design is being proven, or for verification of results obtained in ground testing. An example of this was the NASA X43 \cite{95}, shown in figure 2.2, which became the fastest airbreathing vehicle on March 27th 2004 and was powered by a type of scramjet engine. This vehicle was 3.6 m long and was boosted to flight speed by a rocket which was itself launched from a conventional aircraft. Clearly, this type of test is an expensive operation which required an enormous amount of effort to be expended in the design of the test vehicle, but the 11 second flight was able to unambiguously prove the feasibility
2.2. Scramjet testing

Figure 2.2: The rocket-boost stage of two scramjet flight tests. The photograph on the left shows the HyShot Terrier-Orion launch rocket with a scramjet engine mounted in the nose cone [117]. On the right is the NASA X43 vehicle which is on the nose of a modified Pegasus rocket after being launched from a B52 [57].

of scramjet propulsion at Mach 6.8. In a later flight, a similar vehicle recorded a maximum flight speed of almost Mach 10.

The X43 test represented a test of an entire vehicle, but flight testing is also a worthwhile proposition for testing a scramjet combustor. The University of Queensland HyShot program studied supersonic combustion in a scramjet combustor that was mounted on the front of a two-stage rocket. In August 2002, the rocket flew beyond the atmosphere, turned around and then the experiment was conducted as rocket–scramjet coasted at Mach 7 back towards a crash landing in the Australian desert. The test was instrumented with pressure transducers which were able to prove that supersonic combustion occurred during the flight test and, due to the flight path of the rocket, was able to gather data from a range of flight conditions. Because of the design of the experiment, the data was able to be directly compared with experiments in a ground testing facility [40], as well as with computational simulation [15].

The sensors gathering data in these, and other flight tests need to be able to withstand large acceleration and vibration loading from the rocket launch. The sensors must also be compact enough to fit on-board the test vehicle. In addition, data produced by the sensors should be amenable to being transmitted over a telemetry link since, in both the X43 and HyShot tests, the mission ended with a crash-landing. So, while flight testing is the ultimate method of testing a scramjet design, it is not the easiest way to go about studying supersonic combustion due to the prohibitive cost, logistical difficulties and tight technical requirements on instrumentation. Fortunately possibilities exist for studying supersonic combustion in ground-based facilities.
Blow-down facilities

A common means of testing jet engines is to directly connect the engine to a test facility. This is also appropriate for low-enthalpy testing of scramjets where heated blow-down facilities are commonly used for supersonic combustion testing [23, 118, e.g.], although not always in direct-connect mode [22]. These facilities are characterised by flow durations of tens of seconds or several minutes and this is achieved by allowing a large volume, high-pressure reservoir to expand through a supersonic nozzle.

Blow-down facilities require the addition of heat to the flow prior to expansion through the facility nozzle. Heat addition may be accomplished in a number of ways and burning hydrogen or jet fuel is a common method. The resultant free-stream entering the scramjet combustor differs from atmospheric air because of the presence of combustion products and pre-combustion free-radicals. These contaminants affect the combustion processes in the scramjet combustor [89].

These facilities are also limited in the range of flight conditions they can simulate, with an upper limit on flight Mach number of around 8. Practical considerations of building a high pressure, high temperature pressure vessel are the limiting factor [89].

A sensor designed for these facilities has the advantage of long-running times so that large amounts of data can be gathered even with low sampling rates. However, long running times can be a problem too, as heat transfer to the sensor components needs to be considered in the sensor design.

Pulsed flow facilities

For higher Mach numbers, a different means of generating a test flow needs to be used. A range of facilities exist which produce a hypersonic test flow that lasts for a period of microseconds to milliseconds, where lower enthalpies result in longer test times [110]. These pulsed facilities can cover the entire range of scramjet flight to Mach 25.

Free-piston shock tunnels are a type of pulsed facility whose characteristics are roughly in the middle of the range of pulsed facilities. They are not specific to scramjet testing and deliver test times on the order of 1 to 5 ms, depending on the tunnel size and operating conditions. This is generally a disadvantage when compared with heated blow-down facilities, but means that sensors do not require the same level of thermal protection.

Free-piston shock tunnels also have the advantage that the air flow is more representative of atmospheric air than burner-heated blow-down facilities. This is because, in a shock tunnel, the air is heated and compressed with a shock wave prior to expansion through the facility nozzle and contains no combustion products. The flow still differs from atmospheric conditions, however, due to the formation of NO and other radicals in the stagnation region of the facility. Without sufficient time to re-combine, these species are ‘frozen’ in the flow as it expands out the nozzle. As with burner-related contaminants, these free radicals have the potential to influence combustion [81].
2.3 Diagnostics for scramjet-like flows

Shock tunnels may be operated with a model of the entire scramjet vehicle or, as was the case in this work, with a model of only the combustor. In the latter case, the tunnel is operated to produce conditions that match conditions at the combustor intake in flight, assuming the presence of an intake. This has the advantage of allowing a larger combustor model to be tested.

For a diagnostic, the most challenging feature of shock tunnels is the requirement to sample data quickly because of the short test time. This requirement is critical in a turbulent scramjet flow where multiple measurements are required to build up a mean value for the flow.

2.3 Diagnostics for scramjet-like flows

A wide range of diagnostic techniques exist for measurements in hypersonic flows. In developing a new technique, it is worth briefly reviewing these existing techniques in order to see what new information a proposed technique might offer about the flow.

Surface measurements

Measurements of flows can most easily be made by locating some kind of sensor on the surface of a model, or by placing a probe in the flow [66, e.g.]. Often, a surface is the most important place to find the flow parameters since it is here that the flow imparts force and heat onto a body.

Some possible surface measurements are listed below.

Pressure measurements are among the simplest to implement and are almost always employed in a testing campaign. A variety of pressure sensors exist, but for this work piezoelectric sensors were used. This type of sensor, shown in figure 2.3, contains a piezoelectric crystal which produces an electrical charge when stressed. This can be amplified by on-board electronics to produce a voltage that is proportional to pressure within the operating range. The signal decays with time as the charge on the crystal dissipates, but this discharge is on a longer time scale than a shock tunnel flow. Also significant is the effect of vibration on the sensor, which leads to noisy output, and local heating of the sensor which can lead to thermal expansion and an induced pressure offset.

Heat flux can be measured with thermocouples [37], due to the short test time of shock tunnels. The temperature rise measured over the test time can be differentiated to obtain heat flux.

Making use of piezoelectric again, skin drag [46] can be measured from the shear stress on a crystal. The output voltage needs to be corrected for acceleration and pressure, which also contribute to the signal produced by the crystal.

As well as being limited to the surface of bodies placed in the flow, surface diagnostics are usually limited to relatively coarse spacing because of the physical size of the sensors. The combination of these two effects is that it is difficult to judge what is happening in the flow-field from surface measurements alone.
Optical diagnostics

Optical diagnostics provide a means of flow visualisation, or making quantitative measurements, away from surfaces and without disturbing the flow. The earliest optical techniques exploited variation in the refractive index of the flow due to density gradients. According to Anderson [6], schlieren photographs of shock structures in converging–expanding nozzles were produced by Prandtl and Meyer during 1907–1908.

More recently, lasers have allowed for the development of a variety of techniques based around the interaction of monochromatic light with molecules in the flow. These techniques are generally more demanding to implement than the classical techniques, but can provide a wide range of quantitative data.

Optical techniques have technical difficulties associated with their implementation in scramjet flows. All optical diagnostics have the requirement of optical access to the flow. In scramjets, this usually means that windows have to be incorporated into the design of the test model, resulting in trade-offs in other aspects of the design. The complexity and expense of optical diagnostics can also be a disadvantage when compared with surface sensors.

Shadowgraph and schlieren are classical techniques that both employ a collimated light source that is shone through the flow. Variations in density deflect the beam and these locations show up as light or dark areas in the photographs that the techniques produce. Shadowgraph is less sensitive than schlieren, which can be an advantage when applied to scramjet–like flows with enormous density variations. Shadowgraph has been used to visualise scramjet combustors on several occasions [41, 79, 66]. Schlieren has also been applied successfully with one example coming from Ben-Yakar and Hanson's study [10] of the time evolution of the injection of a hydrogen jet into a supersonic cross flow. In their traditional forms, both techniques are sensitive to variations in density along the entire beam path and therefore are best suited to a 2-D flow field. For 3-D flows, focusing Schlieren [126] can be used to visualise a slice of the flow field.

Planar laser induced fluorescence (PLIF) is more appropriate when studying
2.3. Diagnostics for scramjet-like flows

3-D flows as it restricts its measurement domain to a slice of the flow. In a PLIF experiment, a laser sheet crosses the area of the flow to be investigated while a camera observes fluorescence induced by the laser sheet. In scramjet measurements, OH [11] and NO [86] are common targets since the first indicates the presence of combustion while the second is abundant in shock tunnel flows generally. When set up to probe two different molecular states, NO PLIF can produce a map of temperature allowing for direct comparison with computational simulation. If the experimental setup allows, multiple offset PLIF images can be combined to provide a 3-D temperature map.

As well as temperature, PLIF can be used to make velocity measurements through the use of a flow tagging procedure [24].

Nonlinear optical techniques such as coherent anti-Raman spectroscopy (CARS) [17] are possible candidates for measurements in scramjet flows. For shock tunnel experiments, CARS is important because of its ability to measure vibrational and rotational temperature simultaneously and, in doing so, show the extent of vibrational non-equilibrium in nozzle flows [36]. Another distinctive feature of CARS is that it measures parameters at a single point in the flow. This makes it possible to build up a 3-D map of a flow by moving the interaction region. However, such a process will take quite a while since CARS measurements typically have a repetition rate of around 10 Hz. This is not a feasible proposition in a shock tunnel facility, but it is possible in a direct-connect, heated blow-down facility with a longer running time [23].

Tunable diode laser absorption spectroscopy (TDLAS) can operate at sampling rates of tens of kilohertz. Depending on the choice of laser wavelength, many different species concentrations can be measured. TDLAS can also be used to measure temperature and velocity. Measurements are made along a line-of-sight, and careful interpretation is necessary if the technique is applied in environments where conditions vary along the line-of-sight.

Scramjet engines are complicated to design and test. Design is complicated by the complexity of the flow physics, requiring consideration of turbulent mixing and chemical kinetics. Testing is complicated by the practical issues of generating a high energy flow that simulates the conditions in a scramjet.

Nevertheless, free-piston shock tunnels provide one possible means of generating scramjet-like flows. More details of the facility and scramjet model used in this work are given in chapter 3. Test time is short, and this needs to be considered in the design of diagnostics for such facilities.

Diode laser absorption spectroscopy is one of many diagnostics that can be applied to shock tunnel flows, and the theory underlying this measurement will be considered in chapter 4.
2. Supersonic combustion research
3. T3 flow facility and scramjet model

The experimental study of scramjet flows requires a means of generating a high speed, high enthalpy air flow, as well as a model scramjet to test. For this work, the flow was provided by a pulsed facility, a free-piston shock tunnel known as T3, and utilised a previously-developed scramjet model.

Despite requiring some modifications to allow the laser beam to access the flow, the use of an existing model reduced the mechanical design and manufacture requirements to the level that they were manageable for this project. This also meant that the flow was already relatively well understood, the fuel injection system was well calibrated and CFD efforts that were underway for other work were applicable to this project also.

This chapter describes the T3 shock tunnel, its operation and the flow conditions that the facility was configured to provide. Following from this, section 3.2 describes the scramjet model.

The discussion is relatively brief, since details of both T3 and the scramjet model—albeit in a variety of different configurations—have been presented elsewhere [35, 42, 66, 75, 78, 109].

3.1 The T3 shock tunnel

The T3 free-piston shock tunnel is the third tunnel of its type built. The free-piston shock tunnel was invented by Stalker [108] and T1 was built in 1962 to prove the operational concept.

As mentioned in section 2.2, pulsed facilities are one possible option for scramjet testing. A wide range of pulsed facilities exist with the general properties that the test time is short, $10^{-5}$ to $10^{-2}$ s [110], with higher enthalpy operation resulting in shorter test times. Free-piston shock tunnels are at neither extreme of the test conditions produced by the family of pulsed flow facilities and can produce flows that are applicable to a wide range of possible scramjet operating conditions, although not up to orbital insertion velocities.

Configuration

Modestly sized when compared with newer shock tunnels the T3 shock tunnel, shown in figure 3.1, has a total length of over 20 m. The facility consists of a series of interconnected chambers:
A high pressure reservoir is located behind a piston which is initially stationary but free to move within the next chamber, the compression tube;

The compression tube contains the driver gas and is terminated at its downstream end by a metal diaphragm, known as the primary diaphragm. The diaphragm is chosen according to the desired burst pressure and may be stainless steel or aluminium sheet with typical thickness ranging from 0.7 mm to 2.9 mm;

The primary diaphragm is then followed by a narrower diameter tube, known as the shock tube, which terminates with a thin plastic diaphragm. This ‘secondary diaphragm’ is made from 0.05 mm thick mylar and separates the shock tube from the facility nozzle and test section;

The test section has a cross section of 0.5 m and has windows allowing vertical or horizontal cross-stream optical access; and

Following the test section is a large-volume dump tank.

Operation

Before operation, the compression tube, shock tube and dump tank are evacuated with oil-filled rotary vane roughing pumps to around 0.1 torr (13 Pa), before being filled with gases, as shown in figure 3.2a. The shock tube is filled with the test gas, which was dry air for this work, while the compression tube is filled with the driver gas. Helium was used as the driver gas, chosen for its high sound speed and because it is chemically inert. The piston is then held on a launcher as the high pressure reservoir is filled and, once the pressure here reaches the desired pressure, the tunnel is ready to fire.

From this state, the tunnel can be fired by releasing the piston from the launcher by opening a valve. The pressure behind the piston accelerates it down the compression tube, compressing the driver gas up to the burst pressure of the primary diaphragm. The initial pressure behind the piston is chosen so that the piston retains some forward momentum after the main diaphragm bursts. This is referred to as tuned operation [59] and helps to keep the pressure of the driver gas closer to constant than it would otherwise be.
3.1. The T3 shock tunnel

The flow within the shock tube after diaphragm rupture is described by Gaydon and Hurle [43]. With diaphragm rupture, a shock wave propagates down the shock tube compressing and heating the test gas, as shown in figure 3.2b. Upon arriving at the downstream end of the shock tube, the shock wave reflects off, and vaporises, the mylar diaphragm. The reflected shock then travels back up the shock tube again heating and compressing the flow, as well as slowing it so that the conditions upstream of the nozzle approximate a high temperature, high pressure stagnation region with conditions of the total pressure and temperature of the flow, around 15 MPa and 4500 K for the conditions used in this work. If the reflected shock brings the contact surface to rest, the condition is described as ‘tailored’, however other scenarios are possible [43, p 64]. The test gas then starts flowing out of this stagnation region through the hypersonic nozzle, shown in figure 3.2c.

As well as the shock produced at diaphragm rupture, an expansion wave is produced at the junction of the compression and shock tubes [43, p 60]. Its head travels into the compression tube, reflects off the piston and interacts with the flow structures at the far end of the shock tube. Provided that the shock tube is
not too short, the primary shock reflects from the end of the shock tube before it is overtaken, and attenuated, by the expansion wave.

The nozzle has a throat-to-exit area ratio chosen for the desired Mach number in the test section. After a starting process is complete, quasi-steady flow exists in the test section, for around 3 ms at these operating conditions. This is shown in figure 3.2d. Keeping the dump tank at vacuum minimises the time required for the establishment of quasi-steady flow. The completion of a test is caused by the arrival of driver gas in the test section, indicated by the contact surface in figure 3.2b–d. Driver gas can arrive in the test section earlier than anticipated by consideration of the 1-dimensional flow due to driver gas ‘jetting’ along the edges of the shock tube [83, e.g.] so that identification of driver gas contamination is a major consideration in shock tunnel experiments. This is more of a concern at higher enthalpies than those used in this work. Previous work suggests that driver gas contamination happens sometime after 4 ms after the initial shock reflection for the present operating conditions [76].

Prior to the arrival of driver gas, the pressure in the stagnation region drops steadily as shown in figure 3.3. This pressure signal generally exhibits a plateau for part of the test time, however a significantly longer period of quasi-steady flow can be identified from pressure measurements. This is done by taking the ratio of pressure at a location in the test section to the stagnation pressure and identifying a period where this ratio is a constant. Such a comparison requires the transit time between the two pressure transducers to be taken into account, so that pressure is compared at the same point in the slug of test gas. A measurement of pressure in the stagnation region is also necessary to calculate the free-stream conditions at the exit of the nozzle, as explained next.

The test conditions that were used in this work were chosen to match those used in previous and ongoing work with this scramjet combustor, and tunnel
3.1. The T3 shock tunnel

Table 3.1: Operating conditions for the T3 shock tunnel used for this work. The uncertainty in measured quantities is the shot-to-shot scatter while uncertainty in the effective area ratio, which is calculated from Pitot pressure, is due to Pitot pressure measurement uncertainty.

<table>
<thead>
<tr>
<th>Tunnel operating parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial shock tube fill pressure</td>
<td>$50.0 \pm 0.2$ kPa</td>
</tr>
<tr>
<td>Primary shock speed</td>
<td>$2510 \pm 30$ ms$^{-1}$</td>
</tr>
<tr>
<td>Stagnation pressure at 1.5 ms</td>
<td>$14.3 \pm 0.2$ MPa</td>
</tr>
<tr>
<td>Stagnation pressure at 2.0 ms</td>
<td>$12.9 \pm 0.2$ MPa</td>
</tr>
<tr>
<td>Physical nozzle throat-to-exit area ratio</td>
<td>12.96</td>
</tr>
<tr>
<td>Effective nozzle throat-to-exit area ratio</td>
<td>$12.6 \pm 0.4$</td>
</tr>
</tbody>
</table>

Operation parameters are shown in Table 3.1. For the development of a new sensor, this is extremely useful as it allows measurements to be made in a flow that is relatively well understood from other work. This has the secondary benefit of saving the time it would have otherwise taken to calibrate the tunnel at new operating conditions.

Determination of free-stream conditions

For a number of years the free-stream conditions in both the T2 and T3 shock tunnels have been determined in a roughly similar manner, so there are numerous references describing this procedure [35, 38, 77]. A similar process was followed for this work as outlined below.

Initial pressure and temperature in the shock tube are known and two pressure transducers are used to determine the velocity of the primary shock. The delay between the initial rise of the two transducer signals is measured with a digital counter to within $\pm 1$ $\mu$s. The distance between the transducers was $1438 \pm 5$ mm and the primary shock speed was calculated for each shot.

The shock velocity and conditions in the shock tube are used to solve the conditions behind the shock, assuming 1–dimensional flow and equilibrium chemistry, using a Fortran code known as ESTC [65]. Using these new conditions as input, the same code is then used to solve for the conditions after the reflected shock with the additional constraint that the reflected shock brings the flow to rest.

The pressure measured in the stagnation region will, in general, differ from the conditions predicted by the two passes of ESTC due to the interaction of the reflected shock with the contact surface, so a correction is applied to adjust the conditions to match the measured pressure. This correction, which assumes that the interaction between the reflected shock and the contact surface is isentropic, is done by iteratively applying an isentropic expansion or compression to the model results until the measured and modelled pressure match, therefore fully specifying the conditions in the stagnation region.
A quasi-one-dimensional calculation then follows, using these stagnation conditions and the nozzle geometry as input. This is performed using the STUBE code [121] which incorporates finite-rate chemistry, and therefore chemical freezing, as well as vibrational non-equilibrium. This is necessary since, in a hypersonic nozzle flow, the flow can cool faster than the vibrational relaxation time so that vibrational temperature remains significantly higher than translational and rotational temperature.

Since this is an inviscid calculation, the effect of the boundary layer on the facility nozzle is not predicted. In order to correct for this, the area ratio of the nozzle at the test section is varied until Pitot pressure predicted by the model matches the measured Pitot pressure. Physically, this is justified by considering a boundary layer as a constriction of the nozzle and therefore a modification of the throat-to-exit area ratio.

For this work, this process resulted in the conditions shown in table 3.2 which are quoted at both 1.5 ms and 2 ms after shock reflection. The uncertainties given are calculated by repeating this process at the limits of the uncertainty in the input conditions.

**Additional discussion of free-stream conditions**

Sometime after this thesis was submitted for examination, a problem was discovered with the free-stream conditions. This issue was pointed out by Sean O’Byrne and is discussed, along with its implications, in this additional section.

As mentioned above, the test gas cools rapidly as it expands through the hypersonic nozzle. If the flow speed is great enough, the vibrational temperature of the species in the flow will no longer be in equilibrium with the rotational and translation temperature—it will be higher by an amount determined by the vibrational relaxation time. Since the relaxation time differs between species present in the flow, the vibrational temperature will be different for each species. In the nozzle flow considered here, $N_2$ is the only species for which vibrational non-equilibrium need be considered.

This rather complex situation is treated in STUBE by a so-called ‘sudden freezing’ approximation. As the flow progresses through the nozzle, it stays in equilibrium until the cooling rate is judged to be greater than the vibrational relaxation rate for a particular species. The vibrational temperature is then held constant for that species past this point. Measurements performed in the T3 facility show that this provides a reasonable approximation to the nozzle flow, although better for pure nitrogen flows than air flows [36].

The conditions shown in table 3.2 were inadvertently calculated with the vibrational temperature frozen at the reservoir condition, rather than at some lower-temperature condition part way down the nozzle. Since the vibrational temperature is too high, compared with the actual flow, energy conservation requires that the calculated free-stream temperature is low.

Because of this problem, the free-stream conditions have been re-evaluated and two additional cases appended to table 3.2.
3.1. *The T3 shock tunnel*

Table 3.2: Nominal free-stream conditions at the combustor intake. The ‘vibrational temperature frozen at reservoir temperature’ case shows the free-stream conditions that were used in this thesis with the incorrect belief that the conditions had been calculated under the ‘sudden freezing’ approximation. The ‘vibrational equilibrium’ case shows the conditions that are the most appropriate for use with CFD and the ‘sudden freezing’ approximation is the most physically correct, but has been calculated only for 1.5 ms. See page 20 for further discussion.

<table>
<thead>
<tr>
<th>Freestream quantity</th>
<th>Value at 1.5 ms</th>
<th>Value at 2.0 ms</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Vibrational temperature frozen at reservoir temperature</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mach number</td>
<td>4.16 ± 0.09</td>
<td>4.18 ± 0.10</td>
</tr>
<tr>
<td>Static Pressure</td>
<td>80 ± 6 kPa</td>
<td>70 ± 6 kPa</td>
</tr>
<tr>
<td>Pitot Pressure</td>
<td>1750 ± 80 kPa</td>
<td>1580 ± 70 kPa</td>
</tr>
<tr>
<td>Density</td>
<td>0.23 ± 0.01 kgm(^{-3})</td>
<td>0.21 ± 0.01 kgm(^{-3})</td>
</tr>
<tr>
<td>Velocity</td>
<td>2790 ± 30 ms(^{-1})</td>
<td>2760 ± 30 ms(^{-1})</td>
</tr>
<tr>
<td>Rotational temperature</td>
<td>1160 ± 50 K</td>
<td>1130 ± 50 K</td>
</tr>
<tr>
<td><strong>Vibrational equilibrium</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mach number</td>
<td>3.76 ± 0.06</td>
<td>3.77 ± 0.08</td>
</tr>
<tr>
<td>Static Pressure</td>
<td>101 ± 7 kPa</td>
<td>91 ± 6 kPa</td>
</tr>
<tr>
<td>Pitot Pressure</td>
<td>1805 ± 80 kPa</td>
<td>1624 ± 75 kPa</td>
</tr>
<tr>
<td>Density</td>
<td>0.22 ± 0.01 kgm(^{-3})</td>
<td>0.21 ± 0.01 kgm(^{-3})</td>
</tr>
<tr>
<td>Velocity</td>
<td>2870 ± 30 ms(^{-1})</td>
<td>2850 ± 30 ms(^{-1})</td>
</tr>
<tr>
<td>Temperature</td>
<td>1560 ± 60 K</td>
<td>1510 ± 50 K</td>
</tr>
<tr>
<td><strong>Sudden freezing(^1)</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mach number</td>
<td>3.74 ± 0.03</td>
<td></td>
</tr>
<tr>
<td>Static Pressure</td>
<td>88 ± 2 kPa</td>
<td></td>
</tr>
<tr>
<td>Density</td>
<td>0.217 ± 0.007 kgm(^{-3})</td>
<td></td>
</tr>
<tr>
<td>Velocity</td>
<td>2885 ± 20 ms(^{-1})</td>
<td></td>
</tr>
<tr>
<td>Rotational temperature</td>
<td>1410 ± 30 K</td>
<td></td>
</tr>
</tbody>
</table>

\(^1\) provided by Sean O’Byrne. N\(_2\) frozen at 2468 K, other species in equilibrium.
The first of the additional cases shows the free-stream conditions evaluated under vibrational equilibrium. The temperature of the physical free-stream flow should fall somewhere between the original prediction and vibrational equilibrium. This is seen to be the case for a third calculation showing the free-stream conditions evaluated with a sudden freezing approximation—the calculation that was thought to have been used initially.

Although the sudden freezing approximation is the most physically accurate of the three, there is still value to the vibrational equilibrium case. If computed nozzle exit conditions are to be used as inflow conditions in a CFD simulation, the equilibrium case should be used if the code does not support vibrational non-equilibrium. This approach conserves the total energy of the flow. Furthermore, the physical flow may well approach the equilibrium case inside the scramjet combustor after passing through the inlet shocks.

The use of incorrect free-stream conditions represents a major flaw in the CFD simulations presented later, and it would be interesting to revisit these simulations using vibrational equilibrium inflow conditions. Other results remain valid, however. In particular, mass flux changes by around 2.5% so that equivalence ratio calculations remain valid.

In my opinion, it would be worthwhile to explore alternatives to STUBE for future freestream calculations.

### 3.2 Scramjet combustor model

The scramjet model used in these experiments resembles a rectangular duct with an adjustable floor that can be set so that the duct diverges beyond the half-way point. Previously, this scramjet model has been configured with a strut injector for hyper-mixing studies [35, 66, 79]. The present configuration replaces the previously-used strut injector with injection from the rear face of a cavity. The performance of the cavity in a straight duct has been studied using pressure measurements [75] and OH-PLIF experiments [80].

Apart from the addition of the cavity and the removal of the strut injector, the scramjet model remains essentially the same as in previous work. In particular, the injection system and pressure transducer instrumentation remain the same.

The geometry of the scramjet duct is shown in figure 3.4. The scramjet model was designed with combustor studies in mind and therefore does not include an intake ramp. This allows a more homogeneous airflow to enter the combustor, simplifying the flow-field somewhat, as well as allowing for a larger combustor than would be possible if intake geometry were included.

Since the model does not compress the incoming airflow, the shock tunnel is configured to deliver an airflow that is analogous to the flow that would be present at the entrance to the combustor in flight. For the conditions used in these experiments, the free-stream conditions are equivalent to a vehicle flying at Mach 10.5, with details shown in table 3.2. Equivalent Mach number was calculated from the inlet conditions by applying conservation of enthalpy and
3.2. Scramjet combustor model

assuming a free-stream temperature of 225 K. The high temperature, 1190 K, and pressure of around one atmosphere means that conditions in the combustor are sufficient to initiate combustion.

The flow from the nozzle of the facility is swallowed by the combustor intake, shown in figure 3.5. The intake has sharp leading edges so that, apart from relatively weak shocks attached to these intakes, the flow entering the combustor has similar properties to the free-stream. The flow that does not enter the scramjet is deflected by a bluff plate, also visible in figure 3.5. This plate protects the instrumentation located on either side of the scramjet, however it causes a major disturbance to the external flow. To verify that the plate does not influence flow entering the combustor duct, a photograph was taken of the flow relying on flow luminosity to identify areas of the flow affected by the plate. As shown by figure 3.6, the presence of the plate does not influence the interior flow, with the flow disturbance appearing downstream of the scramjet intake. Pressure measurements taken with and without the duct in place also supported the theory that the duct flow was unaffected by the exterior plate.

The flow within the combustor, meanwhile, travels down the first section of the rectangular duct before encountering a cavity in the floor of the duct. The cavity's main purpose is to provide a recirculating zone holding a hot pool of radicals for flame-holding and stabilisation. Important features of the cavity are its length-to-depth ratio, the sloping rear face and location chosen for fuel injection [49].

The length-to-depth ratio, $L/D$, has a strong influence on the flow structure within the cavity which, in turn, determines drag and mass exchange with the
Figure 3.5: Scramjet inlet viewed from upstream. The duct is 52 mm wide and 25 mm high. The large bluff plate protects sensors mounted on the side of the scramjet and does not disturb the flow entering the duct.

Figure 3.6: False colour luminosity image of the scramjet intake from side-on taken to verify the integrity of the flow entering the combustor. Flow direction is left to right.
3.2. Scramjet combustor model

main flow. This cavity has $L/D = 4.8$, which puts it in the range of minimum induced drag, when fuel injection is off, according to Ben-Yakar and Hanson’s review [9].

The rear face of the cavity is sloped in order to dampen the oscillations that would otherwise be produced in a rectangular cavity of a similar size. Flow oscillations within the cavity are generally undesirable because of the associated increase in drag and instability in the combustion process. Although the flow is certainly turbulent, the sloping back wall of the cavity stabilises the re-attachment of the boundary layer and reduces acoustic wave reflection from the downstream end of the cavity. Both of these features result in reduced oscillations.

Hydrogen injection can also help stabilise the flow. Hydrogen was injected into the cavity from the downstream end, in the opposite direction to the free-stream flow. The model can also be configured for other injection schemes which are expected to be tested in the future. For the generation of thrust, the injection scheme used here is not considered optimal.

Having passed the cavity, the fuel–air mixture is expanded by a 15° corner in the duct floor. Previous work with this scramjet model used a straight duct downstream of the cavity, but the presence of the expansion corner means that the downstream temperature and pressure is reduced, leading to a more suitable environment for spectroscopic measurements.

The laser beam for TDLAS measurements traverses the flow perpendicular to the main flow direction. A fibre optic collimator is located on one side of the combustor with a detector on the other side. These are mounted in a section of the scramjet side-plate that can be traversed vertically across the flow, with the extents of this traverse shown in figure 3.4. The alignment of the beam horizontally across the flow means that the laser is likely to probe a more homogeneous part of the flow than if aligned vertically. Due to the large vertical gradient in flow properties, however, the measurements produced by the sensor were expected to vary significantly as the beam was traversed vertically across the duct.

The laser beam could be located from 5.6 to 50.6 mm above the floor of the duct, covering half of the vertical extent of the duct, which had a total height of 97.6 mm at this location. This was expected to encompass most of the variation in water vapour concentration and temperature across the duct. Further details of how TDLAS was interfaced with the scramjet are given later in section 7.1, prior to the presentation of results.

The fuel injection subsystem is shown schematically in figure 3.7. A Ludwieg tube could be filled with hydrogen to a pressure between 350 and 2500 kPa before the tunnel was operated. A fast-acting valve was opened before the arrival of test flow in the scramjet, triggered from the recoil of the tunnel. The valve opened 30 ms before shock reflection and then shut between 50 and 150 ms after shock reflection. From the Ludwieg tube, the fuel flowed into a plenum chamber underneath the fuel injection ports and then, from the rear face of the cavity, into the scramjet.
Figure 3.7: Important components of the fuel injection system.

Figure 3.8: Details of the pressure transducer mounts in the scramjet floor (figure from [42]). Transducers are recessed to avoid damage.

Instrumentation

Besides TDLAS, the scramjet model is instrumented with multiple piezoelectric pressure transducers. The location of pressure transducers used in this work are shown in figure 3.4 with the details of the mounting shown in figure 3.8. The first of these transducers, referred to as the ‘inlet’ transducer, is mounted on the roof of the duct, upstream of the cavity and 70 mm downstream of the inlet. The results produced by this transducer were noisy compared with the other transducers. Since the flow should be more stable here than at other measurement stations, this is believed to be due to the different mounting configuration of this transducer compared with the others. This theory is supported by the improvement in data produced by this transducer after the vibration isolation of this mount was improved, however this improvement was made after data for this work had been collected.
3.2. Scramjet combustor model

The next transducer in the duct measured pressure on the floor of the cavity—the ‘cavity’ transducer. This transducer produced results that exhibited more fluctuations than the downstream transducers but less than the inlet transducer. Since this transducer was mounted in a similar manner to the downstream transducers, i.e. the configuration shown in figure 3.8, the fluctuations measured with the ‘cavity’ transducer were interpreted as being due to pressure fluctuations at this measurement location.

Downstream of the cavity, a section of the duct was instrumented with 10 pressure transducers spaced 20 mm apart, which was the closest spacing allowed by the size of the transducer mounts. These pressure transducers can be used to test for combustion in the duct by comparing pressure between subsequent experimental runs where fuel is injected into a nitrogen and then air free-stream. The increase in pressure between these two cases can be attributed to combustion.

Apart from the cavity transducer which was 10 mm from the centre-line, the pressure transducers were mounted on the centre-line of the duct and were PCB 113A21 model transducers with built-in amplification circuitry. The output from the transducers was amplified by model 483A02 and 483B03 PCB amplifiers and the results were stored on digital storage oscilloscopes.

As well as the transducers in the duct, the pressure in the plenum chamber was recorded over the operating time of the fast-acting valve. Pressure in the Ludwieg tube was recorded before and after operation of the tunnel, and these three quantities allow the calculation of the fuel–air equivalence ratio.

Calculation of equivalence ratio

The relative proportions of fuel and oxidiser in a combustible mixture are characterised by the equivalence ratio, $\phi$. The equivalence ratio relates the actual molecular fuel/oxidiser ratio to the stoichiometric ratio. By definition, for $\phi > 1$ the mixture is fuel-rich and unburned fuel will remain after combustion, whereas for $\phi < 1$ the mixture is fuel-lean and oxygen will remain after combustion.

The concept of an equivalence ratio is usually applied to closed systems where the fuel and air can fully mix and have time to react. This is not necessarily the case in a scramjet engine where the local equivalence ratio can be quite different from the global equivalence ratio. However, the concept is still a useful means of characterising the operating conditions.

For a hydrogen–air mixture,

$$\phi = \frac{n(H_2)}{2n(O_2)}$$

(3.1)

where $n(\ldots)$ represents the molar concentration of each species.

In a scramjet, this can be rewritten in terms of the input mass flow rates of hydrogen, $\dot{m}_{H_2}$, and air, $\dot{m}_{air}$. In doing so,

$$\phi = 34.23 \frac{\dot{m}_{H_2}}{\dot{m}_{air}}$$

(3.2)
assuming dry air which is 20.95% oxygen by volume, the molecular mass of hydrogen is 2.02 g/mol and the molecular mass of air is 28.97 g/mol.

The mass flow of air is known from the tunnel free-stream conditions, calculated in section 3.1, and the cross-sectional area of the combustor inlet. The calculation of hydrogen mass flow follows an unpublished method developed by Alan Paull and Russell Boyce [16], described briefly here. In this method, we measure the initial pressure in the Ludwieg tube, $p_i$, the final pressure in the Ludwieg tube after it has returned to room temperature, $p_f$, and record the pressure in the plenum, $p_m(t)$, while the fast-acting valve is open. From this, we can determine the total mass of fuel injected

$$m = (p_i - p_f) \frac{V}{R_{H_2} T_0}, \quad (3.3)$$

where $V = 1.419 \text{ L}$ is the volume of the Ludwieg tube, $R_{H_2} = 4124 \text{ J/kg} \cdot \text{K}^{-1}$ is the gas constant for hydrogen and $T_0$ is the Ludwieg tube temperature.

Previously, work at T3 [35, 42, 76] has assumed that the instantaneous mass flow was proportional to the plenum pressure. Using this assumption, the plenum pressure can be numerically integrated and equated to equation (3.3) to find the proportionality constant. The problem with this method is that it implicitly assumes that the temperature in the plenum is constant, which is not a good assumption since the gas cools as it expands out of the Ludwieg tube. Taking cooling into account, we must proceed as follows.

If we assume isentropic flow and treat the injectors as a sonic throat then the temperature at the injectors, $T^*$, is related to the initial temperature in the reservoir, $T_0$ equal to the total temperature, by

$$\frac{T_0}{T^*} = \left( \frac{p_i}{p^*} \right)^{\frac{\gamma - 1}{\gamma}} \quad (3.4)$$

where $p^*$ is the pressure at the throat and $\gamma$ is the ratio of specific heats ($\gamma = c_p/c_v$) for the fuel. This assumption allows the mass flow to be written as

$$\dot{m} = \sqrt{\frac{\gamma}{R_{H_2}}} A \frac{p^*}{\sqrt{T^*}} \quad (3.5)$$

since we know that the velocity here is equal to the local sound speed, $\sqrt{\gamma R_{H_2} T^*}$, and $A$ is the effective cross-sectional area of the injector ports. Equation (3.4) allows us to eliminate $T^*$ from equation (3.5) so that

$$\dot{m} = \left( \sqrt{\frac{\gamma}{R_{H_2}}} A p_0^{\frac{\gamma - 1}{2\gamma}} \right) p^{\frac{\gamma - 1}{2\gamma}} \quad (3.6)$$

where the term in parenthesis is a constant for a particular injector and fill pressure. Furthermore, this shows that the relationship between $\dot{m}$ and $p^*$ is non-linear. If we integrate equation (3.6) to obtain $\dot{m}$ and equate it with equation (3.3) then the constant term in equation (3.6) can be eliminated and we can write

$$\dot{m} = (p_i - p_f) \frac{V}{R_{H_2} T_0} \int_{-\infty}^{+\infty} \frac{(p^*)^{\frac{\gamma - 1}{2\gamma}}}{p^{\frac{\gamma - 1}{2\gamma}}} \, dt. \quad (3.7)$$
3.2. Scramjet combustor model

At this stage we still have the mass flow in terms of the unknown pressure at the injectors, $p^*$. However, if we assume that pressure in the plenum chamber, $p_m$, is proportional to $p^*$ and therefore substitute $p^* = C p_m$ into equation (3.7) then the proportionality constant, $C$, cancels between the numerator and denominator. This provides a useful expression for the mass flow;

$$\dot{m} = (p_i - p_f) \frac{V}{R_{H_2} T_0} \frac{\int_{p_m}^{p^*} \frac{p_{m}^{\gamma+1}}{p_{m}^{\gamma+1}} \, dt}{\int_{0}^{\infty} \frac{p_{m}^{\gamma+1}}{p_{m}^{\gamma+1}} \, dt},$$

(3.8)

where $R_{H_2} = 4124 \text{Jkg}^{-1}\text{K}^{-1}$, $V = 1.419 \times 10^{-3} \text{m}^3$, $\gamma = 1.4$ and $T_0$ is typically 296 K.

Assuming that the isentropic relation holds, the ratio of local static pressure to pressure at the throat is a function of Mach number,

$$\frac{p}{p^*} = \frac{\left(1 + \frac{\gamma - 1}{2} M^2\right)^{\frac{\gamma}{\gamma - 1}}}{\left(1 + \frac{\gamma - 1}{2} M^2\right)^{\frac{\gamma}{\gamma - 1}}},$$

(3.9)

then the assumption that $p_m \propto p^*$ will be accurate provided that the Mach number in the plenum is low.

An example of this calculation is shown in figure 3.9 where equation (3.8) was used to determine the mass flow from the injector pressure trace. A similar calculation assuming that $\dot{m} \propto p_m$, as assumed by several previous investigators [35, 42, 76], is also shown. Although the method outlined in this work is expected to be more precise, it produces almost identical results to the method used previously and therefore validates the previously-reported equivalence ratios. The equivalence ratios reported here do not match those reported by Neely et al. [75], despite the same operation conditions. This was due to an implementation error in Neely’s analysis so that, for hydrogen tests, the equivalence ratio was under-predicted by a factor of two.

Having calculated hydrogen mass flow, the equivalence ratio can be calculated from the mass flow of air predicted by STUBE/ESTC and using equation (3.2). This can be carried out repeatedly as stagnation pressure decays over the test period to obtain the result shown in figure 3.10. As well as showing the repeatability of the shock tunnel, this shows that equivalence ratio rises over the test period due to the stagnation pressure decaying faster than the plenum pressure. This has implications for the interpretation of the TDLAS results outlined later.

Recalling that the determination of the equivalence ratio required the scramjet inlet conditions to be known, the equivalence ratio is the parameter most likely to show shot-to-shot scatter. Since repeatability is good, it can be concluded that the test environment, comprising of the T3 shock tunnel and the scramjet combustor model, are well characterised and well suited to testing a new diagnostic technique.
3. T3 flow facility and scramjet model

Figure 3.9: Hydrogen mass flow calculated by the method outlined in the main text as well as the method used previously by others [35, 42, 76]. The results produced by the two methods are nearly identical at the time of tunnel operation.

Figure 3.10: Fuel-air equivalence ratio calculated from plenum pressure and stagnation pressure traces for fourteen shots, half with 950 kPa and half with 2500 kPa Ludwieg tube fill pressure. Good repeatability is evident between shots, and equivalence ratio always increases over the test.
4. Absorption spectroscopy theory

Spectroscopy describes the interaction of electromagnetic radiation with atoms or molecules. The theoretical base that has been developed to explain this process is voluminous, however it is possible to consider a manageable portion of the theory by focusing on aspects that relate directly to the measurement we want to perform. This means restricting the focus of this chapter to a short outline of the rotational–vibrational spectroscopy of water vapour.

The theoretical background provides an indication of how the measurement is possible and also suggests what the limitations of an optical diagnostic technique based on spectroscopy may be.

The overview presented here is necessarily brief. Molecular energy levels that give rise to the absorption lines that are probed in this study are discussed first, along with the convention followed for labelling the transitions. Following this, aspects of the theory required for making a physical measurement are covered, including the prediction of line strength and line shape. This is used to determine how a measurement of absorption can be used to determine temperature and number density.

4.1 Molecular ro-vibrational energy levels and absorption lines

When a molecule absorbs a photon, its state must change to reflect the energy it has gained. The energy of the photon determines what aspect of the molecule’s state is changed—the electronic configuration, the vibration state, the rotation state or some combination of these may change when a photon is absorbed.

The possible states that a molecule can be in are defined by quantum mechanical considerations, and the energy levels associated with these states are quantised. To be absorbed, the energy of a photon must equal the difference between two states, so it follows that absorption may only occur at particular frequencies

\[ \nu = \frac{E' - E''}{h} \]  

(4.1)

where \( E' \) and \( E'' \) are the energies associated with the upper and lower states respectively and \( h \) is Planck’s constant. Following one of the conventions used in spectroscopy, the units used for \( \nu \) in this thesis are the wavenumber \([\text{cm}^{-1}]\) which is the inverse of the vacuum wavelength, and \( 1 \text{ cm}^{-1} \approx 30 \text{ GHz} \). Also by convention, the energy levels are written in equivalent frequency so that \( h \) can be removed from equation (4.1).
Although not important for this work, it is worth noting that the line position varies slightly as pressure changes due to the change in the energy level of the molecule in the presence of collisions.

In the infrared region of the electromagnetic spectrum, light interacting with molecules results in changes in the rotational–vibrational state of the absorbing molecules. In the case of water vapour, the energy levels of these states can be enumerated by assigning three vibrational quantum numbers ($v_1, v_2, v_3$) and three rotational quantum numbers ($J_{K_a, K_c}$).

The vibrational quantum numbers relate to the modes of vibration shown in figure 4.1. They can take the values $0, 1, 2, \ldots$ and have energy spacings that mean that pure vibrational transitions are seen in the infra-red.

The general form of the rotational quantum numbers is set by the symmetry properties of the $\text{H}_2\text{O}$ molecule. Since each of the three moments of inertia are unique, the molecule is classified as an asymmetric-top. For this class of molecule, there are several ways of characterising the rotational quantum numbers and the form used here is the same as reported in reference [114], which is a major source of line strength data for this work. Other systems for labelling the quantum numbers are $J_{K_a - 1, K_c + 1}$ [128] where $K_a = K_{−1}$ and $K_c = K_{+1}$ or, as Herzberg [51] does, $J_\tau$ where $\tau = K_a - K_c$.

The reason for this variation stems from the physical interpretation of these quantum numbers. $J$ is a good quantum number, in the technical sense, and represents the total angular momentum of the rotating molecule. In contrast, $K_a$ and $K_c$, or their alternate representations, are pseudo-quantum numbers which serve as labels for the different energy within a particular $J$ level. The $\tau$ form simply orders the energy levels while $K_a$ represents the approximate projection of $J$ along the axis with the smallest moment of inertia and $K_c$ represents the approximate projection of $J$ along the axis with the largest moment of inertia [19].

The spacing of rotational energy levels is much finer than the spacing of vibrational energy levels, compared diagrammatically in figure 4.2. Pure rotational transitions are observed in the microwave region of the electromagnetic spectrum however ro-vibrational transitions, where both the vibrational and rotational state changes during a transition, have energy separations that appear in the infra-red. Ro-vibrational transitions were probed in this study, which require the specification of the upper and lower vibrational and rotational quantum numbers to uniquely identify a transition.
4.2 The relationship between line and gas properties

The ro-vibrational energy levels of a molecule determine the frequency at which absorption lines will be present. However, in order to extract temperature and mole fraction information, we also need to know the strength and shape of particular absorption lines.

In reflection of our aim, it is convenient to present the supporting theory in terms of an absorption measurement with the general arrangement shown in figure 4.3.

As a monochromatic laser beam passes through a homogeneous medium, the transmitted intensity of the beam, \( I \), is related to the initial intensity, \( I_0 \), by the
Beer–Lambert relation

\[ I = I_0 \exp(-k_\nu l), \]

where \( k_\nu \) is the frequency-dependant absorption coefficient and \( l \) is the length the beam travels through the absorbing medium. The product \( k_\nu l = \log(I_0/I) \) is termed the spectral absorbance and this is the quantity that is measured in an experiment. Since \( l \) is simple to measure, \( k_\nu \) can be found.

If we consider the attenuation of the beam to be due to water vapour present in the test medium and we are in the neighbourhood of the \( i \)th absorption line, which is sufficiently isolated from other spectral features, then \( k_\nu \) is a function of the strength, \( S(T) \), and shape, \( g(\nu) \), of the absorption line and the number density, \( N_{\text{H}_2\text{O}} \), of water vapour. This relationship is given by

\[ k_\nu = S(T)g(\nu)N_{\text{H}_2\text{O}}. \]

So \( k_\nu \), as well as depending on frequency, depends on temperature, \( T \). The line shape function, \( g(\nu) \), is normalised so that \( \int g(\nu) \, d\nu = 1 \). Where we are interested in a wavelength region with multiple absorption lines, \( k_\nu \) can be treated as a sum over the individual absorption lines, i.e.

\[ k_\nu = N_{\text{H}_2\text{O}} \sum_i S_i(T)g_i(\nu). \]

If we are able to determine \( k_\nu \) over a sufficient frequency range \([\nu_1, \nu_2]\), so that \( \int_{\nu_1}^{\nu_2} g(\nu) \, d\nu \approx 1 \), and there is only one absorption line contributing to \( k_\nu \) over this frequency range, then equation (4.3) leads to

\[ N_{\text{H}_2\text{O}} \approx \frac{\int_{\nu_1}^{\nu_2} k_\nu \, d\nu}{S(T)}. \]

Therefore, number density of water vapour can be found provided that the strength of the absorption line is known. This requires knowledge of the temperature, since line strength is a function of temperature. Also possible is to choose an absorption line which has a small variation in strength over the expected temperature range.

An alternative to taking an integral of the measured absorbance is to fit a theoretical line shape to the measured data. This requires a choice of line shape function, which is discussed below. Despite being computationally intensive, which could be a major consideration for a real-time sensor, this method generally provides better results than taking a direct integral of the data. Furthermore, fitting is the only way of extracting the contributions of individual lines in regions where multiple spectral lines overlap. Temperature still needs to be specified in order to determine number density, however, but this need not be from an independent measurement. Instead, temperature can be found directly from absorption measurements due to the the way in which the strength of different absorption lines depends on temperature.
4.2. The relationship between line and gas properties

Strength of absorption lines

While some headway into the determination of absorption line parameters can be made directly from quantum-mechanical models of water vapour, the theory is not sufficiently advanced to give accurate results \[19, 113\]. A far more practical approach is available due to the existence of spectral databases such as HITRAN \[97, 98\] and reports of observed line strength such as Toth’s \[114\]. Rather than deriving expressions for line strength and other parameters from scratch, the HITRAN database tabulates line position and strength at a reference temperature and pressure, along with parameters that are used to scale strength at a reference temperature to any other temperature. HITRAN also includes line shape parameters, so that a relatively simple model can be used to reconstruct spectra at arbitrary pressure and temperature.

To scale the tabulated strength at temperature \(T_0\), \(S(T_0)\), to strength at an arbitrary temperature, \(T\), we can use the expression \[97\]

\[
S(T) = S(T_0) \frac{Q(T_0)}{Q(T)} \exp \left( -c_2 \frac{E''}{T} \right) \frac{1 - \exp \left( -c_2 \nu_0 / T \right)}{1 - \exp \left( -c_2 \nu_0 / T_0 \right)}.
\]

This scaling function depends on the lower-state energy of the transition, \(E''\), the frequency of the transition, \(\nu_0\), and the total internal partition sum of the molecule, \(Q\). Also appearing in the expression is the second radiation constant, \(c_2 = \hbar c / k\) where \(\hbar\) is Planck’s constant, \(c\) is the speed of light and \(k\) is Boltzmann’s constant.

The partition function for a species at temperature \(T\) can be written as

\[
Q(T) = \sum_i g_i \exp \left( -E_i / kT \right),
\]

where \(E_i\) is the \(i\)th energy level and \(g_i\) is the degeneracy of the \(i\)th level. For this work, the partition function was computed numerically using the method of Fischer et al. \[34\]. In equation (4.6) the ratio \(Q(T_0) / Q(T)\) in conjunction with the next term represents the change in the lower-state population with temperature, as demanded by the Maxwell–Boltzmann distribution. The final term is due to the effect of stimulated emission.

By measuring the strength of two lines we can measure temperature. From equation (4.6), we see that if we choose two spectral lines of different \(E''\) and which are close spectrally (i.e. \(\nu_0\) is similar for both lines) then the ratio of line strengths

\[
R_{ls}(T) \equiv \frac{S_1(T)}{S_2(T)} = \frac{S_1(T_0)}{S_2(T_0)} \exp \left[ -c_2 \left( E''_1 - E''_2 \right) \left( \frac{1}{T} - \frac{1}{T_0} \right) \right],
\]

is a function only of \(T\). Then, knowing \(T\), we can use equation 4.3 to determine \(N_{H_2O}\). Therefore, if an experimental system is arranged in such a way so as to measure the integrated spectral absorption of two spectral lines with different lower-state energies then both temperature and species concentration can be deduced. Furthermore, the sensitivity of the thermometry can be tuned to a particular temperature range by choosing spectral lines with appropriate
4. Absorption spectroscopy theory

Figure 4.4: Pressure (Lorentzian) and Doppler (Gaussian) broadening effects on line shape. Both curves have the same integrated absorption and the same half-width at half-maximum.

$E''$. To find the relative sensitivity, $\frac{dR_{ls}}{dT}/\frac{R_{ls}}{T}$, we can differentiate equation (4.8), following Zhou [129], so that

$$\frac{|dR_{ls}|}{dT} \cdot \frac{R_{ls}}{T} = c_2 \frac{|E_1'' - E_2''|}{T}.$$  (4.9)

If the relative sensitivity is below 1, errors in the determination of $R_{ls}$ couple into larger relative errors in $T$, so high sensitivity is desirable. Maximising $|E_1'' - E_2''|$ is good for sensitivity but transitions with hugely different $E''$ have their peak line strengths at very different temperatures, meaning that if one of the two lines is visible then chances are good that the other is too weak to detect. This implies a trade-off between large $|E_1'' - E_2''|$ and the selection of lines that are strong enough to detect over the target temperature range.

A further implication of this equation is that the relative sensitivity decreases as a factor of $1/T$ meaning that any temperature measurement based on this technique will be more difficult to implement at higher temperatures. Beyond the temperature at which it peaks, the line strength of a particular transition heads towards zero faster than $1/T$, so weak absorption is another difficulty associated with spectroscopic measurements at high temperatures.

Shape of absorption lines

According to the discussion above, molecules may only absorb or emit light at certain frequencies. Observed absorption lines, however, are seen to absorb light over a range of frequencies. Absorption is maximum at the frequency predicted by the energy gap and decreases on either side of this maximum.

There are a number of processes that result in this broadening, and these processes perturb the line shape in different ways.
4.2. The relationship between line and gas properties

Natural broadening

Even if all other sources of line-broadening were eliminated, Heisenberg’s uncertainty principle would place a restriction on the width of absorption lines since

\[ \Delta E \Delta t > \hbar / 2, \]

(4.10)

where \( \Delta E \) is the uncertainty in the energy level, \( \Delta t \) is the lifetime of the state and \( \hbar = h / 2\pi \). In isolation, this is a weak effect but becomes important with the effect of collisions.

Pressure broadening

In a gas sample, molecules are continually colliding with each other and these collisions induce relaxation of the molecules back to the ground state, so that \( \Delta t \) is significantly smaller. Since more collisions occur at high pressure, the line is broadened by increasing the pressure. An analysis of this effect [25, e.g.] for a transition centred on \( \nu_0 \) and with a width at half-maximum of \( \gamma_l \) results in a Lorentzian line shape

\[ g(\nu) = \frac{1}{2\pi} \frac{\gamma_l}{(\nu - \nu_0)^2 + (\gamma_l/2)^2}, \]

(4.11)

as shown in figure 4.4.

For the present work, the Lorentz half-width, \( \gamma_l \), was typically used as a free-parameter when fitting absorption lines. Alternatively, for predicting spectra at expected environmental conditions, values of \( \gamma_l \) can be derived from parameters in the HITRAN database. This is limited to mixtures of air and water vapour and is given in the form

\[ \gamma_l = \gamma_{\text{air}} P_{\text{air}} + \gamma_{\text{H}_2\text{O}} P_{\text{H}_2\text{O}} \]

(4.12)

where \( \gamma_{\text{air}} \) and \( \gamma_{\text{H}_2\text{O}} \) are co-efficients for air and self-broadening respectively and \( P_{\text{air}} \) and \( P_{\text{H}_2\text{O}} \) are the respective partial pressures. Although \( \gamma_{\text{air}} \) and \( \gamma_{\text{H}_2\text{O}} \) are tabulated for all lines listed in HITRAN, it is only a subset these values which are based on measurement. This limits the accuracy of spectra calculated from HITRAN.

Doppler broadening

The translational motion of molecules in a gas sample also contribute to the absorption line shape. Although the molecules emit or absorb radiation at \( \nu_0 \) in their own reference frames, this frequency will be Doppler-shifted in the reference frame of a stationary observer. The resulting line shape perturbation is a direct result of the Maxwellian distribution of velocities in the sample and is given by

\[ g(\nu) = \frac{2}{\gamma_d} \sqrt{\frac{\log(2)}{\pi}} \exp \left[ -\frac{4 \log(2)}{\gamma_d} \frac{(\nu - \nu_0)^2}{\nu_d^2} \right]. \]

(4.13)
This function is shown along with a Lorentzian line shape in figure 4.4. Doppler broadening results in a line shape that has a smaller contribution from the wings of the transition when compared to pressure-broadening.

The Doppler half-width is dependent on temperature, $T$, the molecular mass of the probed species, $M$, and the transition centre frequency, $\nu_0$ so that

$$\gamma_d = \frac{\nu_0}{c} \sqrt{\frac{2RT \log(2)}{M}}$$

where we also have the speed of light, $c$, and the universal gas constant, $R$.

**Combined pressure and Doppler broadening**

If the effect of pressure broadening and Doppler broadening are treated as being uncorrelated, we can convolve equation (4.11) with (4.13) to arrive at an equation, known as the Voigt function,

$$g(\nu) = A \frac{y}{\pi} \int_{-\infty}^{+\infty} \exp\left(-\frac{t^2}{2}\right) \frac{1}{(x - t)^2 + y^2} dt$$

where

$$A = \frac{\sqrt{\log(2)}}{\gamma_d \sqrt{\pi}}, \quad y = \sqrt{\log(2)} \frac{\gamma_l}{\gamma_d} \text{ and } x = \sqrt{\log(2)} \frac{\nu - \nu_0}{\gamma_d}.$$ (4.16)

This function can be calculated using Wells’ algorithm [127] with the addition here of the factor $A$, which normalises the integral of the Voigt function to one.

When fitting the Voigt function to an observed line shape, generally both $\gamma_d$ and $\gamma_l$ are used as free parameters, except when temperature is known independently.

**More advanced line shapes**

Diode laser spectroscopy is an extremely effective means of gaining line shape information [63], so effective that experimental line shapes can be seen to depart from the Voigt function. A brief overview of the hierarchy of line shape models is provided by D’Eu et al. [26] in their comparison of experimental line shapes with models.

In 1953, Dicke [27] proposed that the confinement of a molecule, such as by other molecules in a gas, would result in the narrowing of the line width. Several models have since been developed which reflect this additional complexity.

Both the Galatry [39] and the Rautian and Sobel’man [96] profiles allow the phase of emitted radiation and the translational velocity to change at collisions. Galatry assumes that collisions are soft, so that many collisions are required to result in a large perturbation to the molecule’s motion. In contrast, Rautian and Sobel’man consider collisions to be hard, resulting in a molecule acquiring an essentially random motion after a single collision.
An alternative approach is to consider the dependence of transition collisional width and shift parameters on molecular speeds. This results in the speed-depandant Voigt profile [12], which produces asymmetric line profiles.

While the derivation of these different line models is arrived at from considera- tion of quite different physical situations, the different line models seem to perform similarly when fit to experimental data [26, 63]. The numerical value and meaning of line shape parameters produced by the fit differ between models, which can make it difficult to base conclusions on these values. Where lines are being fit for the purpose of finding the line strength, however, this poses no problem. Fitting a Voigt function to a line shape when a more sophisticated model is required results in characteristically shaped residuals, published in the literature [26, 63, 70]. These are shown in figure 4.5, which has been generated by fitting a Voigt profile to a theoretical line shape generated with a Galatry model. In this example the Doppler width has been fixed to its known value, but allowing the Doppler width to vary results in much smaller residuals as the fitting procedure reduces the Doppler width to better fit the shape of the Galatry profile.

Galatry profiles are the only profiles computed for this work that take Dicke narrowing into account and were calculated using the method reported by Varghese and Hanson [122].

4.3 Spectral model of water vapour

In conjunction with an appropriate spectroscopic database, the theory presented in this chapter is enough to build a spectral model of water vapour. For this work a spectral model known as GENSPECT [94] was used. This is implemented as a MATLAB toolbox and was freely available in mid 2001, however it is not clear if it is still available. Fortunately other models can be obtained, such as RFM [30], which perform a similar function.

These models, in principle, operate in the following manner:
• Line parameters are loaded from a database such as HITRAN [98];

• Equation (4.6) is used to scale the line strength from the tabulated reference strength to the desired temperature;

• A correction is applied to the line centre location based on pressure, as given by Rothman et al. [97];

• Pressure and Doppler broadening parameters are calculated according to equations (4.12) and (4.14) respectively;

• Each spectral line is evaluated individually using a specialised algorithm, such as that given by Wells [127], using the line parameters above. This step is where most of the processing time is taken up, so there are various strategies used to speed evaluation of the line shape while retaining a specified error tolerance, for example the interpolation scheme used in GENSPECT [94]; and

• Contributions from the individual lines are added and the transmission is calculated based on the line strength, absorber density and path length.

Generally the various models have more capabilities than this and may include the ability to simulate absorption across atmospheric paths, calculate absorbance for many species besides H$_2$O or include CO$_2$ line-mixing effects, among other features. For this work, however, the main requirement was simply to obtain a first-estimate of the characteristics of the water vapour spectrum both over a large spectral range, as shown in figure 4.6, and over a small spectral range where measurements would be made but at different temperatures, as shown in figure 4.7.

Since the method of predicting the spectrum relies on a database of line parameters, inaccuracies in the underlying database result in an inaccurate prediction. As a consequence of this ability to predict the spectrum, the theory allows for the measurement of temperature and water vapour concentration provided that the absorbance of two spectral lines can be measured.
4.3. Spectral model of water vapour

Figure 4.6: Water vapour spectrum between 1 and 2 µm. Transitions in the (1, 0, 1) – (0, 0, 0) vibrational band are shown in black.

Figure 4.7: Water vapour absorption at 500, 1000 and 1500 K simulated from HITEMP for a total pressure of 20 kPa and a mixture of 10% by volume of water vapour in air.
4. Absorption spectroscopy theory
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
5. Sensor design

potassium [124, 125]. These species absorb strongly near the operation wavelength 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 converse 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 concentration, 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 turbulent 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 absorption 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

reports of measurements using either the one- or two-line version of the sensor during scramjet tests have not been found in the open literature.

The development of the present sensor can be guided from the wide range of sensors that have been developed previously. Nevertheless, the effectiveness of diode laser absorption spectroscopy, when applied to measurements in a scramjet combustor in a pulsed facility, is largely unknown from the literature.

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),

\[
\left| \frac{dR_{ls}}{dT} \right| = c_2 \frac{|E''_1 - E''_2|}{T}.
\]

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,
5.2. Selection of spectral 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>
<th>Vibrational(^2)</th>
<th>Rotational(^3)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Toth[114] HITRAN[97] Upper</td>
<td></td>
<td>Lower</td>
<td>Upper</td>
</tr>
<tr>
<td>1</td>
<td>7181.15570 7181.1720</td>
<td>(1, 0, 1)</td>
<td>(0, 0, 0)</td>
<td>2(_{02})</td>
</tr>
<tr>
<td>2</td>
<td>7179.7519 7179.7521</td>
<td>(1, 0, 1)</td>
<td>(0, 0, 0)</td>
<td>7(_{62})</td>
</tr>
</tbody>
</table>

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

\(^2\) Vibrational quantum number: \((v_1, v_2, v_3)\)

\(^3\) 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.
Figure 5.1: Line strength (top) and line strength ratio variation with temperature. Calculated using reference line strengths from Toth scaled by parameters given by HITRAN.

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

Figure 5.2: Sensitivity of the line strength ratio, $R_{ls}$, to temperature, plotted as a function of temperature.

If we can measure the integrated absorbances $A_1$ and $A_2$ with an uncertainty of 5%, the corresponding relative uncertainty in $R_{ls}$, $\sigma_{R_{ls}}/R_{ls}$, can be found from the relation for the propagation of errors \[14\]

\[
\sigma_{R_{ls}}^2 = \frac{\partial R_{ls}}{\partial A_1} \sigma_{A_1}^2 + \frac{\partial R_{ls}}{\partial A_2} \sigma_{A_2}^2
\]  

(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.

\[
\frac{\sigma_T}{T} = \frac{\sigma_{R_{ls}}}{R_{ls}} \left\lvert \frac{dR_{ls}/R_{ls}}{dT/T} \right\rvert
\]  

(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

\[N = A_1/(S_1l)\]  

(5.5)

or

\[N = A_2/(S_2l) .\]  

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

\[
\left( \frac{\sigma_N}{N} \right)^2 = \left( 1 - \frac{dS_1 / S_1}{dT / T} / \frac{dR_{ls} / R_{ls}}{dT / T} \right)^2 \left( \frac{\sigma_{A_1}}{A_1} \right)^2 + \left( \frac{dS_1 / S_1}{dT / T} / \frac{dR_{ls} / R_{ls}}{dT / T} \right)^2 \left( \frac{\sigma_{A_2}}{A_2} \right)^2 . \tag{5.7}
\]

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 \( A_2 \).
5.3 Physical sensor design

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

Current flow
Positive contact
n−doped semiconductor
p−doped semiconductor
Active region
Negative contact
Elliptical output beam

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.

Distributed feedback (DFB)
Distributed Bragg reflector (DBR)
External cavity
Grating

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.
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

<table>
<thead>
<tr>
<th>Table 5.2: Characteristics of the DFB laser diodes used in this work.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peak optical power at 25°C</td>
</tr>
<tr>
<td>Side mode suppression ratio</td>
</tr>
<tr>
<td>Line width</td>
</tr>
<tr>
<td>Material</td>
</tr>
<tr>
<td>Temperature tuning coefficient</td>
</tr>
<tr>
<td>DC current tuning coefficient</td>
</tr>
<tr>
<td>Beam divergence (FWHM)</td>
</tr>
<tr>
<td>Supplier</td>
</tr>
</tbody>
</table>
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° to the first one. The net effect on the forward-propagating beam is to rotate the polarisation state by 45°. 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.
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 $\text{H}_2\text{O}$ 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
the laser [3]. Calibration, therefore, is problematic when the system is to make scramjet-based measurements.

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 5.13: 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

\[
V_{\text{out}} = -G \log \left( \frac{i_{\text{ref}}}{i_{\text{sig}}} - 1 \right) \tag{5.8}
\]

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]

\[
f_c = \frac{1}{2\pi G} \left( \frac{i_{\text{sig}}}{1 + \exp(V_{\text{out}}/G)} \right) \frac{R_1/(R_1 + R_2)}{C_f}, \tag{5.9}
\]

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 Q1 and Q2. 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.
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.

$$\Delta l = i\lambda$$  \hspace{1cm} (5.10)

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

$$\Delta l = \frac{ic}{nv}$$  \hspace{1cm} (5.11)

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

$$\Delta \nu = (i + 1) \frac{c}{n\Delta l} - i \frac{c}{n\Delta l} = \frac{c}{n\Delta l}$$  \hspace{1cm} (5.12)

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

$$\nu_{\text{FSR}} = (0.01032 \pm 0.00005) \text{ cm}^{-1}$$  \hspace{1cm} (5.13)

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),
5.4. Data reduction

we can then find

\[ G = -\frac{V_{\text{out}}}{i_{\text{ref}} - i_{\text{sig}}} \]  

(5.14)

In practice, it is difficult to apply known photocurrents to the detector because of losses in the optical system leading up to the detector which, even if characterised, would change with time. Instead, a less direct method was used; requiring the system to be reconfigured as shown in figure 5.18.

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

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

(5.17)
or, from equation (5.15),

\[ V(t) = -G \log \left\{ \frac{\alpha i_{\text{ref}}}{V_1(t)} - 1 \right\}. \] (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

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

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

\[ A_m = \log \left( \exp \left( -\frac{V}{G} \right) - 1 \right). \] (5.20)
5.4. Data reduction

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

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

(5.21)

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

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

(5.22)

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

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

(5.23)

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

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

(5.24)

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.
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

$$A(t) = \log \frac{S(t) - L}{B(t) - L}. \quad (5.25)$$

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

Time can be converted to spectral absorbance from the output of the fibre-interferometer.

**Integrated absorbance from spectral absorbance**

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
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

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

(5.26)

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, \( \gamma_d, \gamma_l \), 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, `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:
5.4. Data reduction

- 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

\[ \ldots \text{you can usually get away with pretending that these are "iid" [independent and identically distributed]}, \ldots \]

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
Figure 5.22: Testing the bootstrap method. For each point in the graph, the width of the 90% confidence interval in fitted integrated absorbance was computed from 1000 synthetic data sets generated from a Voigt profile added to random-number-generator noise. This is plotted on the x-axis and compared, on the y-axis, to a 90% confidence interval generated from 100 bootstrap data sets, identical to the method used in data analysis. The true value of integrated absorbance is 1 and points further from the origin originate from larger amplitude noise. The solid line is $x = y$.

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)
5.4. Data reduction

for temperature, $T$, and water vapour concentration $N_{H_2O}$. 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 $N_{H_2O}$ and $l$ and re-write the equations in terms of the line strength ratio $R_{ls}(T)$. We now have

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

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 $l$, $N_{H_2O}$ 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 $N_{H_2O}$ can be determined by finding $T$ and $N_{H_2O}$ for each pair of $A_1$ and $A_2$ values in the ensemble. In so doing, we build up a distribution for $T$ and $N_{H_2O}$ 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
6. Sensor verification

During the development of any new sensor, it is wise to demonstrate its performance in a known environment before its measurements are relied upon. This is certainly true for the sensor described in the previous chapter.

The verification process is described in this chapter. It was performed in two steps, which are reported in order. First experiments were performed at room temperature at pressures ranging from one atmosphere down to the vapour pressure of water. Following this, the system was used to measure temperature and water vapour concentration in the well-understood environment of a flat-flame burner up to a maximum temperature of 1550 K.

Each of these sections reports the experimental configuration for each of the tests and documents the results of the experiments.

6.1 Measurements at room temperature

Water vapour absorption measurements were made in a low pressure test cell to determine the line strength of transitions at room temperature. The use of a test cell allowed the water vapour concentration to be fixed and allowed measurements to be made at a variety of sub-atmospheric pressures.

At low pressure, spectral lines are narrower and have larger peak absorbance. This allows easier identification of line positions and allows the strength of individual lines to be more easily identified since the overlap between lines is reduced. The signal to noise ratio of the measurement is also improved allowing high-fidelity testing of the line models which are used to fit to the test data.

Measurements were made over several spectral lines over the region accessible by the spectroscopic diode lasers used in the TDLAS system. This meant that a comparison could be made between the line strength measured using this system and two available sources of spectroscopic parameters—HITRAN [98] and Toth’s [114] measurements.

The ability to vary the pressure in the test cell also meant that the analysis technique could be tested for its sensitivity to pressure. This is important since flame experiments were carried out at atmospheric pressure, while scramjet experiments were carried out at sub-atmospheric pressure.

Finally, due to the convenience of such a test, temperature was measured in laboratory room air using the diode laser sensor and compared with the temperature measured using a thermocouple.
Figure 6.1: Experimental layout for low-pressure test cell measurements. Water vapour concentration was fixed by ensuring liquid-phase water was present in the test cell at a known temperature.

Experiment configuration

The TDLAS sensor has been described in general in chapter 5. For absorption measurement of low-pressure water vapour, the log–ratio detector signal beam was passed through a water vapour test cell as shown in figure 6.1. The beam path on either side of the test cell was flushed with dry nitrogen and the test cell was tilted at 7° to prevent étalon effects from the windows. Tilting the cell was able to eliminate étalons since the beam was narrow and the windows were thick, so that internal reflections from the window surfaces did not overlap with the transmitted beam. A wide beam or narrow windows would result in interference even with the test cell tilted. This configuration resulted in a path length of 13.8 cm through the cell.

Water was introduced to the test cell by first pumping down the cell with one of the shock tunnel vacuum pumps, an oil-filled rotary-vane roughing pump, to around 0.1 torr and then placing a drop of distilled water on the vacuum connector and fractionally opening the valve. Enough water was considered to have entered the cell when liquid-phase water was visible inside.

The test cell was returned to the vacuum pump for around an hour and then, with water still visible inside the cell, allowed to equilibrate before measurements were made. The test cell was instrumented with a K-type thermocouple and the water vapour concentration was assumed to be in equilibrium with the liquid-phase water in the test cell. Generally, the dew-point is governed by the coldest place in the cell so the cell was allowed time to come to thermal equilibrium before measurements proceeded. Provided the system is in thermal equilibrium, the water vapour partial pressure is given by an empirically
derived relationship known as the Antoine equation for water,

\[
\log_{10}(P_{H_2O}) = a - \frac{b}{T + c}
\]

(6.1)

where \(P_{H_2O}\) is the water vapour partial pressure [Pa], \(T\) is temperature [K] and the coefficients \(a = 10.40221\), \(b = 1838.675\) and \(c = -31.737\) over the range \(273 < T < 303\) [73].

For calculation of line strengths, this partial pressure is converted into number density according to the perfect gas law in the form

\[
N_{H_2O} = \frac{P_{H_2O} RT}{N_A}
\]

(6.2)

where \(N_{H_2O}\) is the number density of water vapour \([m^{-3}]\), \(R = 8.314 \text{ J mol}^{-1} \text{K}^{-1}\) is the molar gas constant and \(N_A = 6.022 \times 10^{23} \text{ mol}^{-1}\) is Avogadro’s constant.

Absorbance as a function of relative frequency is measured directly from the TDLAS system. The system was operated at low frequency, 11 Hz, which allowed the laser to scan over a wide frequency range. Absolute frequency was determined partly from the tuning curves provided by the laser manufacturer and then determined precisely by comparison with Toth’s [114] measurements.

Laser diode temperature was also varied so that several overlapping spectra could be obtained with overlapping spectral features being used to fix the absolute frequency of each. In order to find the strength of each of these lines, Galatry [39] profiles were fit to the measured spectra using Toth’s measurements as an initial starting guess. A linear background slope was assumed in the model and the Doppler half-width of the fitted lines was fixed based on the measured temperature and equation (4.14).

Applicability of Voigt profile

As shown in figure 6.2, Voigt fits show structured residuals when fit to test cell data. These have a ‘gull wing’ profile which is similar to those seen in other work [63] when observed line shapes depart from Voigt profiles due to simplifications in the Voigt model.

To verify that the limitations of the Voigt profile were indeed the reason for the observed residual, Galatry profiles [39] were fit to the data. Galatry profiles were calculated with the algorithm given by Varghese and Hanson [122]. Moving to the more sophisticated line model improved the fit significantly, as seen by figure 6.2, but the residuals still show structure beyond the background noise. The remaining structure in the residuals indicates that there is still an important physical process that the model doesn’t account for.

A possible cause of the remaining structure in the residuals is due to the emission spectrum of the laser. The line shapes presented here represent the physical shape of the absorption line convolved with the instrument function of the diode laser absorption spectrometer, which is largely dependent on the diode laser emission spectrum.
The instrument function can be determined by making absorbance measurements in a low pressure environment where the line shape is accurately described by a Gaussian profile. In this case, the line shape can be independently predicted by equation (4.13). If the shape of the instrument function is assumed to be a Voigt profile, which provides a good approximation at high injection currents [63], then the observed absorption can be considered as a convolution of a known Gaussian profile with an unknown Voigt profile. This can be solved to find the Voigt Lorentz and Gaussian half-widths, and determine the instrument function.

A further complication is that the emission spectrum of the laser changes with injection current. This consideration meant that Lepère et al. [63] chose to temperature-tune their laser across absorption lines while keeping injection current at its maximum.

An alternative explanation is simply that the Galatry profile does not adequately represent the line shape under these conditions.
6.1. Measurements at room temperature

For this work, the diode laser emission spectrum was not characterised, nor was the laser temperature-tuned across transitions. This was because high-precision measurements of line shapes were not required for the operation of the sensor and because current-tuning was required to achieve high repetition rates. Ultimately, the structure in the residuals can be explained and has no adverse implications for the measurement.

In contrast with line shape parameters, the integrated absorbance of the fitted spectral lines was of great importance. Although using Galatry profiles improves the size of the residuals by a factor of five, the fitted integrated absorbance differs by less than 0.2% between the two methods. Despite showing some structure, the residual values are small at less than 2% of the peak absorbance value even for the less sophisticated Voigt profile. In less controlled environments, such as a scramjet combustor, random noise is well above this level and the error associated with assuming a Voigt profile is not significant to the overall performance of the sensor.

From this investigation, it was concluded that Voigt profiles could be fitted to absorption lines for the purpose of obtaining the integrated absorbance. The Gaussian and Lorentzian half-width returned by the fit were not considered to be reliable, and were not used or required in further analysis. Line shape parameters differed between Galatry and Voigt fits and included a systematic error, possibly due to the emission spectrum of the laser as seen by Lepère et al. [63] or because the Galatry model does not adequately represent Dicke narrowing.

Comparison with literature

Absorption data gathered in the test cell can be compared with simulated data generated from a model based on the HITRAN database. In figure 6.3, this shows that the general features agree reasonably well, however discrepancies are visible. The strong line used for thermometry, line 1 in table 5.1, is over-predicted by the model.

Similarly the line near 7180 cm$^{-1}$, which is line 2 in table 5.1, appears to be over-predicted by the model—although in this case this is due to the presence of an overlapping line in the HITRAN/GENSPECT model. Also shown in figure 6.3 is a part of the spectrum where another line appears in the HITRAN database that is not visible in observations.

Since Toth’s observations are of line strength only, and do not include the pressure broadening coefficients required to generate a spectrum, direct comparison of these results with Toth’s require that the line strength be extracted from the measured spectrum. This comparison is shown in figure 6.4, where observed line strengths are compared against both Toth’s measurements and the strengths tabulated in HITRAN. Where HITRAN and Toth disagree, the measurements made here agree with Toth rather than HITRAN, both in terms of line strength and position. The measurements presented here, however, do not improve on the precision of the strengths measured by Toth since such high precision is unnecessary in the application of this sensor.
This suggests that, in order to predict line strength for thermometry, Toth’s line strengths should be taken as the reference line strength in preference to those given in HITRAN. To scale this to an arbitrary temperature, the value for the lower-state energy level ($E''$) given in HITRAN is still required along with a method of evaluating the partition function, $Q(T)$ [34, e.g.].

**Sensitivity to pressure**

With TDLAS configured to make measurements in a pressure-controlled environment, the opportunity was taken to vary the pressure in the test cell and verify that the measured line strength was not affected. With the presence of liquid-phase water in the test cell, the water vapour concentration depends only on temperature and air could be allowed into the cell, and therefore increase the pressure, without changing the integrated absorption of the transitions.

A Bourdon tube analog pressure gauge provided an approximate indication of the pressure in the test cell, ±2 kPa, so that pressure could be increased from the vapour pressure of water, around 3 kPa at 296 K, up to atmospheric pressure in a number of equal steps.

Integrated absorbance across a spectral line, calculated in three different ways, is shown in figure 6.5. The simplest method determining the total absorbance of the spectral line is to numerically integrate the data over the range where absorbance is noticeable, and this method is compared with the integrated absorbance found with Voigt and Galatry fits. As the pressure increases, the line strength found through direct integration falls as more absorbance is transferred into the wings of the absorption line and out of the integration limits.
6.1. Measurements at room temperature

These limits could not be further increased since doing this would include overlapping lines in the integration region. Curve fits, in contrast, show an approximately constant value for the integrated absorbance over the full pressure range of the test cell.

At the lowest end of the pressure range, Galatry profiles produce results that are closer to constant whereas Voigt profile fits drop slightly at the lowest pressure. This is the regime where Dicke narrowing [27] can be expected to have a noticeable impact, i.e. where pressure is high enough so that molecular confinement has become important to the line shape, but is not yet high enough for the line shape to be dominated by pressure broadening.

At higher pressure, from around 25 kPa, Voigt and Galatry fits produce results that are essentially identical and constant with pressure.

The invariance of integrated absorbance with changing pressure justifies the computational expense of curve fits when performing measurements in a variable-pressure environment. Furthermore, the similarity between Voigt and Galatry fits allows the use of the simpler Voigt profile without the introduction of major errors. This result is also important as it suggests that calibration results from a flame at atmospheric pressure remain valid in a shock tunnel at similar temperatures but lower pressure.

Temperature measurement in room air

Calibration experiments in a low-pressure test cell had suggested that it was:

- Preferable to use Toth’s line strength data over that available in HITRAN 2000; and
- For the purpose of extracting integrated absorbance, Voigt profiles were suitable over the intended pressure range.

A simple test of this analysis strategy was set up in laboratory room-air. This was carried out with the secondary aim of characterising the scatter in results produced by the sensor, in an environment that was completely stable. Measurements in both the shock tunnel and calibration flame exhibit fluctuations in gas properties, which are difficult to decouple from the measurement scatter of the sensor.

After gathering data from 300 scans at 100 Hz, Voigt profiles were fit to each laser scan and 600 temperature measurements were found by taking the ratio of integrated absorbance of consecutive lines and applying the process outlined previously in section 5.4.

Room temperature actually represents a challenging test of the system because of the low strength, and associated decreased signal-to-noise ratio, of the weaker of the two absorption lines, line 2 near 7179 cm⁻¹. Nevertheless, as shown by the histogram in figure 6.6, the system performed admirably. The mean value of all of the single-scan temperature measurements, 297.24 K was within 1% of the thermocouple-derived room temperature of 300 ± 0.3 K. The
6. Sensor verification

Figure 6.4: Comparison of measured line strengths, line strengths reported by Toth and line strengths tabulated in HITRAN at 296 K. Where HITRAN and Toth differ, these measurements agree better with Toth.

Figure 6.5: Integrated absorbance determined from Galatry fits, Voigt fits and direct numerical integration of spectral absorbance. Fitting curves to data is preferable to avoid sensitivity to pressure.
6.2 Flame measurements

While room temperature experiments were able to verify the line strengths reported by Toth for water vapour at 296 K, measurements in the scramjet would...

†This idea is supported by the line data in the recently-released update of HITRAN, discussed on page 89. The latest update of HITRAN was unavailable until after this thesis was submitted for examination.
be carried out at much higher temperatures. A feasible strategy is to use the line reference line strengths reported by Toth and then use parameters in HI-TRAN to scale the line strengths to an arbitrary temperature.

In order to test this strategy at elevated temperatures, measurements were made using the TDLAS system in a hydrogen–air flame and compared against temperatures measured with a thermocouple and equilibrium-chemistry water vapour predictions.

This section describes the experimental configuration, the method of determining flame parameters independently of TDLAS and finally the method used to analyse the TDLAS data taken in the flame.

Experimental configuration

High temperature calibration experiments used a premixed hydrogen–air burner from McKenna products, shown in figure 6.7. Pre-mixed hydrogen and air emanate from a porous, water-cooled disk at the surface of the burner. The flow rates of each gas were controlled using Aalborg variable area flow meters (tube 064-63 with a carboloy float for air, tube 041-96 with a stainless steel float for hydrogen).

Surrounding the main burner plate was an annular co-flow of inert nitrogen. This protected the main flow from the entrainment of room-air, as well as reducing the velocity shear at the edge of the hot burner exhaust. Due to limitations in the flow rate achievable from the nitrogen delivery system, the velocity of the co-flow was lower than the velocity of the combustion products.

During stable operation, the flame front is fixed in position by heat loss to the burner, which increases as the flame front approaches the burner surface. This
6.2. Flame measurements

results in a maximum flame temperature that is generally well below the adiabatic flame temperature but this gap can be closed by increasing the flow rate from the burner or decreasing the equivalence ratio, $\phi$, which decreases the flame front velocity [93].

The instrumentation surrounding the burner is shown in figure 6.8. The laser beam and an S–type thermocouple, composed of a junction between platinum and 90% platinum/10% rhodium alloy, were located 15 mm above the burner surface. According to Prucker et al. [93], this is well outside the zone where combustion occurs. This was verified for the burner used in this work by traversing the thermocouple vertically in the flame to check that temperature variation was indeed small, whereas a steep gradient would be expected in a combustion zone. According to a one–dimensional model of the burner based on Cantera [45], reactions have reached completion by around 2 mm from the burner surface.

This consideration is important, not only because of the steep gradients in the reaction zone but since temperature measurement can be complicated by the catalytic effect of the platinum thermocouple. Ensuring measurements are made in the burner exhaust, therefore, allows measurements to be made in an area of local chemical equilibrium where thermocouple measurements are unaffected by surface chemistry.

As well as shielding with the nitrogen co-flow, the laser beam was housed in tubes on either side of the burner exhaust. These were flushed with nitrogen to prevent ambient water vapour from contributing to the measurement. On the detector side of the burner, an aperture was mounted in the tube to prevent flame luminosity from entering the detector. Because the detector’s gain was affected by temperature, the detector was shielded from flame luminosity to prevent radiant heating of the components.
Independent measurement of flame properties

To enable calibration, flame conditions were determined independently of spectroscopic measurements. The diode laser sensor was able to measure temperature and water vapour number density, so it was these quantities that needed to be characterised in the burner.

Temperature was measured directly with a thermocouple and then the assumption of chemical equilibrium was applied to the gas mixture in order to find species concentrations. The details of these steps are outlined below.

Determining temperature with a bare thermocouple

In general, the junction between two different metals acts as a voltage source which increases with increasing temperature. Thermocouples take advantage of this effect for temperature sensing and, for the junction types used to make thermocouples, the potential across the hot junction is typically tens of millivolts at flame temperatures [20].

For flame measurements, the maximum temperature that can be measured is often determined by the melting point of the metal used in the thermocouple. For the S-type thermocouples used in this work, this meant a maximum temperature of 2040 K could be measured.

The small voltage produced by the thermocouple was converted to temperature using a hand-held digital display unit, an Omega HH200A. This device included cold junction compensation and had a reported precision of $\pm(0.25\% + 0.2 \text{ K})$.

Although this was able to determine the thermocouple junction temperature to high precision, a thermocouple in a flame will not generally be at the same temperature as the gas around it. This can be verified by considering flow of heat into and out of the thermocouple junction.

Heat arrives at the thermocouple junction through convection from the surrounding gas. Convective transfer per unit area, $\dot{q}_c$, is proportional to the difference between the thermocouple temperature, $T_{tc}$, and the surrounding gas temperature, $T_g$. It also depends on the convective heat transfer coefficient, $h$, and is given by

$$\dot{q}_c = h (T_g - T_{tc}).$$

If the system is in a steady state and $T_g = T_{tc}$ then $\dot{q}_c = 0$, which requires there to be no heat loss from the thermocouple junction.

In reality, there are mechanisms of transferring heat away from the thermocouple. Conductive transfer along the thermocouple wires carries heat away from the junction, however by alignment of the wires along an isotherm in the flame, or perpendicular to the flow direction, conductive losses can be minimised. More importantly at high temperature, the thermocouple loses heat through radiation, requiring a large $(T_g - T_{tc})$ to drive a balancing convective transfer. If we label net radiative heat transfer away from the thermocouple per unit surface area as $\dot{q}_r$, then the assumption of steady state implies that

$$\dot{q}_r = \dot{q}_c.$$
The radiation transfer, per unit area, from the thermocouple to its surroundings is given by

$$\dot{q}_r = \sigma \left( \epsilon T_{tc}^4 - \alpha T_s^4 \right)$$  \hspace{1cm} (6.5)$$

where $\sigma$ is the Stefan–Boltzmann constant, $T_s$ is the temperature of the surrounding environment, $\epsilon$ is the emissivity and $\alpha$ is the absorptivity of the thermocouple over all wavelengths.

In a flame that is optically thin, $T_s$ is the temperature of the nearest objects outside the flame, and therefore $T_s \approx 300$ K.

The convective transfer is more complicated to evaluate since $h$ depends on flow properties. Evaluation is based on correlations, determined from experimental data, that exist between the dimensionless numbers $\text{Nu}$, $\text{Pr}$ and $\text{Re}$ [20, 55]. The Nusselt number, $\text{Nu} = \frac{h d}{k}$, is proportional to the ratio of total heat transfer to conductive heat transfer, the Prandtl number, $\text{Pr} = \frac{C_p \mu}{k}$ is proportional to the ratio of momentum diffusion to thermal diffusion and the Reynolds number, $\text{Re} = \frac{\rho u d}{\mu}$, is proportional to the ratio of inertial to viscous forces in the flow. Parameters appearing in these definitions that have not been introduced previously are the thermocouple wire diameter, $d$, and properties of the surrounding gas: thermal conductivity, $k$, specific heat capacity, $C_p$, viscosity, $\mu$, velocity, $u$, and density, $\rho$.

If the thermocouple is considered as a cylinder in a cross-flow, as shown in figure 6.9, one of the many experimentally-derived correlations that exists between $\text{Nu}$, $\text{Pr}$ and $\text{Re}$ can be used to determine $\text{Nu}$. Many of these are cited in textbooks with Holman [55], for example, listing correlations that are valid over the range $0.4 \leq \text{Re} \leq 400,000$.

Strictly speaking, the Prandtl number is a function of gas properties, however in combustion gases, $\text{Pr} \approx 0.7$ [20]. This allows the use of the correlation between $\text{Re}$ and $\text{Nu}$ reported by Lange et al. [60, 61] for low-Reynolds number air flow around a cylinder since, for air, $\text{Pr} = 0.715$.

Lange et al. derived their correlation from numerical simulation, verified against experiments, and reported

$$\text{Nu} = \left( \frac{T_f}{T_g} \right)^{0.17} \left( 0.082 \text{Re}_t^{0.5} + 0.734 \text{Re}_t^{0.05} + 0.226 \text{Re}_t^{0.083} \right)$$  \hspace{1cm} (6.6)$$
where \( T_i = (T_g + T_{tc}) / 2 \) is the film temperature and \( \text{Re}_i \) is the Reynolds number evaluated at \( T_i \). This correlation is valid for \( 10^{-4} \leq \text{Re} \leq 200 \), which is appropriate for this work where \( \text{Re} \approx 0.1 \). Furthermore, \( T_i \approx T_g \) for this work, so the final temperature correction changed by less than 1\% if \( T_i = T_g \) was set in equation (6.6).

Equating convective input with radiative output leads to

\[
 k \frac{\text{Nu}}{d} (T_g - T_{tc}) = \sigma \left( e T_{tc}^4 - \alpha T_s^4 \right).
\]

(6.7)

Since \( T_s^4 \ll T_{tc}^4 \) for flame temperatures, we can neglect \( \alpha T_s^4 \) in equation (6.7) and set \( e = 0.2 \), a value averaged over the measurement temperature and over the two different metals in the thermocouple [18].

The convective heat transfer coefficient still depends on the post-combustion gas properties: the flow velocity, density and thermal conductivity. These properties are themselves dependent on temperature, so an iterative approach is taken to find the convective heat transfer.

Starting with an initial guess of \( T_g = T_{tc} \), a corrected value for \( T_g \) is calculated. This proceeds as follows:

1. Flow composition is determined by first assuming a mixture based on the metered inputs of air and hydrogen and then using Cantera [45] to predict the gas state assuming chemical equilibrium and a temperature \( T_g \). Cantera implements Smith and Misson’s algorithm [107] for solution by the method of element potentials;

2. Density, \( \rho \), viscosity, \( \mu \), thermal conductivity, \( k \), and heat capacity, \( C_p \), are calculated for the gas mixture based on Cantera’s implementation of the multi-component transport model by Kee et al. [58];

3. Velocity is calculated by converting the metered input flow rates of air and hydrogen total mass flux, \( \dot{m} \), and then assuming that the flow is one-dimensional and applying the incompressible continuity equation so that \( u = \dot{m} / (A \rho) \) where \( A = 2.83 \times 10^{-3} \text{ m}^2 \) is the cross-sectional area of the burner;

4. The non-dimensional numbers \( \text{Re} \) and \( \text{Pr} \) are evaluated and equation (6.6) is used to determine \( \text{Nu} \); then

5. Equation (6.7) is then solved for the gas temperature, \( T_g \). The process is repeated with the new value of \( T_g \) until convergence, although in practice \( T_g \) only changes by around 1 K between the first and last iteration.

The magnitude of the temperature correction increases with increasing wire diameter and temperature. Because of this, narrow thermocouple wires with \( d = 25 \mu m \) were chosen for the measurement. The relatively low maximum temperature attained with the burner also meant that the radiation correction was relatively small. At the highest temperatures used in this work, 1568 K, the
flow velocity was $1.45 \text{ms}^{-1}$ and this procedure found $\text{Re} = 0.131$, $\text{Nu} = 0.480$ and $(T_g - T_c) = 28.2 \text{K}$.

This calculation is expected to be of relatively low precision because of the approximations in its derivation. The emissivity of the thermocouple junction, for instance, uses a representative average value over the entire temperature range of interest and assumes the thermocouple surface to be clean and shiny. While the hydrogen–air flame is soot-free and generally clean, some degradation of the thermocouple surface and therefore modification of the emissivity could be expected.

The uncertainties in the correction are hard to specify precisely, however if we set the uncertainty to 25% then the uncertainty in the gas temperature, $T_g$, is 7 K, or below 0.1%, at the highest measured temperature.

Determining water vapour number density

The number density of water vapour is calculated in the process of determining the gas temperature as the gas composition must be calculated in order to calculate the transport properties of the gas. As mentioned above, the gas composition is determined by taking the known input rates of hydrogen and air and performing a chemical equilibrium calculation with the atomic composition fixed, the pressure fixed to one atmosphere and the temperature fixed from thermocouple measurements.

The uncertainty in water vapour concentration was caused by the uncertainties in the measured air and hydrogen flow rates. These varied between $\pm 10\%$ for the coldest flame temperatures, which required low flow rates of hydrogen, and $\pm 2\%$ for the hottest flame temperatures which had higher flow rates.

Spectroscopic measurements of flame properties

The derivation of temperature and water vapour concentration from diode laser absorption spectroscopy has been described previously in section 5.4 on page 63, however this analysis assumes homogeneous gas properties across the beam path, which is not a correct assumption for measurements in the burner. Whilst most of the beam path is through the homogeneous region of the flame exhaust, the beam also passes through the edge of the burner exhaust where hot combustion products mix with the nitrogen co-flow. Analysis based on the assumption of a homogeneous beam path will therefore find a different temperature to that measured by the thermocouple in the hot core of the burner exhaust.

With the addition of some more information, however, the core temperature can be deduced from spectroscopy. With two-line thermometry, as used in this work, the specification of the shape of temperature and water vapour profiles along the beam path provides enough information to deduce temperature and water vapour concentration in the core. Zhou et al. [129] demonstrate this approach in a two line measurement, and Sanders et al. [101] show that more degrees of freedom can be introduced to the line-of-sight profile by probing more spectral lines.
With the availability of only two spectral lines, however, the shape of the line-of-sight profiles needed to be determined.

Radial temperature and concentration profiles

The radial temperature profile of the exhaust gas was measured along the laser beam path, 15 mm above the burner surface, using an S-type thermocouple and applying a correction for radiation as specified above. The burner was configured with equivalence ratio $\phi = 0.37$ to produce a central exhaust temperature of 1250 K with hydrogen and air flow rates of 5.71 lmin$^{-1}$ and 36.6 lmin$^{-1}$, respectively.

Following Zhou’s approach, a trapezoid was fit to this temperature distribution as shown in figure 6.10.

The fitted temperature distribution was then scaled to obtain a non-dimensional distribution, $\tau(x)$, where

$$\tau(x) = \frac{T_g(x) - T_0}{T_g(0) - T_0}. \quad (6.8)$$

In this relation, $x$ is the horizontal distance from the burner centreline, $T_0 = 300$ K is the initial temperature of the burner inputs and $T_g(x)$ is the radiation-corrected gas temperature measured during the thermocouple traverse.

Assuming that the shape in the temperature distribution is similar for different operating conditions of the burner, the measured temperature distribution can be scaled to an arbitrary core temperature according to

$$T_g(x) = \tau(x) \left( T_g(0) - T_0 \right) + T_0. \quad (6.9)$$

Assuming it follows a similar profile to temperature, the water vapour concentration is given by

$$N_{H_2O}(x) = \tau(x)N_{H_2O}(0). \quad (6.10)$$
The integrated absorbance for the two spectral lines, \( A_1 \) and \( A_2 \) is then given by the integral along the beam path, or from \(-l/2\) to \(l/2\) where \( l \) is the total distance travelled by the beam. Therefore, the line ratio is given by

\[
R_{ls} \equiv \frac{A_1}{A_2} = \frac{\int_{-l/2}^{l/2} S_1 \left(T_g(x)\right) N_{H_2O}(x) \, dx}{\int_{-l/2}^{l/2} S_2 \left(T_g(x)\right) N_{H_2O}(x) \, dx}.
\] (6.11)

This can be simplified by noting that when equation (6.10) is substituted into equation (6.11), the water vapour concentration at \( x = 0 \) cancels out between numerator and denominator and

\[
R_{ls} = \frac{\int_{-l/2}^{l/2} S_1 \left(T_g(x)\right) \tau(x) \, dx}{\int_{-l/2}^{l/2} S_2 \left(T_g(x)\right) \tau(x) \, dx}
\] (6.12)

is a function only of temperature, since we assume \( \tau(x) \) to be constant. Water vapour concentration in the burner core can then be found from integrated absorbance of either of the two lines, taking line 1 for example,

\[
N_{H_2O}(0) = \frac{A_1}{\int_{-l/2}^{l/2} S_1 \left(T_g(x)\right) \tau(x) \, dx},
\] (6.13)

which is the measured absorbance divided by the modelled absorbance per unit concentration.

Although this is an approximation to the burner profile, Zhou et al. [129] were able to determine temperature with a relative error of 1.2% and concentration with a relative error of 0.3%, which is a sufficient level of accuracy for the calibration of this sensor.

Calibration results

The comparison between temperature measured with a thermocouple, applying the previously-described radiation correction, and measured using the diode laser sensor is shown in figure 6.11. Temperature measurements made assuming a homogeneous beam path show a systematic offset below the thermocouple-derived temperatures. This is the effect of the shear layer on the edge of the flame where cooler nitrogen mixes with the combustion products in the centre of the flame.

When the mixing layer is accounted for, the comparison improves significantly. Best agreement is seen at 1050 K where the temperature difference between the burner and mixing layer is lowest. Agreement is still good around 1250 K, the temperature at which the temperature profile was taken. This suggests that the worsening agreement at higher temperatures may well be due to the assumption that the temperature profile retains its shape as flame operating conditions change.

Despite this approximation in determining the flame profile, the systematic error between the two measurement techniques is around 5% at the highest
temperature and 1.6% at 1250 K, which compares well with the error of 1.2% that Zhou et al. [129] found using the same technique.

A similar comparison for water vapour concentration is shown in figure 6.12 where the ratio of measured to predicted water vapour concentration is plotted against temperature.

Figure 6.12 shows good agreement near 1250 K but shows systematic offsets away from this temperature. Large uncertainties exist in the experimental data at low temperature. This is because low hydrogen flow rates were required to obtain low temperatures in the burner, resulting in an increased relative error. Scatter is lower than the uncertainty since several data points were taken consecutively without re-adjusting the flow rate.

Notwithstanding the large uncertainties, a downwards trend is apparent from the data. Since agreement is especially good at 1250 K, which is where the burner temperature profile was measured, the disagreement away from this temperature is likely to be due to the assumption that the burner profile stays the same with changing operating conditions.

The burner profile was only measured at one temperature since this was found to be the operation conditions that produced the most stable flame. The flame temperature tended to drift at other operation conditions making it impractical to measure a temperature profile without resorting to more sophisticated techniques.

Much of the scatter in both of these comparisons is due to fluctuations in the flame. These fluctuations were visible when viewing the flame with an infra-red viewer, and seemed more pronounced at high temperatures.
6.2. Flame measurements

To within the limitation of the calibration method, the strategy of taking Toth’s data as reference strengths and then scaling with HITRAN parameters delivers accurate temperature and water vapour concentration measurements. Agreement was found to be within 5% for both temperature and water vapour concentration. This was limited primarily by the uncertainty in independently determining the water vapour concentration and temperature along the laser line of sight.

Time-resolved measurements

Fluctuations in the burner, while irritating for making a calibration measurement, provide a convenient way of demonstrating the time-resolution of the sensor in a high temperature environment.

Hydrogen and air flows were set to induce a large instability in the flame—much larger than the smaller fluctuations in the flame temperature that were present during calibration.

With the system acquiring data at 1 kHz, the temperature and concentration fluctuations are clearly visible, as shown in figure 6.13. These results show a major frequency component at around 8.9 Hz with temperature leading concentration in phase. No correction was applied for the mixing layer on the edge of the burner, so reported temperatures are lower than those in the centre of the flame and water vapour concentrations are reported as relative rather than absolute.

Resolution of the temporal instability of the flame allows the component of the measurement variation due to measurement noise to be identified. If the flame variability is assumed to be well-described by a sinusoid fit to the measured
temperature, then the difference between observed temperature and the sinusoid fit is due to the measurement noise.

After subtraction of the sinusoid fit, with peak-to-peak temperature fluctuations of 20 K, the standard deviation of the measurement noise is 1.2 K. This is shown as a histogram in figure 6.14 which compares well with the measurement of temperature in room air, shown in figure 6.6 on page 85, where the temperature measurement standard deviation was 0.93 K.

The results of the time-resolved measurement, when combined with the significant effect of the flame mixing layer correction, indicate that the calibration of the sensor is limited by the temporal instability of the flame as well as uncertainty in the characterisation of the mixing layer.

A number of conclusions can be drawn from these verification experiments. During experiments at room temperature, observed line shapes were seen to depart from Voigt profiles due to Dicke [27] narrowing. Nevertheless, the departure was reasonably small and integrated absorbance could be found accurately by fitting Voigt profiles. Line shape fitting was found to be necessary to avoid dependence on pressure and measured line strength agreed better with Toth [114] than HITRAN 2000 [98].

Using the line strengths given by Toth [114] at 296 K, scaled to arbitrary temperature using the parameters given by HITRAN [98], temperature measurements with the sensor in laboratory room air had an accuracy of within 1%.

Flame measurements were complicated by the variation in gas properties along the beam path. When a simple model was used to account for this variation, temperature and water concentration measurements were accurate to within
5%. Fluctuations in the flame were the major cause of measurement scatter and the simplicity of the mixing layer correction has the potential to explain the systematic disagreement.

From these experiments, the performance of the sensor in a flame is considered to be good. However, the correction required for the relatively thin mixing layer in flame experiments shows that variation along the beam path is important and may need to be considered in later applications of the sensor.
6. Sensor verification
7. Scramjet-based measurements

Calibration experiments, while necessary, do not test how a diagnostic will perform in a shock tunnel measurement. Measurement of temperature and water vapour in a scramjet combustor was the primary focus of this work and this chapter describes the results obtained during scramjet-based measurements.

Descriptions of the shock tunnel and the scramjet have been given earlier in chapter 3, so these are not dealt with again. Similarly, the design and operation of the diode laser sensor has been described in chapter 5 so, in section 7.1, only additions to the sensor which were required for integration with the scramjet are described. In addition, section 7.1 reviews the operation conditions for the test.

Raw absorbance data from a representative tunnel run are presented in section 7.2. These data were obtained with the log–ratio detector and were affected by luminosity. To determine the extent of this effect, a direct measure of luminosity from a linear detector is presented next.

In section 7.4, line fits to absorption data at a variety of conditions are shown along with time series showing how absorbance changes over tunnel runs. Absorbance is then converted into temperature and concentration time-series, which are examined for repeatability in section 7.5. Temperature and concentration is then averaged over part of the tunnel run and plotted for different heights in the duct. Finally, time-series taken with ethylene fuel are shown and compared with those obtained when fueling the combustor with hydrogen.

7.1 Test outline and sensor configuration

A wide parameter space is available for investigation, variables include the location of the beam in the duct, operation conditions of the tunnel, fuel injection rates and fuel types. In order to limit this to something manageable, as well as maximise the chance of obtaining useful data from the diode laser sensor, the following approach was taken:

- Tunnel operation conditions were held constant, with values given in section 3.1, to correspond with work done by others [75] on a similar scramjet geometry;
- Two equivalence ratios were tested, a ‘low’ case with Ludwieg tube fill pressure of 950 kPa and a ‘high’ case with Ludwieg tube fill pressure of 2500 kPa, further details were provided in section 3.2;
7. *Scramjet-based measurements*

- Position within the duct was varied along a vertical traverse, but a reference location was chosen 10.6 mm above the duct floor for testing repeatability;

- Absorption was generally measured with a log–ratio detector. Measurements were also made with a linear detector to investigate the contribution of luminosity and for comparison with results obtained with the log–ratio detector; and

- The combustor was fueled with hydrogen, except for two runs of the tunnel which used ethylene to verify the operation of the sensor in an ethylene-fueled environment.

Compared with flame measurements, experiments in the scramjet required more consideration to be given to how the probe beam would be introduced to the measurement location. The scramjet model was mounted inside a vacuum-sealed shock tunnel test section, without direct optical access. Access to awkward locations, however, is one of the major technical benefits of diode laser-based spectroscopy.

In general, two methods can be employed. One option is to use fibre-optics to transmit the laser output to the test location, which means that the laser system can be built from off-the-shelf components. Alternatively, the system can be miniaturised and built into the scramjet model, which can result in a system that doesn’t need optical fibre.

Both approaches have their relative advantages and disadvantages, and refinement of a sensor may see a change between the two methods. For a system that needed to be dropped 27 m and withstand deceleration loads of 100 g, Silver, Kane and Greenberg’s first generation sensor [106] used fibre-optics to transmit laser light in both directions between the top of the drop tower to the falling test rig. In their next refinement of their sensor [105], the electronics were built into the test rig which required better integration but did not require fibre-coupling.

For this work, light was coupled into fibre-optics which meant that:

- Less time was required for the mechanical design of the diode laser system;

- Only small changes, unplugging and plugging in connectorised fibre optics, were required to switch between flame and tunnel measurements;

- There was convenient access to the laser and optical system for diagnostics and fine tuning; and

- The majority of the optical components were away from the dirty and harsh environment inside the tunnel test section.

The use of fibre optics can increase the cost of the system when compared with using bulk optics. Fibre is also wavelength-specific which limits the possible wavelengths that can be used, as well as making it difficult to change the system to a new operating wavelength.
7.1. Test outline and sensor configuration

If the entire system had been built inside the tunnel, more care would have been required for protecting the diode laser system from the environment and access to the lasers would have been restricted. Because a log–ratio detector was used, requiring the input of both signal and reference channels, the optical system would have been more complex than if a simpler detection scheme was used. It would have been impractical to build an interferometer inside the tunnel, so wavelength scanning would not have been measured for each run. Without an interferometer built into the sensor, the wavelength scanning behaviour of the lasers could be measured before installation but, as the scanning range is dependent on the details of the laser drive current, such an approach would have limited the flexability of the system.

The laser system was arranged on an optical table outside the shock tunnel and light was transmitted to the scramjet through single-channel, receptacle-style Oz Optics fibre-optic vacuum feed-throughs. The beam was then collimated by a Newport fibre-pigtailed gradient index, or GRIN, lens (F-COL-9-13). This collimator directed a 0.5 mm diameter beam through a wedged BK7 window (Oriel/Newport, 0.5° wedge, diameter of 12.7 mm) and into the scramjet duct as shown in figure 7.1. Wedged windows were used to avoid étalon effects, in preference to anti-reflection coatings which may have been degraded after exposure to the flow.

On the far side of the duct, shown in figure 7.2, the beam passed through a similar window and then an optical interference filter (Thorlabs FB-1400-12 with 12 nm FWHM bandpass) to exclude flow luminosity. The centre wavelength of the passband of interference filters is dependent on the incident angle of the transmitted light, and decreases as the incoming beam moves away from normal incidence. This filter was tilted at 14° to shift the centre of the passband from the specified 1400 nm to around 1392 nm, where the lasers were operating. The optimum angle was found experimentally by maximising laser transmission in a bench-top test.

The beam then illuminated the 'signal' photodiode on a log–ratio detector. An alternative would have been to couple the beam back into a fibre optic and transmit the signal back outside the shock tunnel. Power transmission into single mode fibre optics, however, is extremely sensitive to alignment, and others have generally found better results by directly illuminating the detector photodiode [3] due to beam steering effects in flows with density gradients.

Nevertheless, some applications have coupled light back into fibres such as the first sensor developed by Silver, Kane and Greenberg [105]. In contrast with the detection scheme used here, their sensor used wavelength modulation spectroscopy which is better at rejecting noise introduced by beam steering [123], and the measurement was in a less turbulent environment than the supersonic combustor studied in this project.

Some initial runs with this configuration showed that stray light was overwhelming the diode laser signal. The stray light was determined to be coming from outside the scramjet duct and was eliminated by winding optical blackout tape around the detector circuit board supports and around the back of the detector circuit board.
Figure 7.1: Cross-section of the fibre-optic launch module. Some of the fastenings have been excluded from the drawing for clarity. Co-designed with and built by Paul Walsh.
Figure 7.2: Cross-section of the detector module. Optical blackout tape is wound around the PCB supports and the rear of the PCB during operation to prevent stray light from contributing to the photodiode signal. Co-designed with and built by Paul Walsh.
7.2 Absorbance before processing

Unprocessed absorbance signal from the log–ratio detector is shown in figure 7.5. This is from a high equivalence ratio run, i.e. Ludwieg tube fill pressure of 2500 kPa, with the probe beam located 10.6 mm above the duct floor. In the first half of each scan one of the lasers crosses the line near 7179 cm$^{-1}$, designated as line 2. In the second half of each scan the other laser crosses the line near 7181 cm$^{-1}$, designated as line 1. Line 1 is visibly asymmetric due to the contribution of the additional high temperature line. Over the run time, line 1 becomes stronger relative to line 2, indicating a fall in temperature.

Spikes are evident in the data when the lasers switch on and off, at the start and in the middle of each scan. This noise does not contribute to the absorption measurement; its presence is actually useful to indicate that the maximum bandwidth of the detector and digitisation system is well above what is necessary to capture the absorption line shape.
Figure 7.4: Photograph of the scramjet with protective covers in place.

Figure 7.5: Absorbance during a high $\phi$ run with probe beam at 10.6 mm from the duct floor taken directly from log-ratio detector output without further processing. Line 1 is on the right of each scan.
The baseline absorption over each scan, as well as between scans, is not completely flat. The curve in the baseline, or a changing background absorbance with changing laser frequency, is characteristic of optical interference such as étalon fringes. For this system, the interference was tracked to passband ripple in the narrow-band filter.

While not visible in figure 7.5, other optical interference problems were also observed in the system. On occasion, when the beam was aligned with the detector, the alignment was sufficiently precise to form an étalon across the duct. When observed, this induced a peak-to-peak absorbance modulation of 0.02, but only required a very small de-alignment of the system to eliminate.

Another étalon formed in the system between the fibre-optic feedthrough and the termination of the signal channel optical fibre. While angled fibre connections were preferred for all parts of the system, component availability meant that these connections were flat polished. Since the length of fibre here was long, around 2 m, the étalon signal appeared at a very high frequency when compared with the laser scan rate. Since it was only within the detector bandwidth when the sensor was scanning at low frequency, it was initially mistaken an electronics problem. Once the signal was identified as optical interference, however, it was of no concern since it was outside the detector bandwidth when scanning at 10 kHz. Nevertheless, it emphasises the preference for angled connectors when using fibre in spectroscopy-based sensors. The presence of this étalon meant that the sensor, when installed in the shock tunnel, could not be operated below around 1 kHz. This would have been far too slow to acquire data from the shock tunnel.

Other sources of background interference are flow luminosity and beam steering from density gradients in the flow. Flow luminosity decreases both the mean value of absorbance over a scan and the peak height relative to baseline. Beam steering changes the overlap of the beam with the detector, causing fluctuations in the detected intensity as gas of different density is advected across the beam path. Furthermore, since the centre of the band-pass of the interference filter depends on the angle of incidence, beam steering interacts with the interference filter. If the passband ripple of the filter is thought of as a sinusoid waveform, changing the angle between the filter and the beam changes the phase of this sinusoid. This effect is evident in the results shown in figure 7.5 as the background in the first half of each scan changes from a curve which increases over each scan, for scans that begin near 1 ms, to be nearly flat in the last of the scans shown.

Flow luminosity does not appear to influence this data much, maybe being responsible for a decrease in the mean absorbance over scans starting near 2 ms. With the presence of beam steering and passband ripple, luminosity is difficult to estimate from this data. To better characterise the contribution of luminosity, some experiments were performed using a standard detector and a different analysis strategy.
The use of the log–ratio detector helps to reduce noise and provides a signal that is simple to convert to absorbance. However electronic processing has the potential to hide certain features of the data. In particular, the log–ratio detector only provides an indirect measure of flow luminosity.

Broadband luminosity is present in the flow due to combustion as well as emission produced by the shock tunnel operation, mostly due to impurities in the flow [85]. Although laser output is spectrally narrow, the detector is sensitive over a wide wavelength range so that luminosity can be a problem if it is not considered in the sensor design.

In order to determine the importance of luminosity to the results shown above, the log–ratio detector was replaced with a standard photodiode detector—the low-noise design given by Gray et al. [47]—which was tested for linearity against a commercial power meter (Newport 840-C). The scan rate was reduced from 10 kHz to 5 kHz for this test and the scan broken into three segments: laser 1 on, laser 2 on and both lasers off. The signal, shown in figure 7.6, was then analysed following the procedure given in section 5.4 on page 63.

The luminosity signal was extracted from the portion of the scan where both lasers were turned off and then plotted as a ratio of the laser signal in figure 7.7. These results show that the luminosity contributes, at most, 1.5% to the detected signal. By modelling the luminosity as described in section 7.1 on page 99, curve fits to synthetic data show that the systematic error in the integrated absorbance introduced by ignoring the contribution of luminosity also turns out to be around 1.5%. If the two lasers are operated at similar power, this error cancels out in the determination of the line ratio, $R_{ls}$. Therefore,
the temperature measurement is unaffected by ignoring luminosity and water vapour concentration is underestimated slightly if luminosity is ignored. As it was small, this systematic error was accepted and lines were fit to absorption data without applying a correction for luminosity.

While the signal-to-noise ratio was worse for the direct-absorption measurements, the results were consistent with the results obtained with the log–ratio detector.

### 7.4 Integrated absorbance

Having established that the effect of luminosity could be neglected during analysis, absorbance was determined from log–ratio detector output and Voigt line profiles fit to these data. Profiles were first fit to absorbance averaged for all of the scans taken over the run time and then the result of this fit was used as an initial guess for each individual scan. This approach provided a good initial guess for each individual scan, speeding up the processing and reducing the chance of fitting a line shape to noise.

The quality of line fits varied considerably due to the wide variety of flow conditions over each shot and in different parts of the duct. Locations where temperatures was near 800 K, where both absorption lines are relatively strong, and water vapour concentration was high provided the highest absorption signal and correspondingly best fits. These conditions were best met near the bottom of the duct at the high equivalence ratio.

Examples of fits to several single-scan line shapes are shown in figures 7.8 and 7.9. Figure 7.8 shows data acquired at the high equivalence ratio, 10.6 mm from the floor of the duct, while figure 7.9 shows data acquired at the low equivalence ratio.
ratio in the same location. Absorbance for the high equivalence ratio is double what is observed for the low equivalence ratio case.

The magnitude of the residuals in figures 7.8 and 7.9 are similar for all of the fitted data. This indicates that variation in the signal-to-noise ratio is dominated by the changing absorption signal, and this is highest at 2.5 ms in the high equivalence ratio case.

The residuals seem unrelated to whether or not the laser is scanning through an absorption line. This is in contrast with the residuals observed during test cell measurements, shown in figure 6.2 on page 80, where the largest residuals were observed as the laser scanned across the absorption line. The magnitude of the residuals in scramjet measurements, therefore, was primarily due to effects which are not frequency-dependent such as beam steering and background luminosity fluctuations; not fluctuations in absorbance from turbulent temperature and concentration variation.

Also visible in the line fits is the changing influence of the weak line, which appears near line 1. This is at its strongest, compared with line 1, in figure 7.8(a) which corresponds to the highest temperature out of these cases. The increasing influence of this line has the potential to degrade the fit at high temperature, since the quality of the fit of the main absorption becomes more dependant on how well the weaker overlapping line is fit.

As was described in section 5.4, the uncertainty in the fit parameters can be estimated by the bootstrap Monte-Carlo method. This was used to provide an estimate of the 90% confidence interval for integrated absorbance for each curve fit. The integrated absorbance, with uncertainty, is shown as a function of time in figures 7.10 and 7.11 for high and low equivalence ratio cases respectively. This data is from the same two shots as the line shape data presented above and shows the changing absorbance due to the two spectral lines over the runs.

In each of the cases, unsettled conditions preclude line fits before around 1 ms, but conditions settle rapidly after this. Much more absorption is observed in the high equivalence ratio case, which provides lower relative uncertainty than the low equivalence ratio case. After around 3 ms, first for the low equivalence ratio case and then for the high equivalence ratio case, absorbance decreases for both spectral lines and line 2 becomes too weak to measure slightly after 4 ms.

Mean relative uncertainty between 1 and 3 ms at the high equivalence ratio is 4.4% for line 1, 5.3% for line 2 and, at the low equivalence ratio, 7.5% for line 1 and 6.7% for line 2. Uncertainty is controlled mostly by the line strength, so that the stronger line generally exhibits the lower relative uncertainty. However, line 1 exhibits more uncertainty than line 2 at times where both lines are of similar strength. This reflects the increased uncertainty in the fit caused by the line that overlaps line 1, since this fit requires more free parameters.

Generally, the uncertainty in the fits is smaller than the scatter in the data. This has the implication that, despite the smoothing effect of the line-of-sight integration, the fluctuations in the flow are larger than the measurement uncertainty. The fluctuations are largest in the low equivalence ratio case, despite uncertainty being similar. This analysis does not, however, indicate the level
7. Scramjet-based measurements

Figure 7.8: Curve fits to high equivalence ratio data, 10.6 mm above combustor floor: (a) shows line 1 at 1.5 ms, (b) shows line 2 at 1.5 ms, (c) shows line 1 at 2.5 ms and (d) shows line 2 at 2.5 ms. Data is shown as dots, the fit is shown as a solid line. Line 1 requires two Voigt profiles to be fit to the data, and these are shown as dashed lines. ‘Obs-fit’ means ‘Observed−fitted absorbance’, equivalently, the unnormalised residuals.

Figure 7.9: Curve fits to low equivalence ratio data where the panels have the same meaning as figure 7.8. Absorbance is scaled between 0 and 0.05, half the range of figure 7.8.
7.4. Integrated absorbance

Figure 7.10: Integrated absorbance from 1 to 4 ms, 10.6 mm above the combustor floor for a high equivalence ratio run. Error bars show the 90% confidence interval of the fit.

Figure 7.11: Similar to figure 7.10 but for the low equivalence ratio condition.
of fluctuations present on time scales smaller than the time required to scan across an absorption line, around 0.01 ms. Small time-scale variations in the flow are instead interpreted as a contribution to measurement noise by the present analysis.

Since the line strengths change relative to each other over the course of the run, it is apparent that temperature and water vapour number density changes over the run. This is better considered, however, after the absorbance data is converted to temperature and number density.

### 7.5 Temperature and water vapour time series

The procedure explained in section 5.4 was used to convert the absorbance data to temperature and water vapour concentration. Since the system is time-multiplexed, the two absorbance measurements are not made at precisely the same time and interpolation was used to calculate the line strength ratio $R_{ls}$. For each point that $A_1$ was measured at, $A_2$ was found by linear interpolation between the two closest points where $A_2$ was measured. A similar process was followed to obtain $R_{ls}$ for each point where $A_2$ was defined with the result that $R_{ls}$, along with temperature and water vapour concentration, was obtained twice for each laser scan.

The analysis procedure also assumes constant properties along the beam line-of-sight since, unlike flame measurements, there was no other information about the spatial variation of properties along the beam path. Temperature calculated in this manner is shown in figure 7.12. This was calculated from the same data as above taken at 10.6 mm from the duct floor.
7.6. Traverse across duct

The repeatability of this result was tested over a total of seven shock tunnel runs, and produced the temperature and water vapour concentration results shown in figures 7.13 and 7.14 respectively.

Two of the cases shown in figures 7.13 and 7.14 show data taken at the low equivalence ratio while the other five are from the high equivalence ratio. Most of the runs were acquired at 10 kHz, however one of each of the high and low cases was acquired at 20 kHz.

The result is repeatable between the runs of the tunnel, and appears unaffected by the use of the higher sampling rate. Over all of the shots, for both high and low equivalence ratio, the temperature signal fluctuates about an approximately linear decrease. Water concentration, meanwhile, is relatively unchanged between 1 and 3 ms, especially in the low φ case, but decreases after 3 ms.

Temperature is higher in the low equivalence ratio case, 1100 K compared with 800 K at 2 ms, while water vapour concentration is around two-thirds of the high equivalence ratio case. The low equivalence ratio case also shows larger fluctuations in temperature and water vapour concentration, indicating larger fluctuations in the flow at this condition.

7.6 Traverse across duct

As well as data from 10.6 mm from the duct floor, several more shots were taken at the two equivalence ratios at different heights in the duct. Sufficient water vapour was present in the duct to obtain measurements up to 25.6 mm from the duct floor for the low equivalence ratio and up to 40.6 mm from the duct floor for the high equivalence ratio.
Temperature and concentration were obtained at 2 ms by regression-fitting a line to data between 1.5 and 2.5 ms and then evaluating the value of the line at 2 ms. This approach resulted in the same value as simply taking the mean over 1.5 to 2.5 ms, but meant that fluctuations could be represented in terms of their standard deviation about the fitted linear trend. Since 10 measurements contribute to each point, the uncertainty in the mean at each point is less than the standard deviation by a factor of around $\sqrt{10}$ if normal distributions can be assumed.

Temperature and standard deviation is shown in figure 7.15 for the two equivalence ratio cases. The maximum temperature of over 2000 K was observed for the low equivalence ratio case, 15 mm above the duct floor. This is the most uncertain of the measurements presented, with some of the points making up the fit reaching 3000 K, which is well outside the optimal range for this pair of transitions. Despite uncertainty in the temperature at this point, it is nevertheless the point where the highest temperature was observed, provided that the assumption of a homogeneous beam path is just as true as at the other measurement locations.

Either side of this maximum, the temperature for the low equivalence ratio case falls to more manageable temperatures, dropping off both towards the wall and towards the middle of the duct. Temperature for the high equivalence ratio case shows a similar decrease towards the duct floor but increases towards the centre of the duct, reaching a maximum at 30.6 mm from the floor and then showing a decrease at the topmost measurement location, 40.6 mm from the duct floor.

The low equivalence ratio data is limited to the lower part of the duct because of a lack of signal, presumably due to low water concentration, higher in the duct. Concentration across the duct is plotted in figure 7.16. These data show
larger variability and poorer shot-to-shot repeatability than the temperature measurement, although trends are still visible in the data.

Compared with temperature, there is less delineation between the two cases. Water vapour concentration tends to decrease with increasing distance from the duct floor. The low equivalence ratio shows a peak at the same location as the peak in temperature. However, this point will be overestimated if the temperature is overestimated due to the dependence of water vapour concentration on temperature.

The high equivalence ratio case shows no significant peak in water vapour concentration, the highest concentration is located closest to the wall but is within the scatter of the other points. The sawtooth structure is also too small to necessarily be significant, especially when compared with the shot-to-shot scatter in the repeated measurement at 10.6 mm.

Better understanding of these results can be achieved through more consideration of the scramjet flow-field, and this will be tackled in the next chapter.

7.7 Measurements in ethylene-fueled combustor

Because of the importance of hydrocarbons as fuels in conventional jet engines, as well as the interest in using hydrocarbons for fueling scramjets [49], the present water vapour sensor was also used to gather data when fueling the combustor with ethylene instead of hydrogen.

Measurements were carried out at the same location used for most of the measurements, 10.6 mm above the scramjet floor, at two equivalence ratios. For the low equivalence ratio, the Ludwieg tube was filled with ethylene to 510 kPa and to 1450 kPa for the high equivalence ratio.
Since combustion products besides water were expected for ethylene, less water vapour was expected when compared with the hydrogen measurements. This turned out to be the case and, as a result, the temperature measurements shown in figure 7.17 have higher uncertainties than for the hydrogen cases. Low absorption makes measurements impossible sooner in the test, at around 3.5 ms instead of after 4 ms.

Similar trends to the hydrogen fueled cases are apparent, with the low equivalence ratio recording a higher temperature as well as temperature decreasing over the test time.

Concentration also follows similar trends to the hydrogen case, as shown in figure 7.18. Water vapour concentration is lower in the low equivalence ratio case although, for both the low and high equivalence ratio, there is around one quarter as much as in the hydrogen fueled cases.
7.7. **Measurements in ethylene-fueled combustor**

Figure 7.17: Temperature for an ethylene-fueled run. High equivalence ratio here means a fill pressure of 1450 kPa and low equivalence ratio means a fill pressure of 510 kPa.

Figure 7.18: Water vapour concentration for an ethylene-fueled run. High equivalence ratio here means a fill pressure of 1450 kPa and low equivalence ratio means a fill pressure of 510 kPa.
7. Scramjet-based measurements
8. Interpretation of results

The temperature and water vapour concentration measured in a scramjet combustor were presented in the previous chapter. The measurements were able to resolve trends over the test time of the facility, showed that different conditions existed at different heights in the duct and were repeatable between shots. Nevertheless, since the temperature and water vapour concentration were derived from a line of sight measurement, it is not clear how well the measured temperature and concentration relate to the conditions present in the scramjet duct.

The purpose of this chapter is to establish whether or not the measurements are useful, given this limitation. This is done by comparison with other information sources. As part of this work, scramjet experiments were carried out with pressure transducer instrumentation, providing wall pressure data that can be compared with TDLAS results. Other experiments, documented by Stotz and O’Byrne et. al. [80, 111], used OH–PLIF to visualise the location of OH radicals near the cavity.

Since the different techniques provide different information, a direct comparison is not possible. Instead, it is first shown how the techniques can be used independently to determine the presence of combustion. Following this, pressure and TDLAS measurements are combined to obtain an estimate of the mixing ratio of water molecules.

Next, a situation where a direct comparison is possible is considered by comparison between TDLAS and computational fluid dynamics results, or CFD. CFD is able to predict the variability of the water and temperature along the line of sight, and this can be used to simulate a TDLAS experiment. The simulated TDLAS measurements are then compared with the simulated mean temperature and water concentration along the lines-of-sight. Finally, in a demonstration of how TDLAS results are applicable for verification of CFD results, the simulated TDLAS measurements are compared with experiment.

8.1 Confirmation of combustion

The presence of water vapour in the scramjet engine, as detected by the diode laser sensor, is a strong case for the presence of combustion. The scramjet freestream was obtained from bottled gases. Therefore, water vapour in the beam path would be explainable, if not from combustion, then only due to out-gassing from the shock tunnel walls or residual water vapour inside the dump tank.
In this work, residual water vapour was indeed detectable in the pumped-down shock tunnel prior to a shot. Furthermore, a test without injection showed that water vapour was present in the free-stream at low levels. In each of these cases, only absorption due to line 1 was visible. This indicates low temperatures, indeed the temperature was known to be around 300 K for residual absorption before a shot, so that the line strength of line 1 was at least a factor of three higher than during the main scramjet tests. Despite the increased line strength, the absorption signal was well below what was observed during fuel-on scramjet tests, indicating combustion was present upstream of the sensor.

Wall pressure along the duct centre-line is shown in figure 8.1. The two equivalence ratio cases are shown along with the pressure observed without injection. Injecting fuel results in an increase in pressure which is larger when injecting at a higher equivalence ratio. This pressure rise can be attributed to the heat released by combustion and the addition of mass to the duct.

In order to determine the relative size of these two effects, hydrogen was injected into a nitrogen free-stream, inhibiting combustion, and this was compared to the same amount of hydrogen being injected into an air free-stream. The pressure difference between these two cases, then, is due only to the effect of combustion and is plotted in figure 8.2.

In confirmation of the TDLAS result, a combustion-induced pressure rise is observed for both the high and low equivalence ratio. The high equivalence ratio shows a 15 – 20% pressure rise along the duct while the low equivalence ratio results in a pressure rise that is smaller and shows more variation along the duct, with one point showing drop in pressure. In a more comprehensive pressure survey of the scramjet operating as a straight duct, Neely et al. [75] noted a similar variability in the pressure increase. This was attributed to movement of shocks in the duct due to the presence of combustion.
Visualisation experiments were also carried out by others in the vicinity of the cavity. These experiments used OH–PLIF [103] and are described in detail by references [80, 111]. Briefly, the output from a pulsed laser is formed into a sheet which illuminates a plane of the flow for a period of nanoseconds. A camera detects the luminosity emitted as molecules, having been excited by the laser sheet, relax back to their ground state. The luminosity signal is dependent on the concentration of the excited species, which was OH in this case, but also on several other parameters of the flow including temperature and pressure. Therefore, in the configuration discussed here, OH–PLIF provides an indication of the location and relative abundance of OH in a plane of the flow, but does not provide quantitative species concentration.

The PLIF images provided by Stotz and O’Byrne were corrected for pulse-to-pulse variation in the total laser energy and the spatial variation in the laser sheet. Flow luminosity was not subtracted, so that the images include a contribution from the flow luminosity as well as the fluorescence signal.

PLIF images from a plane centred on one of the central fuel jets are shown in figures 8.3 and 8.4 for the high and low equivalence ratios, respectively. For hydrogen combustion, OH is an important species to visualise since it is present only as an intermediate species in the combustion reaction. The distribution of OH, therefore, indicates the parts of the flow where combustion is occurring. Abundant fluorescence is visible in each of the images above and downstream of the cavity, and is limited downstream by the extent of the laser sheet. The high equivalence ratio shows more fluorescence, and therefore has a higher OH concentration, and higher penetration of OH into the duct. The presence of OH fluorescence is another indicator that the fuel is burning at this condition.
8. Interpretation of results

Figure 8.3: OH–PLIF for high $\phi$ run with laser sheet directly above one of the central fuel jets, from references [80, 111].

and that H$_2$O measured downstream is a result of combustion and not simply ambient water vapour.

8.2 The source of measurement uncertainty

As well as information about the OH presence, PLIF images also provide information about the turbulence of the flow. In figure 8.3, the stream-wise spacing between consecutive maxima in the luminosity signal is $\lesssim 20\, \text{mm}$. Assuming that these structures are transported by the main flow at the free-stream velocity of $2760\, \text{m/s}$ then the time between consecutive maxima passing a stationary point is $\sim 7\, \mu\text{s}$. From figure 7.5 on page 105, the time taken to scan across an absorption line is $10\, \mu\text{s}$ while, at $10\, \text{kHz}$, the time required to scan over both absorption features is $100\, \mu\text{s}$.

Assuming that the turbulence timescale at the TDLAS measurement location is similar to that near the cavity, the diode laser sensor would be unable to resolve the high frequency turbulent fluctuations in the flow. If the flow properties change in the time between the laser scanning across line 1 and line 2, a measurement error can be introduced. In a flow with steady temperature, for example, if the water vapour concentration changes between the time that the two lines are scanned then the line ratio, $R_{ls}$, would depend on the changing water vapour concentration as well as the temperature. In the temperature and water vapour time-series presented earlier, this effect shows up as random variability in the measurement.

Changes in the flow conditions over a single scan are also important and can contribute to the noise in the absorption data as well as changing the line shape and reducing the quality of the fit. Since the time-scale associated with turbulent fluctuations is similar to the time taken to scan across a single absorption
line, the flow properties can change considerably during this time. Some fraction of the uncertainty in the fitted absorbance, therefore, is due to turbulent variation in flow properties changing the absorbance of the flow.

Turbulence also affects the measurement away from spectral lines. Upschulte, Miller and Allen [118, 119] found that beam steering determined their signal-to-noise ratio when measuring water vapour in a scramjet combustor. Beam steering changes the fraction of the probe beam that arrives on the active surface of the detector and its effect can be reduced by using a de-focused lens [72] in front of the detector or by using a larger detector and large aperture. Reducing sensitivity to beam-steering, however, increases the relative amount of luminosity that is captured by the detector.

In the present sensor, an interference filter was used to reject broadband luminosity. This filter caused a sinusoid-like ripple in absorption which changed in phase from scan to scan. In bench-top experiments, a very small change in incident beam angle resulted in a large change in the phase of the ripple. Therefore, it is believed that the change in beam angle due to beam steering is sufficient to interact with the interference filter and produce undesirable changes in the shape of the absorption baseline. The interaction of turbulence, beam steering and the interference filter are believed to be major contributors to the measurement uncertainty.

8.3 Water vapour mixture fraction

While comparison with pressure and PLIF measurements provides some experimental confirmation of the results obtained with TDLAS, the information that these measurement techniques provides is complimentary. A possible reality
check on the TDLAS results is to use the measured temperature and number density to estimate the water vapour mixture fraction.

If we assume that the pressure of the components can be represented by Dalton’s law, then the partial pressure of water vapour is given by

$$P_{H_2O} = \frac{N_{H_2O}RT}{N_A10^{-6}}$$

(8.1)

where $N_{H_2O}$ is the number density of water vapour [molecules cm$^{-3}$], $R = 8.314$ J mol$^{-1}$ K$^{-1}$ is the molar gas constant, $T$ is temperature [K], $N_A = 6.022 \times 10^{23}$ mol$^{-1}$ is Avogadro’s number and the factor of $10^{-6}$ is present since $N_{H_2O}$ is expressed in molecules cm$^{-3}$.

Close to the combustor wall, we assume that the local pressure is well approximated by the wall pressure. This is shown for the two equivalence ratios, and for no injection, in figure 8.5. At this location, there is a periodic modulation about a steady decay which is present in only some of the upstream traces. Neely et al. [75] noted similar features in their pressure measurements and attributed this to shock reflection off the wall in the vicinity of the pressure transducer. Slight variation in the position of the shock over the course of the shock tunnel test time would result in varying pressure as observed in figure 8.5.

By normalising water vapour partial pressure by the wall pressure, we obtain an approximation to the water vapour mixing ratio. This is the fraction of water molecules in the gas mixture, and is shown in figure 8.6. Figure 8.6 was calculated from the same data as was used to demonstrate repeatability in the previous chapter, which were from 10.6 mm above the scramjet floor.

If we were to start with a stoichiometric mixture of hydrogen and air, the mixture after combustion would contain about 35% water vapour by volume. Al-
though the global equivalence ratio is below 1 in each of the cases, some parts of the duct would have a local equivalence ratio of 1 and therefore, if combustion is complete, it is feasible for parts of the duct to reach 35% water vapour. Measurements that indicate more than this, however, are physically impossible and would indicate an error in the measurement.

Shown in figure 8.6, after 1.5 ms the water vapour ratio is well below the theoretical maximum of 35% in both the high and low equivalence ratio cases, although the larger scatter before 1.5 ms takes some measurements above this. Having been determined for two fluctuating data sets, the inferred water fraction is highly variable but appears close to 0.08 at 2 ms for both equivalence ratios. Apart from the variability in the measurement, which declines over the test time, the water fraction appears relatively constant until 3 ms when it starts to decline rapidly in the low equivalence ratio case.

Water concentration at this location is close to the maximum recorded in the duct. Therefore, these measurements indicate that it is unlikely that combustion reaches completion in the scramjet duct and unburned hydrogen and oxygen are expelled from the duct. The measurement also has some credibility, since it is is physically reasonable to have 8% water in the duct. Still remaining, however, is the uncertainty in how accurately the temperature and water concentration are measured, given the assumption of constant properties along the beam path.
8. Interpretation of results

8.4 Comparison with CFD

Comparing TDLAS and CFD results is useful for two reasons:

- CFD provides full details of the flow-field within the scramjet and the 3-D CFD results can be used to find out how the assumption of homogeneous line-of-sight properties affects a simulated TDLAS measurement in the CFD flow; and

- Experimental results can be used to verify the accuracy of the CFD simulation.

Both of these aspects are considered in this section, although the comparison is limited by the apparent poor correspondence between the CFD result and conditions in the scramjet duct.

Before experiments were conducted, GASP version 3.2 [1] was used to compute the 3-D, chemically-reacting flow within the scramjet combustor. Attempts to obtain a turbulent solution were unsuccessful, however a solution was obtained using a laminar solver and this was used as an approximate guide to the possible flow-field in the combustor during sensor design.

The laminar CFD results performed by the author were superseded by the ones presented here which were computed by Stotz using CFD++ version 4.2 [67]. Apart from the geometry changing downstream of the cavity from a straight to diverging duct, the computational model was identical to that described in references [80, 111].

Taking advantage of the symmetry of the combustor, the 3-D flow solution was computed for half of the duct using a Reynolds–averaged Navier–Stokes solver, using wall functions and a three-equation turbulence model (the $k – \epsilon – R$ model [44]). The combustor geometry was modelled with a rectangular mesh of 2.3 million cells. The cells were clustered in the cavity, particularly around the injector ports, and at the duct walls. The boundary layer of the duct was resolved in the model and contained around 15 cells near the TDLAS probe location. Cells were not tightly clustered in the vertical direction at the TDLAS beam location, however grid spacing was still much finer than the separation between individual probe beam locations.

Flow chemistry was simulated with the model by Drummond et al. [29] which includes 9 species and 18 reactions and treats nitrogen as inert. Since dissociation of nitrogen and formation of NO$_x$ was not allowed by this chemistry model, the flow entering the scramjet was modelled as a 20%O$_2$, 80%N$_2$ mixture. This is a simplification of the actual flow delivered by the facility which contains chemically frozen radicals generated in the stagnation region.

Other conditions at the CFD-model inlet were: pressure 91.1 kPa, temperature 1215 K, and velocity 2811 m s$^{-1}$. These nominally matched the free-stream conditions at 1.5 ms, although comparison with table 3.2 on page 21 shows that these parameters are slightly higher than the experimental free-stream. Injection was set to simulate a high equivalence ratio run with hydrogen being
8.4. Comparison with CFD

injected at 5.65 gs$^{-1}$ at a temperature of 250 K. This is half of the flow rate of experiments since the computational model included only half of the combustor.$^1$

The pressure along the duct centre-line, as predicted by the CFD model, is slightly lower than the measured pressure at the 'inlet' transducer and in the cavity, as shown by figure 8.7. The standard deviation of pressure fluctuations at each measurement location is shown, indicating the large fluctuations in the cavity as well as the measurement noise associated with the inlet transducer. The inlet measurement also shows poor shot-to-shot repeatability which is not matched by the measurements further down the duct. Since the cavity transducer was off-centre, the comparison between centre-line pressure is slightly misleading. According to the CFD prediction, pressure at the transducer location is 10% lower than along the center-line. When this is taken into account, the CFD under-predicts the cavity pressure by a similar amount to the inlet pressure.

Pressure measurements beyond the cavity have mixed agreement. The first few upstream and furthest downstream measurements match CFD. However, the shape of the pressure distribution is not particularly well predicted by CFD. The CFD indicates a steadily decreasing pressure towards the end of the duct whereas measurements show the pressure to be almost constant in this region. Despite the noted differences however, the overall agreement between measurements and simulation is relatively good.

$^1$Note also that the freestream conditions used for the CFD underestimated the temperature significantly—conditions assuming vibrational equilibrium would be more appropriate. See page 20 for more information.
Temperature predicted by the model is shown in figure 8.8. The wall temperature is constant at 300 K to match the experimental scramjet, which has insufficient time to heat significantly over the 3 ms test. Along the scramjet centreline, the left of the model in figure 8.8, the shock structure is visible in the vicinity of the cavity. The flow then cools as it encounters the expansion fan after passing the diverging corner in the duct floor. The lower part of the duct contains a cool stream of gas which is mostly unburnt hydrogen. A second cool pocket is visible near the top of the duct, cooler due to the expanding flow, while a hot layer adheres to the wall of the duct at the right of the image.

The mole fraction for water vapour predicted by the model is shown in figure 8.9. This shows less structure than the temperature plot with water vapour visible only in the lower part of the duct. Although not visible at this scale, the model predicts water vapour all the way up the duct. Near the top of the duct, water vapour is mostly confined to the boundary layer.

Although the spatial distribution of water vapour in the model looks reasonable, the concentration predicted by the model is low. The maximum predicted water fraction, 0.3%, occurs above the cavity and near the wall, which is out of sight in the image. According to the CFD, 0.15% is more typical for the area where temperature and water vapour were measured.
8.4. Comparison with CFD

Figure 8.9: Water mole fraction predicted by CFD. CFD by Stotz.

Figure 8.10 shows temperature and water concentration in the measurement plane, overlaid with the probe beam locations. The traverse takes the beam through the cool pocket of gas near the duct floor and passes through the hot layer near the duct wall at each location.

As the beam moves up the duct, it passes through regions with decreasing water vapour concentration so that the topmost location passes through a region with comparatively little water. While temperature varies considerably along each line-of-sight, water concentration is relatively constant.

The data in figure 8.10 can be used to simulate a TDLAS measurement. Temperature and water concentration provide the information necessary to predict absorbance from each of the spectral lines, as described in section 4.2. The absorbance from a measurement can then be calculated by integrating this absorbance along each of the beam paths and the analysis procedure used for the experimental data can be applied to this simulated experiment.

Horizontal mean compared with simulated TDLAS temperature and water concentration are shown in figures 8.11 and 8.12 respectively. Near the bottom of the duct, measured temperature is low compared with the mean temperature because of the stronger absorption of line 1 at low temperature. Further up the duct, temperature is reported higher than the horizontal mean since the water vapour is located only in the hot boundary layer.

The concentration measurement is largely unaffected by the systematic error in temperature. Figure 8.12 shows good agreement between the concentration
8. Interpretation of results

Figure 8.10: Temperature (left) and water vapour (right) in the measurement plane, predicted by CFD for the high equivalence ratio case. Horizontal lines indicate the probe beam locations. CFD by Stotz.

Figure 8.11: CFD-predicted line-of-sight mean temperature, apparent temperature from TDLAS simulated from CFD data and measured temperature. Plotted measurements indicate the average and standard deviation from 1 to 2 ms and therefore have larger variability than those reported in the previous chapter. CFD by Stotz.
8.4. Comparison with CFD

measured with simulated TDLAS and the mean concentration across the duct. Water concentration is highest near the duct floor and decreases with increasing distance up the duct.

For both temperature and water vapour concentration, this suggests that the error with assuming a homogeneous beam path is relatively small provided that the CFD is producing a representative line-of-sight variation in flow properties. A limitation of this analysis is that the result produced by CFD represents a time-averaged solution to the turbulent flow-field. As such, the line-of-sight variability in flow properties is underestimated somewhat compared with the instantaneous variability in flow properties. This conclusion should also be tempered by the knowledge that the CFD massively underpredicts the water vapour concentration, as discussed next.

Besides providing an indication of how line-of-sight variability affects the measurement, the usefulness of the temperature and water vapour measurements can be illustrated by direct comparison with the CFD results.

As well as the simulated TDLAS results, experimental results are shown in figure 8.11. These are from the same data as the results presented in the previous chapter, with the difference that data extracted from the time-series was centred on 1.5 ms instead of 2 ms to match the CFD boundary conditions.

Diode laser measurements had large fluctuations early in the experimental run, so that the variability indicated in figure 8.11 is larger than that reported in the previous chapter. As before, the error bars indicate the standard deviation of the variability of the measurements rather than the error in the mean. Shot-to-shot variability is indicated by the repeated measurements at 10.6 mm.

Despite the large fluctuations, measured temperatures are significantly higher than the temperature predicted by CFD. Furthermore, the simulated TDLAS
results differ from the measurements. Turbulent line-of-sight variability does not help explain this discrepancy either, since increasing the variability along the line of sight tends to decrease the measured temperature, suggesting that CFD is indeed predicting a low temperature.

The gulf between measurements and CFD predictions is considerably larger for water vapour concentration. Measured water concentration is not plotted in figure 8.12 since it is approximately $10^2$ larger than the concentration predicted by CFD—TDLAS results were shown in figure 7.16. The extent of the water vapour is similar, with measured water vapour dropping to 25% of its maximum at 40 mm from the duct floor, whereas CFD predictions put this point nearer 30 mm. The distribution shape is also similar. Although the measurements suggest that a peak in water concentration may be present at some distance from the wall, a monotonic decrease in concentration is within experimental uncertainty.

The main purpose of presenting these CFD results here is to illustrate the utility of TDLAS in verifying the results from a simulation. The CFD result is taken to be at fault here since PLIF results, presented earlier in this chapter, show strong combustion within the duct. This is inconsistent with water vapour concentrations of 0.15% or less.

Nevertheless, it is worth considering some possible reasons why the discrepancy is so large, with a view to making improvements to the CFD simulation in the future.

Comparison with experiments saw that the simulation was under-predicting both water concentration and temperature. Since heat is released with the formation of water vapour, an increase in water production should result in an increase in temperature, and take both quantities towards better agreement.

In order for more hydrogen to react in the duct, it must first mix with oxygen from the free-stream. Although not shown, examination of the hydrogen mole fraction indicated that this mixing is indeed occurring—enough so that it is unlikely to be the limiting step.

Assuming that the mixing is modelled reasonably, the chosen chemistry model seems a likely candidate for further investigation. As noted above, the chemistry model is comparatively simple and treats nitrogen as inert. In experiments, the free-stream contains a fraction of radicals and nitrogen compounds. These are formed in the stagnation region of the shock tunnel and have insufficient time to recombine before encountering the scramjet flow. In some reaction models, the presence of small amounts of radicals has the ability to significantly decrease the ignition delay time [81]. If this were to happen, heat released before the expansion might be sufficient to maintain a high enough temperature for combustion to continue after the expansion. In this way, a threshold could be reached where a small change could result in a disproportionate increase in water vapour concentration.†

In a simulation of a scramjet combustor, however, we encounter a supersonic, turbulent, chemically-reacting flow so there is ample opportunity for problems

†It is also likely that the CFD would agree better with observations if a hotter, and more physically appropriate, free-stream condition was used. See page 20 for more information.
to arise in the simulation which produce results that differ from observations. Therefore, further investigation is required before a cause for the discrepancy can be definitely assigned.
8. Interpretation of results
9. Conclusions

The aim of this work was to test the effectiveness of TDLAS as a diagnostic for a scramjet combustor operating in a free-piston shock tunnel. At the onset of the project, no such diode laser sensor was available so a considerable fraction of the project was spent designing, building and testing the sensor. Measurements in a hydrogen–air flame were able to verify the accuracy of the sensor with a maximum systematic error of 5% at 1550 K. Validation uncertainty was limited by flame fluctuations as well as the variation in flame properties along the beam line-of-sight.

The validated sensor was used to make measurements in a scramjet combustor, and the effectiveness of the sensor was discussed in the previous chapter. Measurements were possible at all four conditions tested, which included high and low equivalence ratio cases of hydrogen and ethylene fuel. The success of the sensor in ethylene was limited by the reduced amount of water vapour present in the flow when compared with hydrogen tests. However, the measurement was selective enough not to be affected by the additional species present in the ethylene-fuel case.

Measurements were limited to the lower part of the scramjet duct, where the most water vapour was present. Measurement of other species, such as oxygen, would compliment the present sensor and allow measurements to be made through the entire duct. With the present sensor, trends were resolved over the test time, and different results were obtained at different locations within the duct and at different equivalence ratios.

Comparison of TDLAS results with pressure measurements, OH fluorescence measurements and CFD were used as the basis for judging the usefulness of the TDLAS sensor. The conclusions that arise from this discussion are given below.

Evidence of combustion was observed by TDLAS at both of the scramjet operating conditions through the detection of the water vapour combustion product. The presence of combustion was supported by pressure and OH–PLIF measurements, validating the result inferred from the diode laser sensor.

As expected from theory, the uncertainty in the temperature measurement increased with increasing temperature. While dependent also on water concentration, typical values ranged from ±2% at 500 K to ±10% at 1500 K. This is higher than the uncertainty in flame verification experiments, which was a maximum of ±5% at 1550 K. Calibration experiments, therefore, were able to
characterise the sensor with sufficiently high precision for the intended application of the sensor.

Improved precision in scramjet experiments might be possible if the effect of the interference filter were eliminated. In the present configuration, this filter was essential for blocking broadband luminosity from the flow. Nevertheless, improvement of this feature of the system could provide the largest improvement in future measurements.

Turbulent fluctuations also influenced the measurement. Comparison with PLIF images showed that the sampling rate of the sensor was a factor of $10^2$ below what would be required to resolve turbulent fluctuations in the duct. A decrease in the time between the two absorption measurements would improve the sensor. This could be achieved by increasing the scanning rate or selecting new spectral lines that are close enough to be scanned with a single diode laser.

The previous chapter also presented a simulation of the scramjet flow. The simulated flow-field was used to simulate the absorption along lines-of-sight. The simulated absorption was then used to find apparent temperature and water vapour concentrations, based on a hypothetical TDLAS measurement along that line of sight.

This showed that the error associated with assuming constant properties along the line-of-sight results in a small error, for this simulated flow. Temperature was low by 5% and concentration by 3%. Despite the 3–D nature of scramjet flow fields, therefore, TDLAS can be used to effectively determine mean temperature and water concentration provided that the beam path is chosen carefully. This conclusion, however, is limited to the CFD-predicted flow and is only valid in the experimental case if the simulation correctly predicted the variability in temperature and water concentration along the line of sight.

The value of the TDLAS measurement is best demonstrated by comparison with CFD results. Diode laser measurements showed that CFD temperature predictions were low. More strikingly, water concentration was under-predicted by a factor of $10^2$.

The diode laser sensor, therefore, is effective at producing data which can be used to verify CFD predictions. Without the availability of the diode laser sensor, the under-prediction of water vapour would have been difficult to discover from the PLIF or pressure measurements. It produces quantitative data which compliments other experimental techniques. With the possibility of future enhancements to the sensor, diode laser sensors seem to be a valuable tool for scramjet research.
References


References


References


References


[112] The Math Works Inc. 3 Apple Hill Drive, Natick, MA 01760-2098, USA http://www.mathworks.com/. 51, 72


Glossary of symbols

Symbols used in this thesis are listed below. Units, where given, refer to the most common usage and other units were sometimes used when convenient. Values of constants are from NIST standard reference database number 69, March 2003, http://webbook.nist.gov/chemistry/.

\( A \) Integrated absorbance due to a spectral line \([\text{cm}^{-1}]\)
\( A \) Area \([\text{m}^2]\)
\( A_m \) Measured, or apparent, integrated absorbance \([\text{cm}^{-1}]\)
\( c \) Speed of light \((2.997 \times 10^8 \text{ ms}^{-1})\)
\( c_2 \) Second radiation constant, \( c_2 = hc/k \)
\( C_f \) Feedback capacitor.
\( C_p \) Specific heat capacity
\( d \) Characteristic length scale, cylinder diameter \([\text{m}]\)
\( e \) The electronic charge \((1.602 \times 10^{-19} \text{ C})\)
\( E' \) Upper state energy level \([\text{cm}^{-1}]\)
\( E'' \) Lower state energy level \([\text{cm}^{-1}]\)
\( G \) Detector gain
\( g(\nu) \) Absorption line shape
\( h \) Planck’s constant \((6.626 \times 10^{-34} \text{ Js})\)
\( h \) Convective heat transfer coefficient
\( I \) Initial beam intensity
\( I_0 \) Transmitted beam intensity
\( i_{\text{ref}} \) Reference beam photocurrent
\( i_{\text{sig}} \) Signal beam photocurrent
Glossary of symbols

$I_{\text{ref}}$ Reference beam intensity

$I_{\text{sig}}$ Signal beam intensity

$J_{K_a,K_c}$ Rotational quantum numbers, see section 4.1

$k$ Boltzmann’s constant ($1.381 \times 10^{-23}$)

$k$ Thermal conductivity

$k_v$ Frequency-dependant absorption coefficient [cm$^{-1}$]

$l$ The length the beam travels through the absorbing medium [cm]

$L/D$ Length-to-depth ratio (of a cavity)

$M$ Molecular mass [g mol$^{-1}$]

$n$ Refractive index

$N_A$ Avogadro’s number ($6.022 \times 10^{23}$ mol$^{-1}$)

$N_K$ Number density of species $K$ [molecules cm$^{-3}$]

$Nu$ Nusselt number, $Nu = h d / k$

$P$ Pressure [kPa]

$P_K$ Partial pressure of species $K$ [kPa]

$Pr$ Prandtl number, $Pr = C_p \mu / k$

$Q(T)$ Partition sum

$Q_1, Q_2, \ldots$ Semiconductor device 1, semiconductor device 2, \ldots

$q_c$ Convective heat transfer per unit area

$q_r$ Radiative heat transfer per unit area.

$R_{ls}$ Ratio of line strengths, $R_{ls}(T) = S_1(T) / S_2(T)$

$R$ The molar gas constant (8.314 J mol$^{-1}$ K$^{-1}$)

$R_K$ The specific gas constant for species $K$ [J kg$^{-1}$ K$^{-1}$]

$R_1, R_2, \ldots$ Resistor 1, Resistor 2, \ldots

$Re$ Reynolds number, $Re = \rho ud / \mu$

$S(T)$ Line strength [cm$^{-1}$(molecule cm$^{-2}$)]

$T$ Temperature [K]

$T_f$ Film temperature $T_f = (T_g + T_{tc}) / 2$

$T_g$ Gas temperature [K]

$T_s$ Temperature of surrounding environment [K]
Glossary of symbols

$T_{tc}$  Thermocouple junction temperature [K]
$u$     Velocity [ms$^{-1}$]
$v_1, v_2, v_3$  Vibrational quantum numbers, see section 4.1
$V_{out}$  Output signal [V]

$\alpha$  Absorptivity
$\gamma_d$  Gaussian, or Doppler broadening, width at half-maximum [cm$^{-1}$]
$\gamma_l$  Lorentzian, or pressure broadening, width at half-maximum [cm$^{-1}$]
$\epsilon$  Emissivity
$\lambda$  Wavelength [nm]
$\mu$  Viscosity
$\nu$  Frequency [cm$^{-1}$]
$\nu_0$  Transition centre frequency [cm$^{-1}$]
$\nu_{FSR}$  Free spectral range [cm$^{-1}$]
$\rho$  Density
$\sigma_K$  Standard deviation in variable $K$
$\sigma$  Stefan–Boltzmann constant ($5.6704 \times 10^{-8}$ Wm$^{-2}$K$^{-4}$)
$\phi$  Fuel–air equivalence ratio