REMOTE SENSING MEASUREMENTS OF
THE ATMOSPHERIC BOUNDARY LAYER

DEVELOPMENT OF A NOCTURNAL BOUNDARY
LAYER TEMPERATURE LiDAR

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Abstract

A LiDAR instrument to monitor the evolution of the urban boundary layer capping inversion over Manchester has been developed from a previous instrument. This LiDAR uses a frequency-tripled Nd:YAG laser, operating at low pulse energy but high repetition frequency. Rotational Raman scattering of this laser light is parsed into two channels by narrowband interference filters, before detection by photomultiplier tubes operating in photon-counting mode.

The receiving telescope was refocused to operate in the boundary layer, and an interference filter was replaced following modelling work. The calibrations of this instrument use locally-launched sondes to determine corrections due to operating in the near-field region of the receiving telescope. The LiDAR receiver was thoroughly calibrated under laboratory conditions to construct a lookup table. Locally-launched sondes were used to correct for mirror shading by instrument components, as well as constrain the overlap function of the BLT.

A temperature resolution of better than 0.4K arising from Poisson noise was achieved for data collected for the mean temperature profile measured over the course of a night, with temperature inversions being identifiable down to a height of 500m. A total temperature error of less than 3K was achieved by taking the whole-night mean, which is significantly less than the size of the smallest identified temperature inversion (7.6 ± 2K).

The LiDAR instrument data was compared with locally-launched sondes to validate the collected data, agreeing with the sonde measurements to within the uncertainty of the instrument. A WRF model temperature output was compared to both the BLT and sonde data and found to poorly capture the boundary layer temperature profile. The inversion strength was always underestimated by several K, and when the inversion height is below 300m the model underestimates the inversion height by 100-500m.
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Chapter 1

Introduction

1.1 Boundary Layer

The boundary layer is the lowest layer of the atmosphere - the portion of the atmosphere in contact with the ground. The air in this layer is in direct contact with the non-marine biosphere - used for respiration and photosynthesis, as well as forming the air-sea interface through which pass carbon dioxide and oxygen (necessary for photosynthesis and aerobic life).

On a human scale, all agriculture relies on boundary layer air as well as (the vast majority of) the human population who breathe this air. Further, almost all human atmospheric emissions enter the boundary layer as do natural emissions - pollen, fungal spores, sea spray, biomass burning products, etc. In regions of low ambient boundary layer wind these ground-based emissions can build up to potentially dangerous levels, such as smogs forming in large cities, or smoke from fires.

The interface between the boundary layer and the planetary surface is most obviously visible in the form of winds - gusts creating sea swells, rippling crops, and powering windmills. These are good examples of the atmosphere transferring momentum to the planetary surface - energy being removed from the boundary layer.

Understanding the structure of the boundary layer is critical to our understanding of how emissions are distributed throughout the atmosphere - whether they will accumulate, increasing to dangerous concentrations or mix into the surrounding air. Additionally, by identifying the evolution of this structure, forecasts of air quality can be constructed, and any necessary actions taken.
1.1.1 Structure of the Boundary Layer

Within the boundary layer a sublayer forms during the day, mixing air from the surface vertically through the atmosphere. This sublayer is called the convective boundary layer and its evolution is driven by the diurnal temperature variation which alters the energy supplied to the boundary layer. Because the atmosphere is largely transparent to solar radiation, it passes through to warm the planetary surface (while clouds can block incoming solar radiation, suppressing the development of the boundary layer, this discussion assumes a cloud-free sky). Any temperature gradients between the ground and the atmosphere are reduced by energy transfer, either from the ground to the surface layer, or vice versa. Sensible heat is passed through conduction, while latent heat is transferred through evaporation or condensation. When energy is transferred from the ground to the atmosphere, convective motions (see below) transfer this energy further into the boundary layer.

The energy added to the bottom of the boundary layer drives convective motions which circulate materials throughout the range of the circulation. This convective mixing determines the bulk properties of the boundary layer - see figure 1.1.1.

The potential temperature of an atmosphere provides a quantitative measure of the stability of of an atmosphere, to a greater degree than the absolute temperature profile. The potential temperature of an air parcel is the temperature it would carry if moved adiabatically from its original altitude to a reference pressure \(P_0\), typically 1000hPa.

Equation 1.1.1 (Stull, 1988, p.7) describes the calculation of the potential temperature. For air, \(\frac{R}{c_p} \approx 0.286\).

\[
\theta(h) = T(h) \left( \frac{P_0}{P(h)} \right)^{\frac{R}{cp}}
\]  

(1.1.1)

To remove the necessity for a reference pressure and instead convert from an absolute temperature profile to a potential temperature profile the pressure profile of the atmosphere can be removed through the consideration of the changing pressure with altitude (equation 1.1.2).

\[
P(h) = P_0 \exp \left( \frac{-gh}{RT(h)} \right)
\]  

(1.1.2)

Combining equations 1.1.1 and 1.1.2 yields:
\[ \theta(h) = T(h) \left[ \exp \left( \frac{gh}{RT(h)} \right) \right]^{0.286} \]  

When the potential temperature of an air parcel is greater than that of the air below it the air is stably located (small perturbations in its altitude will not produce an extended vertical motion). The limits of this instability define the limits of convective motions throughout the boundary layer.

The mean potential temperature (\( \theta \)) of each of stages A-E of the diurnal cycle (shown in figure 1.1.1ii) are plotted below, which additionally highlights the changing stability of the boundary layer over the course of a diurnal cycle.
Evolution of the Boundary Layer Structure

Because the boundary layer is in direct contact with the ground, any change in ground conditions necessarily manifest in a modification of the properties of the boundary layer air close to the ground. This can be conduction of heat from the ground, or a radiative transfer of longwave radiation from the warming ground during the course of a day, or an increase in moisture due to surface water presence. Trace gases and pollutants emitted at
ground level also enter the lowest reaches of the boundary layer.

Convective motions within the atmosphere are driven by buoyancy differences, themselves driven by temperature (and thus density) differences between an air parcel and that of the local atmosphere. The evolution in the surface radiative forcing can be summarised as follows:

1. Beginning when the radiation terrestrial flux first becomes negative (the ground begins warming) early in the morning following sunrise, sensible and latent heat is passed to the lower region of the atmosphere, warming it. This increase in temperature raises the buoyancy of the air adjacent to the ground, resulting in short-scale convective motions. These convective motions extend by entraining air from above. The region of the boundary layer which feels the direct effect of the surface radiative forcings is known as the surface layer.

2. By noon the radiation flux will be most negative (vertically downwards), and thus the ground heating is at its maximum. As such, the radiative forcing is strongest and the thermals become much more extended, reaching the temperature inversion marking the limit of the boundary layer. The region of the boundary layer over which the convective motions extend is known as the convective mixed layer when vertical motions are dominated by convective motions. If, instead turbulent processes dominate the vertical motions of the boundary layer this region is called the mixed layer (Stull, 1988, p.450). The green shaded region of figure 1.1.1 shows where the boundary layer is well-mixed, without presuming the dominant vertical mixing mechanism. See, for example, the work of Barlow et al. (2011) (their figure 5) for empirical measurement of the depth of the convectively mixed layer in London, observed to reach a maximum altitude of 800m.

3. Later in the afternoon the intensity of the illuminating solar radiation will decrease and the radiation flux will reduce, eventually reaching a point where the net upward flux from the surface will become zero. At this point there is no net transfer of energy (including latent and sensible heat) between the surface and the adjacent air. With no radiative forcing, no further surface-forced convection can occur and the boundary layer begins to become neutrally stratified.

\[1\text{This temperature inversion is typically a few } \text{K per } 100\text{m in the midlatitudes - see Chen et al. (2011), Hammann et al. (2015), Imaki et al. (2012) for a few examples.}\]
4. As the illuminating solar radiation continues to weaken, the net radiation flux becomes positive (vertically upwards) as the ground begins to cool. Latent and sensible heat flow from the air to the surface in the form of cooling the air and condensing any moisture present at ground level, cooling the lower air more rapidly than air further aloft due to the closer proximity to the cooler ground. This region of the atmosphere adjacent to the ground over which the temperature increases with height is known as the **stable boundary layer** or the **stable nocturnal boundary layer**.

Existing thermals are dissipated by turbulence (random eddy motions within the atmosphere) within the boundary layer resulting in a region which homogenises with respect to mean virtual potential temperature (see figure [1.1.1](#)). This region is known as the **residual layer** because its properties (temperature, water vapour, trace gas and aerosol loading) are defined by the mixed layer from which it forms.

5. At sunset the solar illuminating radiation ceases altogether. The stable boundary layer continues to grow in depth as air further aloft from the ground passes its energy to lower air in response to the low-level cooling.

6. Following sunset the surface continues to emit longwave radiation as the ground cools and the limit of the stable boundary layer increases logarithmically. The residual layer aloft from this stable region retains the characteristics from the convectively mixed layer from which it formed, the turbulent motions within acting to homogenise this region throughout the night.

7. After sunrise the illuminating solar radiation begins to increase, but the ground temperature cannot increase until sufficient energy has been absorbed to raise the ground temperature.

8. Once sufficient energy has been absorbed by the ground to raise its temperature, the surface radiation flux returns to negative and latent and sensible heat can be passed to the stable boundary layer. The previous night’s stable air is entrained into the growing convectively mixed layer over the course of the day - see figure [1.1.1](#) - allowing the mixed layer to grow steadily until the stable layer is fully entrained. Entrainment (mixing in) of the residual layer is much more rapid due to
the unstable\textsuperscript{2} nature of this region of the atmosphere (see figure 1.1.1).

The limits of convective mixing in the boundary layer necessarily determine the limit to which atmospheric components can be mixed (both upwards from ground-level emissions as well as downwards motion of materials aloft). When the boundary layer temperature profile resembles that of case A in figure 1.1.1\textsuperscript{i} all ground-based emissions can be mixed throughout the boundary layer within a typical time of approximately 10-20 minutes (Stull [1988], p.450).

Before sunrise (case C in figure 1.1.1\textsuperscript{ii}) the opposite is true - the strong stability of the boundary layer means that the surface layer will not be convectively mixed. These pollutants will instead remain at the altitude to which they were mixed by convective motions during the day, or emitted during the course of the night.

If we consider the shaded regions of the potential temperature profiles in figure 1.1.1\textsuperscript{ii} we can see that the potential temperature is greater than (or equal to) at the surface than in the layers directly above it. However once the potential temperature equals the surface potential temperature the convective motion is halted and the mixing layer terminates. This height is where air from the above the boundary layer is being mixed down (entrained), and across this entrainment layer the potential temperature increases with height - forming a capping inversion for the convective motions.

The convective motions may transfer water vapour from lower in the boundary layer to regions where the temperature is sufficiently low for the water vapour to condense, forming clouds. The tops of boundary layer clouds clearly delineate the level at which the potential temperature begins increasing with height (the temperature inversion). This can conveniently be used to determine the depth of the boundary layer where there are clouds available (using ceilometers or vertically-directed high frequency RADARs, for example).

1.2 Boundary layer over rural areas vs over a city

Of the world’s population, 53\% of people live in urban environments - and this rises in the developed world (73\% of Europe’s population live in urban environments) (Kaneda and

\textsuperscript{2}If air aloft is of a lower temperature than lower-altitude air then convective motions are supported and thus develop swiftly.
Additionally, many major cities in the world experience pollution problems - from smogs and other large-size aerosols to high concentrations of gases harmful to human health (nitrous oxides, carbon monoxide, sulphur compounds, etc) (Lodgejr, 2006). Understanding the distribution of these pollutants is imperative to controlling and predicting health risks across a city from these compounds (Lodgejr, 2006).

Understanding the temperature profile of the boundary layer over a city (the urban boundary layer) is therefore critical - and is linked to the differences in land use within the city compared to rural environments. In urban areas there is often a persistent heat transfer to the boundary layer due to the increased heat capacity of the urban fabric. This heat transfer produces an urban heat island (a region of atmosphere of a few degrees higher temperature than the surrounding regions located over an urban area) (Bohnenstengel et al., 2011; Bornstein, 1968; Knight et al., 2010; Park, 1986; Stull, 1988, p.610) which can support the convective mixed layer for longer than figure 1.1.1 would suggest. Further to this, because of their extensive sewer and drainage systems urban environments are significantly more water-permeable than surrounding rural land and thus there is significantly less moisture available at ground level to be mixed into the boundary layer from urban environments, and a corresponding reduction in evaporative cooling (resulting in a greater sensible heat emission from urban environments). The urban heat island is more pronounced overnight than during the day, as found by Bohnenstengel et al. (2011); Collier (2006); Knight et al. (2010); Oke (1982).

There are significant challenges to measuring the real-time temperature distribution across a city, but the work of Knight et al. (2010) promoted a ‘citizen science’ project to collect temperature data across the city of Manchester. Data was obtained through the use of vehicle external thermometers, upon advisement from the European Automobile Manufacturers Association - which concluded that so long as the vehicle had been moving for a period of time to measure the air unaffected by engine heat. Participants were asked to submit their temperature readings and the postcode at which the measurements were taken. From these data, figure 1.2.1 was constructed. Additionally, individuals were asked to measure the temperature approximately 3m from buildings and 1m above the ground within a short time window, and submit this temperature reading, again with the postcode of the measurement site.

3Anthropogenic heat sources such as residents commuting and/or use central heating, are additional ground-level heat sources. Depending on the latitude of the urban environment in question this surface heating can vary in importance.
Figure 1.2.1: Manchester’s heat island. Colours indicate the difference from the mean temperature measured (shown yellow) Green colours indicate lower temperatures measured and the urban heat island is clearly visible in the red colours (indicating higher temperatures than the mean of measured temperatures). The data has been smoothed using linear Kriging interpolation. 

Taken from [Knight et al. (2010)].

This data revealed a greater than 6K difference in temperatures from the countryside to the city centre - red colours indicate higher than average temperatures, and green colours lower than average. Another study by [Smith et al. (2011)] also found this phenomenon in Manchester. This is, however, not a practical long-term monitoring method for urban temperature distributions due to the extended commitment needed to be made by the participants.

In the work of [Collier (2006)] a greater temperature difference (8°C between urban and rural regions) was found using satellite temperature measurements. This measurement was made using satellite data which are affected by a number of factors such as viewing angle and sampling techniques. These factors preclude an accurate measurement of the urban heat island magnitude, but do serve to indicate whether one exists.
The extension of the lifetime of the mixed layer allows pollutants/other aerosols emitted later in the day/night to be mixed thoroughly into the boundary layer, which can lead to wider dispersion of urban pollution into the surrounding rural regions, along the *urban plume*, the extension of the mixed layer downwind away from an urban environment (see figure 1.2.2). This plume is of the order of the city width (when viewed normal to the local wind direction) and can extend for over 100km (Collier, 2006).

Figure 1.2.2: Urban boundary layer structure. The extent of the urban plume is shown by the dashed lines. Swirling air motions are indicated by curved arrows. The dashed lines delineate two important heights when considering urban boundary layers; the blue line shows the height of the urban boundary layer, while the purple line shows the height of the urban canopy (defined by the height of buildings within the urban area).

Adapted from Markowski and Richardson (2010, p.104).

Any pollutants (or other materials/moisture) carried by the urban plume over rural regions will be mixed into the rural atmosphere when the following day’s convective motions extend sufficiently to ‘join up’ with the plume and mix the material down to lower levels, spreading urban pollutants into otherwise typically clean rural air.

In addition to this heat plume, the urban environment defines a canopy at the mean building height which defines the tops of *urban canyons* which direct any surface level winds along streets. Winds crossing buildings tend to produce local low pressure areas on the lee side of the building (Collier, 2006). The low pressure regions behind buildings (and other structures) draw air vertically down and cause swirling of air in their lee side and potentially trap pollutants, leading to concentrations greater than would be expected from the distance from the pollutant source (see the eddy motions in figure 1.2.2).
Because buildings present a significantly greater surface area to passing winds than flat land common to rural environments, winds passing through urban areas are typically 5-10 ms\(^{-1}\) slower than in rural areas upwind (Markowski and Richardson, 2010, p.105).

The urban heat plume may also be the cause of increased precipitation rates downwind of cities (Collier, 2006) - the increased concentration of pollutants and other cloud condensation nuclei are likely to be convected upwards in the urban plume and correspondingly form clouds some distance downwind of the urban environment (Markowski and Richardson, 2010, p.105).

Pal et al. (2012) found that the nocturnal boundary layer over a major city (Paris) is up to 19% higher than in surrounding rural areas (and as much as 600m higher) - corresponding to a temperature difference of between 2\(^\circ\)C and 4.5\(^\circ\)C between Paris and its surrounding rural areas. This difference in the boundary layer height and temperature was attributed to the urban heat island effect.

1.3 Does the boundary layer become stable over a city at night?

Boundary layers over cities have been observed previously (see, for example Barlow et al. (2011); Bohnenstengel et al. (2015); Kolev et al. (2000); Pal et al. (2012); Piringer et al. (2007)), with the effect of the urban heat island on the development of a stable boundary layer investigated in Pal et al. (2012); Piringer et al. (2007). The motivation for these studies was to identify whether stable layers can form over cities, potentially trapping pollutants near the surface (see, for example, Banta et al. (1998)) due to the uncoupling of winds aloft of the boundary layer from the urban fabric. This can lead to concentrations hazardous to health (or in violation of local clean-air laws).

Barlow et al. (2011) found that the convective boundary layer above London varies in height from a little under 1km to almost 1.5km. Further, overnight stable layers were observed, typically under 500m thick - defined by the height at which ground-emitted aerosols were observed. This is in agreement with the more recent Clean Air for London (ClearfLo) project, also assessing London boundary layer properties, which found that the winter mixing height varied between 400m (summer and winter nights) and 1100m (winter day) or 1800m (summer day) (Bohnenstengel et al., 2015).
In their work in Basel, Piringer et al. (2007) found that in less than 10% of observations, the nocturnal urban boundary layer became stably stratified, compared with similar experiments in rural areas which found stable boundary layers 60% of the time.

Whether the Manchester urban boundary layer becomes stable during the course of a night is one of the fundamental questions this study will aim to answer.

Measuring temperature profiles directly over a city is hampered by the difficulty in erecting structures such as towers due to planning and safety regulations. Launching radiosonde balloons brings its own challenges - if there are nearby airports, or the local authorities regularly fly helicopters (or similar) over the city then launching standard-sized weather balloons may be impossible due to local aviation regulations.

Remote sensing tools allow the monitoring of the atmosphere without the resource-heavy approach of in situ measurement approaches. Therefore, this work seeks to develop a rotational Raman LiDAR to measure the boundary layer temperature profile.

1.4 Thesis overview

This work will briefly discuss the different types of measurements which can be made using the LiDAR technique. Starting from the original concept and summarising the evolution of the measurement technique since its conception this discussion will include a discussion of the different properties which can be investigated using LiDAR instruments. Both elastic and inelastic scattering mechanisms are highlighted, before going onto discuss Raman scattering. The rotational Raman spectrum and its relationship with temperature will be discussed - highlighting that it is a suitable mechanism to determine atmospheric temperatures. The LiDAR equation will be discussed with regards to rotational Raman scattering, and previous works will be discussed relevant to this project.

Following the theoretical discussion, the Manchester Boundary Layer Temperature LiDAR will be introduced, with each component of the instrument identified. A LiDAR instrument was made available for this project which was originally designed for stratospheric work (Vaughan et al. 1993). Changes to the original instrument will be discussed (some components of the instrument were not redesigned due to cost and time constraints), and the calibration of the receiver optics outlined, as with the challenges faced by the calibration approach.
This instrument is intended to answer the following questions:

1. Can the LiDAR instrument be modified to use a low pulse energy, high repetition laser be used and identify the boundary layer capping inversion over an urban environment?

2. Can this instrument resolve the temperature profile of the boundary layer below this inversion and thus identify the development of residual/stable layers from the mixed layer?

3. Does the nocturnal boundary layer over Manchester become stably stratified during the course of a night?\footnote{Note that question 3 assumes that the question 2 is achieved.}

4. Is the nocturnal urban boundary layer properly resolved in forecast models?

An interference filter of the receiving optics was replaced during the course of this work, and a discussion of the work identifying the properties of a suitable replacement is presented. Following this the approach of converting atmospheric signals into a temperature is outlined, taking direction from previous works, and highlighting the shortcomings of our approach and the solution found to these shortcomings.

Analytical corrections to the collected data are discussed, addressing calibration constraints and the limitations of using the LiDAR configuration chosen for this instrument. Random and systematic errors are discussed, as well as a discussion regarding averaging, and how it affects both the uncertainty of the measurement and the representability of the data.

Data are presented for several nights under different synoptic conditions, as well as varying cloud-cover regimes. The ability of the instrument to identify the boundary layer capping temperature inversion is assessed, utilising locally-launched sondes to provide a measured temperature profile. A locally-run weather forecasting model is compared with the data collected to quantify how necessary this sort of instrument is in the context of supporting computer modelling of air quality for which good understanding of the boundary layer is essential.

Finally, the future of the instrument is discussed, from proposed upgrades to comparison with other models with differing boundary layer schemes outlined.
Chapter 2

Rotational Raman LiDAR

2.1 LiDAR theory

2.1.1 Introduction to LiDAR

Similar to atmospheric RADAR (radio detection and ranging), LiDAR is an acronym of the term “light detection and ranging”, and they both operate in essentially the same manner. Pulses of electromagnetic radiation are directed at a medium of interest and the scattered signals are gathered. The difference between RADARs and LiDARs is the wavelength of light used. RADARs use only radio waves - typically from 3-10GHz (Markowski and Richardson 2010, p. 369) - corresponding to wavelengths of 3 - 10mm - which limits the size of the particles it can detect to the mm scale.

LiDARs, on the other hand, operate at a number of different frequencies - most often in the infra-red, visible and ultraviolet regions of the electromagnetic spectrum (250nm to 11µm), corresponding to sub-micron wavelengths. This allows a rich world of sub-micron target investigation - from large aerosols down to gas molecules. As a result of this range of measurement scales LiDARs have become popular tools for a large range of investigations.

The concept of using visible light as a as an active remote sensing tool predates the laser (Hulburt 1937, Johnson et al. 1939) who used searchlights to illuminate the atmosphere at a 30° angle above the observation station several kilometers from the searchlights. Hulburt (1937) used a camera to capture the scattered light, with Johnson et al. (1939) using a photoelectric cell as their receiver.

The invention of the Q-switched laser allowed for a very bright and collimated light source to be used, starting with Piocco and Smullin (1963), who developed a system to
observe scattering from volcanic ash in the stratosphere using a ruby laser. Following this work, LiDAR techniques were developed rapidly, using a variety of different approaches to identifying atmospheric properties.

**Scattering Regimes**

Light returned from the atmosphere at the same wavelength as the emitted light has been *elastically* scattered - no energy has been passed between the photons and the scattering medium. If instead the returning light has a different wavelength the scattering is *inelastic*, which means energy has either been passed from the laser light to the scattering medium, or vice versa (see red arrows in figure 2.1.1). The exact difference between the emitted laser light wavelength and the collected wavelength(s) can be used to determine physical properties of the scattering medium.

![Figure 2.1.1: Energy levels of a medium scattering elastically and inelastically.](image)

Elastic scattering occurs when light interacts with matter, raising the matter to a virtual energy state \( V \) in figure 2.1.1. This energy state is described as ‘virtual’ energy state because it does not correspond to an electronic, vibrational, rotational (etc) energy state. The relaxing of the matter from this virtual energy state produces a photon of the same energy as the illuminating light and leaves the matter in the original energetic state. Fiocco and Smullin (1963) used the elastic scattering of laser light from atmospheric molecules in their investigation of scattering layers in the atmosphere.

Inelastic scattering occurs when there is an available energy state for the illuminated medium to be excited/relaxed into. The change in the energy state of the illuminated matter can be a change in any energy state (electronic, rotational, vibrational) of the atoms.
and molecules, and each carries its own distinct signature visible in the wavelength difference between the illuminating light and the scattered light. Some LiDAR experiments use this energy difference (and the intensity of the collected light at the shifted wavelengths) to investigate the medium of interest - see section 2.3.

2.2 LiDAR experiments

LiDAR uses a laser to illuminate the scattering medium of interest and collects the scattered light. Lasers used in LiDAR experiments range in wavelength range from infrared to ultraviolet - depending on the experiment. Most LiDARs use a pulsed laser which allows the signals from different heights to be separated by the collection electronics. The time taken for signals to return determine the height from which they have been scattered as per:

\[\text{Range} = \frac{\Delta t c}{2}\]  

(2.2.1)

Here \(t\) is the time elapsed since the laser pulse was emitted and \(c\) the speed of light - the factor of two is required to accommodate the full ‘round trip’ rather than the single trip distance to the scattering medium. The collection of the returning signals is achieved using a telescope which is directed at the laser beam.
LiDARs can be configured in one of two arrangements - with the optical axis of the telescope colocated with the laser emission path (*coaxial*) or with the laser offset by a small distance (*biaxial*).

Coaxial LiDARs carry the advantage that the laser is within the field of view of the telescope at all times - however either the laser itself or a directing mirror will block a portion of the telescope field of view, and the detectors can be overloaded from scattering at very low altitudes. While this saturation can be avoided by adjusting the focus of the telescope, it will not be examined because the LiDAR used in this work is arranged in biaxial configuration.

Biaxial LiDARs (see figure 2.2.1 for an example schematic) make the trade off that the telescope field of view is not obscured by the laser (or its directing mirror), but there will be a region where the laser beam is not entirely within the field of view of the telescope - see figure 2.2.2.
Figure 2.2.2: Biaxial LiDAR overlap schematic. The black trace shows the telescope field of view, the red trace shows the laser beam divergence.

In this example between the telescope (0 on the scale) and point A the telescope will not see direct backscattering from the laser. Between heights \( A \) and \( B \) there is only a partial overlap between the telescope field of view and the laser - above \( B \) the entirety of the laser beam is within the telescope field of view and all backscattering events will be visible to the telescope.

Following the collection by the telescope, many LiDARs separate the backscattered signals by wavelength or polarisation - in the case of figure 2.2.1 a beamsplitter is used which allows two channels to be illuminated. Spectrally selecting optical components may be used to select a narrow wavelength range (to reject background light or isolate a certain inelastic scattering band) or a polariser to select a certain polarisation of the backscattered light, or both. Following the filters are photodetectors - commonly photomultiplier tubes, and some form of sampling electronics.

Two basic types of electronics are used in LiDAR - analogue detection and photon-counting. In an analogue detector the current from the photomultiplier is digitised with a fast analogue-digital converter, while in a photon-counting detector individual pulses of electrons are counted, corresponding to individual photons reaching the photocathode.

The collection electronics of a LiDAR separate the signals from the photodetectors into discrete range bins - determined by the time taken for the signals to return as per the above relationship.

The advent of high speed electronics allowed the range bins of atmospheric LiDAR
experiments to be reduced in size from the initial range bins of Fiocco and Smullin (1963) - 10km - down to 3.75m in the case of Imaki et al. (2012).

It should be noted that while single lasing pulses can be very powerful there is a corresponding risk of using such lasers. The attraction of using strong pulses to deliver enough energy to the atmosphere is to provide a strong backscattered signal, but a trade off must be made between practical constraints (such as operational safety, cost and lifetime of the laser) and signal strength. By using rapidly pulsing lasers the individual pulse strength can be significantly reduced (vastly reducing the eye safety risks (see Appendix A) associated with using the laser) and the signals scattered from multiple lasing pulses can be combined to ameliorate the lower power of each pulse.

The tradeoff of using a lower power per pulse lasers is that the range over which the LiDAR instrument can operate is significantly reduced - as are the strength of the collected signals.

2.2.1 Nd:YAG lasers

A Neodymium:YAG (yttrium aluminium garnet) laser emits in the infrared region of the electromagnetic spectrum (1064nm). Lasing is achieved by pumping the medium into excited states which decay rapidly to the $^{4}F_{3/2}$ electron shell before the lasing transition is induced between this shell and the $^{4}I_{11/2}$. 
Figure 2.2.3: Energy states in Nd:YAG lasers. The lasing crystals are pumped from the initial energy state $^4I_{\frac{9}{2}}$ into pumping states which rapidly relax into the $^4F_{\frac{3}{2}}$ state before lasing at 1064nm (red line) to the $^4I_{\frac{11}{2}}$ state, before relaxing into the original state. Adapted from Silfvast (2003, p. 162) with permission from Cambridge University Press.

Nd:YAG lasers are often frequency-doubled (see below) and used in LiDAR experiments (see Behrendt and Reichardt (2000); Martinsson et al. (1996); Vaughan et al. (1993)) due to the high power available and efficiency of the receiver optic system over IR wavelengths (Radlach et al., 2008).

Di Girolamo et al. (2004) and Hua et al. (2005) investigated the use of a frequency-tripled (see below) Nd:YAG laser (355nm) with regards to temperature probing of the atmosphere, motivated by an improvement in daytime performance due to reduced background signals and, in part, eye safety - UV lasers represent a significantly smaller eye safety risk compared with visible-wavelength lasers. Further advantage of using a higher frequency is that the backscatter cross section (see section 2.5.1) depends on $\lambda^{-4}$ - increasing by a factor of 5 when moving to the third harmonic from the second.

### 2.2.2 Frequency multiplying

Lasers can be induced to lase at integer-divisions of their fundamental frequency. If one considers the induced polarisability of a material due to an imposed electric field (Measures, 1984, p. 16) to be:

$$P = P_1 E + P_2 E^2 + P_3 E^3 + \ldots$$

(2.2.2)
Where $P_x$ denotes the $x^{th}$ order of polarisability, it should be noted that $P_2, P_3 << P_1$ but at high field strengths (such as in a laser) the non-linear properties can become important.

With the electric field taking the usual form of $E(r, t) = E_0(r) \sin(\omega t)$ it can be shown that:

$$P = P_1 E \sin(\omega t) + \frac{1}{2} P_2 E^2 \left[1 - \cos(2\omega t)\right] + \frac{1}{4} P_3 E^3 \left[3 \sin(\omega t) - \sin(3\omega t)\right] + \ldots \ (2.2.3)$$

Examination of the sine arguments clearly shows the frequency-doubled and tripled terms. While there are higher order terms, because $P_1 >> P_2 > P_3 > \ldots$ they contribute very little to the total polarisability. Figure 2.2.4 shows the energy levels available in the non-linear crystal and how the frequency doubling and tripling occurs.

![Figure 2.2.4: Higher order generation schematic. The lower black line indicates the non-linear crystal ground state with other energy levels shown by the dashed lines. Transitions between the states is shown by the coloured arrows. Adapted from Silfvast (2003, p. 608) with permission from Cambridge University Press.](image)

In figure 2.2.4 the non-linear crystal (for example lithium triborate) is excited from the ground state (solid line) to a first virtual excited state ($V_1$) by a photon of the exciting laser frequency ($\omega_1$). From this state the crystal may relax to the ground state, emitting a photon of the same frequency as the exciting photon. Alternatively, if the photon flux is sufficiently high the crystal may be further excited by another photon of the exciting laser, exciting the crystal into the second virtual state ($V_2$) - as shown in case A. Decay
from this second virtual excited state produces a photon with twice the energy of the first and thus radiation with twice the frequency ($\omega_2 = 2\omega_1$).

Alternatively once the crystal has been excited into its second virtual excited state (again assuming a sufficiently high photon flux) another $\omega_1$ photon may excite the crystal into the third virtual excited state (example B) and subsequently relaxation into the ground state will emit a photon with $\omega_3$ with three times the energy and frequency of $\omega_1$.

Other excitations to $V_3$ are possible once radiation with $\omega_2$ has been produced, and those cases are shown in examples C and D in figure 2.2.4.

### 2.3 Atmospheric LiDAR applications

#### 2.3.1 Elastic LiDAR

The first LiDAR investigation used elastic scattering as the means to probe the upper atmosphere (Fiocco and Smullin, 1963) - and the principle has varied very little since this experiment. The improvement of high-speed electronics and increase in available laser power has allowed much smaller range bins compared to Fiocco and Smullin (1963) - finding use in ceilometers and cloud base height monitors. Improvements in spectral selective optical components results in narrower spectral ranges (and thus a weaker signal strength) can be separated from the received signals which, when coupled with the improvements in detectors has allowed these weaker signals to be detected, allowing these narrow spectral regions to be detected.

**Cloud measurements**

The strong backscatter from clouds not only allows LiDARs to monitor cloud base height, but also (provided the optical thickness of the cloud is not too great) cloud thickness, and identifying higher layers of cloud. Further to the location of cloud layers, returns from clouds can carry different polarisations to the outgoing laser light, which allows for determination of the cloud type.

**Polarisation LiDAR**

By considering the polarisation of the returning signals, compared to the laser polarisation, LiDARs can be used to investigate the shapes of the scattering particles. Spherical
particles do not change the polarisation relative to the incident light, but non-spherical scatterers do so (Sassen, 2005). Scattering from air molecules also introduces a small amount of depolarisation. The degree of depolarisation of the received signals with respect to the emitted laser light can be used to measure the depolarisation properties of the scattering particles (Behrendt, 2005; Sassen, 2005) and correspondingly compare the depolarisation ratio to laboratory measurements to identify the shape of the scattering species.

**Aerosol measurements**

By modelling the expected LiDAR return from a ‘clean’ atmosphere one can use the elastic return from the atmosphere to determine the presence of aerosols by considering the deviation from the ‘clean-air’ modelled return. See, for example Behrendt et al. (2004); Whiteman (2003a,b). More empirically, Raman scattering can be used to measure the ‘clean-air’ profile.

High spectral resolution LiDAR (HSRL) takes an elastic return and separates out the contributions from aerosol and molecular species. Light scattered from molecules is Doppler broadened by the root mean squared (RMS) velocity of the molecules (approximately 300 ms\(^{-1}\)) whereas the aerosols detected by the LiDAR are usually hundreds of nm in diameter so have much smaller thermal RMS (Eloranta, 2005). This leads to a difference in Doppler broadening of the elastic return, which allows the aerosol loading of the atmosphere to be determined.

**Stratospheric and mesospheric measurements**

Above 30km, in cloud-free skies, one can make the assumption that there are no (or infinitesimally small amounts of) aerosols so the expected LiDAR signal returns from this region will be a measure of atmospheric density. Correspondingly, one can use such measurements along with the Ideal Gas Law to determine the atmospheric temperature profile in the upper stratosphere and mesosphere (see Hauchecorne and Chanin (1980), for example). However, Neely III et al. (2011) identified dust arising from meteor ablation at approximately 35km which would affect such observations. By considering their data and the latitude of the experiment the effects of this dust can be taken into account.
Differential Absorption LiDAR

One can construct a LiDAR experiment utilising the wavelength variation of the absorption cross-section of a molecule of interest. Such LiDAR experiments require the use of two (or more) output laser wavelengths (either from multiple lasers, or lasers emitting at multiple different wavelengths), each tuned to a region of the absorption spectrum of the molecule of interest.

The lasers of a differential absorption LiDAR (DIAL) investigation are tuned such that one laser beam is strongly absorbed by the atmospheric species (for example, ozone), while the other laser beam is less strongly absorbed (Gimmestad, 2005). The absorption cross-section of the molecule of interest is known from laboratory experiments so the ratio between the returning signals can be used to determine the number density profile of the species under investigation (see, for example, Browell et al. (1981)).

Doppler LiDAR

Doppler LiDAR utilises the relative motion of the scattering medium to shift the wavelength of the scattered light - the amount of wavelength shift is used to determine the speed of the wind. Because the typical wind speeds in the atmosphere are not sufficient to change the wavelength of the scattered light by much, very high precision instruments must be used (Bissonnette, 2005).

2.4 Molecular energetic transitions

Atmospheric LiDAR experiments often investigate the distribution of molecular species, which have different regimes in which their energy can be distributed, most notably, electronic, vibrational and rotational energy. Transitions can occur between these states, individually (eg. between two vibrational energy states) as well as between multiple states (eg. between two rotational energy states and simultaneously between two vibrational energy states).

Electronic transitions

Electronic transitions occur when molecules (or atoms) receive (or give) enough energy from the illuminating photons to allow electrons to move between different energy levels. By tuning a laser to the electronic absorption line of a species of interest, for example
one of the D-lines (589.6nm) of sodium present in the mesosphere, the density profile of mesospheric sodium can be determined (Rosenburg et al., 1969). In this investigation the sodium ions were excited into the higher energy state before rapidly decaying into the original electronic energy state. This approach only allows investigation of the specific species (and specific electronic transition) to which the laser has been tuned, but the reaction cross section for the electronic excitation is much larger than other inelastic scattering cross sections (Rosenburg et al., 1969) enabling remote sensing of meteor debris such as sodium, iron and calcium.

Vibrational transitions

Molecules can also move between vibrational energy states - although at atmospheric temperatures nearly all molecules are in the ground vibrational state, so scattering of laser radiation can only induce a transfer to the first vibrationally excited state. This induces a wavelength shift which is characteristic for each molecule and by isolating the vibrationally-shifted returns the concentration of the corresponding scattering species may be determined (Behrendt et al., 2002) - see figure 2.4.1.

Rotational transitions

Unlike vibrational excitations, rotationally-excited molecules may be found at atmospheric temperatures. Scattering of a laser beam can excite transitions between these states, leading to inelastic scattering. The spectrum of the scattered light is temperature-sensitive (see equation 2.4.10), which provided the basis for temperature measurements using LiDAR.
Figure 2.4.1: Example Raman spectrum of 532nm light backscattered from the atmosphere. The Cabannes line showing the elastically scattered laser light is shown as well as the vibrational Raman spectral lines for a number of atmospheric components. The rotational Raman spectrum is shown by the ‘humped’ structures centred on the Cabannes and vibrational spectral lines.

After Behrend et al. (2002).

The vibrational transitions of molecular oxygen, carbon dioxide, molecular nitrogen and water vapour are clearly separated in the spectral of the scattered signals - the envelope surrounding each of the vibrational lines is the rotational spectrum.

2.4.1 Raman Spectroscopy

Discovered by Sir Chandrasakara Raman in 1928 (Raman, 1928), Raman transitions are those in which either the rotational or vibrational energy state (or both) of the scattering particle is changed, with the change being induced by light with wavelength smaller than the particle. The initial discovery of this scattering was in liquids, but subsequent work extended the observations to solids and gases as well (Menzies, 1930).

Figure 2.4.2 shows an example of energy levels available to a nitrogen molecule. The $v$ states (labelled on the right side of the diagram) indicate the vibrational energy states available. It can be clearly seen that the difference in vibrational energy levels (the spacing of the vibrational energy states compared with the spacing of the rotational energy states) is significantly greater than the difference between rotational energy states (labelled $J$), as suggested by the spectral line distribution in figure 2.4.1. The lower axis shows the frequency of the scattered light resulting from the Raman transitions.
Yellow transitions indicate Raman scattering in which the vibrational energy state does not change. The central line in the frequency plot is far larger than the other lines due to the dominance of elastic scattering over inelastic. The side lobes of the plot show transitions in which the rotational energy state of the nitrogen molecule has increased (left of the Rayleigh line) and decreased (right of the Rayleigh line). Green transitions indicate a Raman transition which increases the vibrational energy state, and the blue transitions are for a reduction in the vibrational energy state.

Note that the vibrational Raman transitions also contain side lobes in their spectra - these indicate that the rotational energy state has changed in addition to the change in the vibrational energy state.
Figure 2.4.2: Vibrational and rotational Raman energy states for molecular nitrogen. The Stokes branch of the Raman spectra are for transitions where the scattering molecule increases its energy state, with the anti-Stokes branch for where the molecule moves to a lower energy state following the scattering interaction.

Reproduced after figure 9.1 of Wandinger (2005b) with permission from Springer.

The letters Q, S and O in figure 2.4.2 refer to the Cabannes scattering lines, and the Stokes (following the scattering event the scattering molecule is in a higher energy state than prior to the scattering) and anti-Stokes (following the scattering event the scattering molecule is in a lower energy state) branches of the spectra, respectively. See table 2.4.1 and the surrounding discussion for further information.
2.4.2 Rotational Raman Spectroscopy

To properly consider rotational Raman spectroscopy the quantum mechanics of a transition must be explored:

\[
[P]_{nm} = \int \Psi_n^* P \Psi_m d\tau
\]  
(2.4.1)

where \(\Psi_n\) and \(\Psi_m\) are the wavefunctions of two states, transition between which is determined by the transition matrix \(P\). The square of the matrix element \([P]_{nm}\) determines the transition probability, and thus the intensity of any emission lines this transition may produce.

Rotational Raman transition rules

For homonuclear diatomic molecules (which is a good assumption of the state of the atmosphere\(^1\)) the following rotational Raman transition rules apply:

In nuclei such as those of oxygen or nitrogen the wave equation of the molecule does not change. Similarly the total eigenfunction either does not change, or only changes its sign (Herzberg and Spinks, 1951, p.130). Additionally, the assumption can be made that atmospheric molecules will be in their electronic ground state (at least at the altitude of interest for boundary layer investigations).

Reproducing the argument from Herzberg and Spinks (1951, p.131) and Hollas (2004, p.129-130), adjacent rotational energy states for diatomic homonuclei have symmetry described in figure 2.4.3.

---

\(^1\)Rotational symmetry is mainly a feature of diatomic molecules which represent the Earth’s atmosphere (which is composed of approximately 98% diatomic molecules in the form of nitrogen and oxygen (Behrendt, 2005, p.283)) so this simplification is appropriate in the case of atmospheric investigations, which commonly utilise Raman scattering.
Here the rotational states for case (a) are those in which the eigenfunction does not change when the atomic nuclei are exchanged (denoted a symmetric state). Conversely (b) shows the case of the eigenfunction reversing its sign following the exchanging of the nuclei positions (antisymmetric).

Rotational Raman transitions are forbidden if the molecule moves from a symmetric (labelled s in figure 2.4.3) to antisymmetric energy state (labelled a) - thus the selection rule for rotational Raman transition rule can be summarised as:

\[ \Delta J = 0, \pm 2 \]  \hspace{1cm} (2.4.2)

**Polarisability tensors and Raman transitions**

For the cases of electromagnetically-induced transitions we must consider the polarisability of a molecule and in particular the shape of the polarisability tensor, \( \alpha \).

If the molecule is rotating (often the case for atmospheric temperatures) with a rotational frequency \( \nu_{\text{rot}} \) then the polarisability of the molecule can be represented as a mean value \( \alpha_{o,r} \), with a first-order perturbation \( \alpha_{1,r} \) resulting from the rotation added (Hol-\[ las] 2004 p. 84):

\[ \alpha_{\text{rot}} = \alpha_{o,r} + \alpha_{1,r} \sin \left( 2\pi c \left| 2\nu_{\text{rot}} \right| t \right) \]  \hspace{1cm} (2.4.3)
By considering an electric field illuminating a molecule, an electric dipole can be induced, as described by:

$$\mu_{\text{rot}} = \alpha_{\text{rot}} E$$

where $E$ takes the form $A \sin (2\pi c \tilde{\nu} t)$.

It can therefore be seen that the resultant electric dipole induced in a rotating molecule illuminated by a laser is given by [Herzberg and Spinks (1951), p.84]:

$$\mu_{\text{rot}} = A_0 \alpha_0, r \sin (2\pi c t \tilde{\nu}) + \frac{1}{2} A_1, r \cos (2\pi c t [\tilde{\nu} - 2\tilde{\nu}_{\text{rot}}]) - \frac{1}{2} A_1, r \cos (2\pi c t [\tilde{\nu} + 2\tilde{\nu}_{\text{rot}}])$$

(2.4.4)

The first term of equation 2.4.4 describes the Cabannes scattering - scattering at the illuminating frequency. The second and third terms refer to scattering at lower and higher frequency than the illuminating light, producing the spectrum seen in figure 2.4.4. The second term of equation 2.4.4 corresponds to the O-branch region of the spectrum of figure 2.4.4, while the third term corresponds to the S-branch of the spectrum.

![Rotational Raman spectrum of oxygen acquired using 514.5nm laser.](image)

Figure 2.4.4: Rotational Raman spectrum of oxygen acquired using 514.5nm laser.

Adapted from Compaan et al. (1994).

Reproduced with the permission of the American Association of Physics Teachers.

This is known as either Stokes or anti-Stokes scattering depending on whether the photon has transferred energy to- or taken energy from the atom/molecule from which it was scattered. The Stokes and anti-Stokes branches are not symmetric, and the brightness of the spectral lines are described by equation 2.4.10.
Figure 2.4.4 shows a measured Rayleigh spectrum of a diatomic atmospheric component illuminated by a laser (see the central feature). There is an extremely large peak (passes beyond the limits of the intensity scale) located at a frequency shift of 0 cm\(^{-1}\). This is the *Cabannes line* as discussed above and represents purely elastic scattering from the atmospheric component. To the positive and negative sides of the Cabannes line are the Rotational Raman spectrum; the *Stokes* lines located to the negative (because energy is lost to the scattering body) and the *anti-Stokes* lines located to the positive (energy is gained from the scattering body).

The different branches of the rotational Raman spectrum are referred to as S- Q or O-branches - see figure 2.4.2. Table 2.4.1 summarises the nomenclature below:

<table>
<thead>
<tr>
<th>Change in rotational quantum number</th>
<th>Scattering body energy change</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\Delta J = +2)</td>
<td>Stokes branch S-branch Scattering body gains energy</td>
</tr>
<tr>
<td>(\Delta J = 0)</td>
<td>Rayleigh line Q-branch No energy change</td>
</tr>
<tr>
<td>(\Delta J = -2)</td>
<td>anti-Stokes branch O-branch Scattering body loses energy</td>
</tr>
</tbody>
</table>

Table 2.4.1: Nomenclature relevant to the rotational Raman spectrum.

Reproduced from *(Measures, 1984, p.106)*.

**Raman Scattering Energies**

Because quantum mechanics determines the energy levels of matter one must consider the allowable states. It should be noted that because of their dominance of the Earth’s atmosphere (98% of the atmosphere *(Behrendt, 2005, p.283)*) investigated by this work this discussion focuses on the diatomic molecules of oxygen (O\(_2\)) and nitrogen (N\(_2\)) and the following discussion is based on the quantum mechanics of these molecules.

The transitions in molecular energy levels allowed for Raman scattering:

\[
\Delta J = 0, \pm 2
\]

\[
\Delta \nu = 0, \pm 1
\]

Note that here the transition selection rules have 0 as an option. This is to allow for purely rotational or vibrational transitions.
Figure 2.4.5: Rotational Raman energy level transitions. Net change in energy state of
the scattering body shown in red.

Figure 2.4.5 shows on the left edge a transition in which the molecule is excited to a
virtual energy state and returns to a state of higher rotational quantum number (J=0 →
J=2). By considering the rotational energy states of a rigid rotator (one that does not
longitudinally deform under rotational motion) it can be shown that the energy \( E_r \) of a
rotational energy level is given by \cite{Hollas2004} p.105 as:

\[
E_r = \frac{\hbar^2}{8\pi^2 I} J(J + 1)
\]  

(2.4.5)

where \( \hbar \) is Boltzmann’s constant, \( J \) is the rotational energy state of the molecule and
\( I \) is the moment of inertia of the molecule.

In the case of the rotational quantum number changing by \( \pm 2 \) the molecule expe-
riences a change in energy, which is caused by the Raman interaction with an incident
photon. By introducing the rotational constant \( B \) the equation 2.4.5 is simplified:

\[
E_r = BJ(J + 1)
\]  

(2.4.6)

Conventionally the upper rotational state is referred to as \( \Psi_{J+2} \), with the lower state
\( \Psi_J \). From this it is clear that a Raman transition \( \Psi_{J+2} \rightarrow \Psi_J \) produces an energy change of:

\[
\Delta E_r = E_{r1} - E_{r2} = 2B(2J + 3)
\]  

(2.4.7)
Clearly a rotational Raman interaction in which the rotational state of the molecule does not change does not correspond to a change in energy, so there is no change in wavelength of the interacting photon.

**Centrifugal Correction**  The rigid rotor approximation provides an acceptable approximation for low rotational quantum numbers (small rotational speeds) but one must consider the *axial deformation* of molecules to fully comprehend any rotational Raman spectrum. To account for the molecular deformation under rotation correction must be made (Hollas 2004, p. 111):

\[ F(J) = BJ(J + 1) - DJ^2(J + 1)^2 \]  

(2.4.8)

Where \( D \) is known as the *centrifugal distortion constant*.

With this factor included the change in rotational energy of a molecule following a Raman interaction will be:

\[ \Delta E_r = 2B(2J - 3D)\left(J + \frac{3}{2}\right) - 8D\left(J + \frac{3}{2}\right)^3 \]  

(2.4.9)

This energy difference will be reflected in the energy of the scattered photon, as a frequency shift away from the illuminating frequency.

**B and D values**

Several studies have been carried out to quantify the rotational constants of diatomic molecules. Being the two most abundant atmospheric components we have included some values for Nitrogen and Oxygen (\(^{16}\)O\(_2\) and \(^{14}\)N\(_2\)) as shown in table 2.4.2.
**Rotational Raman Spectral Intensity**

From the values of B and D tabulated above the theoretical frequency shifts for nitrogen and oxygen from equation can be calculated using 2.4.9 remembering that to change from an energy shift to a frequency one must divide by Planck’s constant, \( h \).

Knowing the energy and frequency shift due to rotational Raman scattering is of use, but additionally knowing the spectral intensity allows investigations to spectrally tune their receiving optics to the most intense return. The spectral intensity of the returned signal is governed by Penney and Peters (1974):

\[
P_J = \frac{3(J + 1)(J + 2)}{2(2J + 1)} \frac{2hcB}{(2I + 1)^2k_BT} \omega_J^2 \gamma^2 g_J \exp \left[ -\frac{hcB}{k_BT} J(J + 1) \right] \quad (2.4.10)
\]

where \( B \) is the rotational constant for the scattering molecule, \( \omega_J \) the Raman-shifted wave number of line \( J \) and \( I \) the nuclear spin quantum number (0 for molecular oxygen and 1 for molecular nitrogen). Note the Maxwell Boltzmann distribution containing the temperature sensitivity. \( \gamma \) is the anisotropy of the molecular polarisability tensor of the molecule in question, and \( g_J \) the statistical weight factor (Vaughan et al., 1993):

---

<table>
<thead>
<tr>
<th>Study reference</th>
<th>Oxygen B (cm(^{-1}))</th>
<th>Oxygen D (10(^{-6})cm(^{-1}))</th>
<th>Nitrogen B (cm(^{-1}))</th>
<th>Nitrogen D (10(^{-6})cm(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Edwards et al. (1976)</td>
<td>1.437685 ± 4.61 ± 0.09</td>
<td>0.00005</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fletcher and Rayside (1974)</td>
<td>1.4376478 ± 4.806 ± 0.225</td>
<td>0.001765</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Babcock and Herzberg (1948)</td>
<td>1.43777 ± 4.91 ± 0.02</td>
<td>0.000015</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mcknight and Gordy (1968)</td>
<td>1.43688 ± as Babcock and Herzberg (1948)</td>
<td>0.000007</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Butcher et al. (1971)</td>
<td>1.437682 ± 4.85 ± 0.01</td>
<td>1.98950 ± 5.48 ± 0.05</td>
<td>0.000009</td>
<td></td>
</tr>
<tr>
<td>Stotcheff (1954)</td>
<td></td>
<td>1.9898 ± 6.1 ± 0.5</td>
<td>0.0003</td>
<td></td>
</tr>
<tr>
<td>Bendtsen (1974)</td>
<td>1.989574 ± 5.76 ± 0.03</td>
<td>0000012</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Butcher and Jones (1974)</td>
<td>1.923604 ± 5.29 ± 0.3</td>
<td></td>
<td>0.000020</td>
<td></td>
</tr>
</tbody>
</table>

Table 2.4.2: Rotational constants for \(^{16}\)O\(_2\) and \(^{14}\)N\(_2\).
The statistical weight factor is a measure of how many available nuclear spin states exist for the molecules in question. Molecular nitrogen carries a nuclear spin quantum number of \( I = 1 \), while for molecular oxygen \( I = 0 \) (Hollas, 2004, p.129-131). Correspondingly nitrogen can carry both odd- or even-\( J \) wavefunctions, with twice as many available wavefunctions with even \( J \). Oxygen cannot exist in even \( J \) states, and there are only one third as many available energy states for odd-\( J \) states. Greater detail of determining the statistical weight factor is given in Hollas (2004, p.129-131).

Behrendt (2005, p.285) quotes the values for the anisotropy of the polarisability tensor (\( \gamma \)) for molecular oxygen and nitrogen from Buldakov (1979):

\[
\gamma = \begin{cases} 
\pm 0.51 \times 10^{-48} \pm 0.016 \times 10^{-48} \text{cm} & \text{for Nitrogen} \\
\pm 1.27 \times 10^{-48} \pm 0.06 \times 10^{-48} \text{cm} & \text{for Oxygen}
\end{cases}
\]

Note that these values for the anisotropy of the polarisability tensor were measured at a wavelength of 488nm.

From equations 2.4.9 and 2.4.10 and the values given above, the theoretical rotational Raman spectra for nitrogen and oxygen at different temperatures, illuminated by a laser of wavelength 354.7nm were calculated:
Figure 2.4.6: Rotational Raman spectrum of $O_2$ and $N_2$ at different temperatures excited by a frequency-tripled Nd:YAG laser (355nm). The 1000K spectra is presented to highlight the temperature variation of the spectral line brightness.

Note that the spectrum for oxygen has fewer peaks than that of nitrogen, and a reduced intensity. The intensity variation is due to the fact that these spectra have been calculated accounting for the atmospheric abundance of each molecule (and weights the scattered power accordingly. There are fewer scattered frequencies because the $g_J$ values for nitrogen are non-zero for any value of $J$, but for oxygen this is only the case for odd $J$ values. Further, the temperature sensitivity of the rotational Raman spectrum indicated in equation 2.4.10 is shown by the changing lengths of the spectral lines - (the ‘peak’ of the line spectrum moves to wavelengths further from the laser line at higher temperatures).

2.4.3 Raman backscattering cross sections

The differential backscattering cross sections for single lines in each Raman branch are presented below (Behrendt, 2005, 284).

$$
\left( \frac{d\sigma}{d\Omega} \right)_{RR,i}^{\pi}(J) = \frac{112\pi^4}{15} \frac{g_i(J)hcB_{0,i}(v_0 + \Delta v_i(J))^{4}\gamma_i^2}{(2I_i + 1)^2kT} \times \frac{X(J)}{\exp\left(-\frac{E_{rot,i}(J)}{kT}\right)}
$$

(2.4.11)

with

$$\gamma = \begin{cases} 
X(J) = \frac{(J+1)(J+2)}{2J+3} 
& \text{for Stokes (J=0,1,2...)} \\
X(J) = \frac{J(J-1)}{2J-1} 
& \text{for anti-Stokes (J=2,3,4...)} 
\end{cases}$$
Subscripts denote the $i^{th}$ scattering species. $\nu$ denotes the vibrational energy state.

Here it is very clear that there is a temperature dependence of the backscatter cross section for rotational Raman scattering - see the denominator and the exponential argument.

## 2.5 LiDAR equation

At the heart of all LiDAR investigations is the LiDAR equation. It governs the theoretical return from a scattering medium. It accounts for the laser system’s parameters, the optical system’s capabilities (the collective optical characteristics of any mirrors, lenses, beam splitters, etc), atmospheric effects on the transmitted (and scattered) signal and the actual laser:matter interactions.

The exact form of the LiDAR equation depends on the particular investigation to be carried out, the scattering form being of most use for this discussion. The elastic scattering form of the LiDAR equation is quoted in Measures (1984, p.243) as:

$$P(\lambda_L, h) = P_0(\lambda_L) \frac{A_0}{h^2} c \tau E \Xi(h) \xi(\lambda) \beta(\lambda_L, h) \exp \left[ -2 \int_0^h \kappa(\lambda_L, r') dr' \right]$$

(2.5.1)

$P(\lambda_L, h)$ is the power of the signal scattered from an atmospheric component at range $h$ illuminated by a laser (lasing at wavelength $\lambda_L$).

$P_0(\lambda_L)$ represents the power of the emitting laser, which is defined by the energy output of a laser pulse $E_L$ and the pulse length $\tau_L$:

$$P_0(\lambda_L) = \frac{E_0(\lambda_L)}{\tau_L}$$

The term $\frac{A_0}{h^2}$ represents the acceptance angle of the receiver optics (as adjusted for the sphere over which radiation is scattered from a scattering centre a distance $h$ from the receiver optics).

$\Xi(h)$ describes the probability of the radiation scattered from range $h$ reaching the detector and is often referred to as the geometrical form factor (see Halldorsson and Langer-holc (1978) for an in-depth discussion of the geometrical form factor).

$\tau_E$ is the time interval of the collection electronics which determines the width of the range bin. By multiplying this factor by $c$ the time step is converted into the spatial range. The factor of 2 is required to accommodate the two way path of the light. From this...
expression it can be seen that the range resolution of a LiDAR with $\tau_E$ of 100ns duration is approximately 15m (Wandinger [2005a]).

$\xi(\lambda)$ describes the spectral transmission of the receiving optics, and is contributed to by any spectrally selective components - monochromators or interference filters, for example.

The exponential factor accounts for the extinction of the signals as they pass through the atmosphere (through other scattering events or absorption). $\kappa(\lambda, r')$ is known as the atmospheric extinction coefficient for light of wavelength $\lambda$, and must be integrated over the entire path of the laser and return signal. This is discussed in section 2.5.2.

$\beta(\lambda, h)$ is the volume backscattering term at a range $h$ and position $r$ and is discussed in section 2.5.1.

2.5.1 Scattering from molecules and particles

Because the motivation of this work is to investigate the boundary layer temperature profile, backscatter discussion will be limited here to that from molecules and aerosols present within the atmosphere.

The change in direction experienced by scattered light is not limited to any particular plane - scattering can redirect light into any direction. It is for this reason that we must consider spherical coordinates. Figure 2.5.1 shows an example of an incident photon following vector $k_i$ (defining the $z$ axis) scattering and being diverted along vector $k_s$ at an angle $\theta$ from the $z$ axis and $\phi$ above the $yz$ plane:

---

2The aerosol contribution is only important when considering elastic scattering because any wavelength shift due to aerosol elastic scattering typically shifts light further than rotational Raman shifts from molecules.
Figure 2.5.1: Scattering in spherical coordinates. The pre-scattering vector is shown in orange, with the scattered vector shown in green.

With the appropriate coordinate system established, scattering processes in general can be considered.

Rayleigh scattering is scattering of light when the wavelength is much greater than the size of the scattering body. A convenient parameter to introduce here is the size parameter for scattering (Measures, 1984, p.48) linking the wavelength of the illuminating light and the characteristic size of the particle ($a$):

$$\alpha = ka = \frac{2\pi a}{\lambda}$$ (2.5.2)

For atmospheric components which are of interest to this study (molecular nitrogen and oxygen) $\alpha < 0.5$ and therefore we can use Rayleigh scattering.

Measures (1984, p.48) derives the differential elastic scattering cross section for air to be:

$$\frac{d\sigma(\theta, \phi)}{d\Omega} = a^2 \left(\frac{2\pi a}{\lambda}\right)^4 \left\{\frac{n^2 - 1}{n^2 + 2}\right\}^2 \left[\cos^2 \phi \cos^2 \theta + \sin^2 \phi\right]$$ (2.5.3)

Here $n$ is the refractive index of air and $\lambda$ the wavelength of the illuminating light.

By setting $\theta = \pi$ and $\phi = 0$ (see figure 2.5.1) we see that this corresponds to an elastic backscattering event with differential cross section.

$$\frac{d\sigma(\theta, \phi)}{d\Omega} = a^2 \left(\frac{2\pi a}{\lambda}\right)^4 \left\{\frac{n^2 - 1}{n^2 + 2}\right\}^2$$ (2.5.4)

We can consider the volume backscattering from a particular atmospheric species $i$ to
be determined by the number density of that species $N_i(h, r)$, multiplied by the differential backscattering cross section $\beta_i$ (Measures 1984, p.239):

$$\beta(\lambda, h, r) = \sum_i N_i(h, r) \left\{ \frac{d\sigma(\lambda)}{d\Omega} \right\}^{\text{backscatter}}_i$$

(2.5.5)

$N$ is the scattering species number density at range $h$ and position $r$. $\left\{ \frac{d\sigma(\lambda)}{d\Omega} \right\}^{\text{backscatter}}_i$ is the differential scattering cross section. The summation indicates there are multiple species $i$ which contribute to the scattering.

**Mie scattering**

Elastic scattering from particles of similar wavelength to the illuminating light is called Mie scattering. In the case of using ultraviolet lasers (for example, frequency-tripled Nd:YAG lasers, which many LiDARs use - see table 3.6.1) Mie scattering is from atmospheric aerosols which are of comparable size to the illuminating radiation. This is different from elastic scattering from gas molecules in which there is an energy level change within the scattering molecule (see figure 2.1.1).

In more practical terms it can be assumed that the contribution to LiDAR-collected elastic signals from Rayleigh scattering will be constant from one experiment to another, but the contribution from Mie scattering will vary due to varying atmospheric aerosol loading which typically varies from day-to-day (especially within urban environments).

**2.5.2 Atmospheric Extinction**

Extinction is the reduction of light intensity as it passes through a medium. In the case of the planetary atmosphere this can be caused by scattering from molecules (Rayleigh scattering - which provides the blue colour of the sky), aerosols (Rayleigh or Mie scattering, depending on the size parameter of the scattering aerosol) or absorption of the light (by smog-like events, for example). The exact cause of the extinction is not important for consideration in the LiDAR equation - the extinction reduces the intensity of the collected light.

The form that the atmospheric extinction factor takes in the LiDAR equation is taken from the Lambert-Beer-Bouguer law (Wandinger 2005a, p.10), and for elastic scattering takes the form:
\[ \kappa(\lambda, h, r) = \sum_i N_i(h, r) \left\{ \frac{d\sigma(\lambda)}{d\Omega} \right\}_i^{\text{ext}} + \sum_j N_j(h, r) \left\{ \frac{d\sigma(\lambda)}{d\Omega} \right\}_j^{\text{ext}} \] (2.5.6)

Similarly to the backscatter discussion, the amount of extinction from each species (the \(i^{\text{th}}\) atmospheric molecular species, and \(j^{\text{th}}\) aerosol species) is the product of the number density of the species and its extinction cross section.

The contribution to extinction from atmospheric molecules and aerosols must be accounted for separately; the molecular contribution can be assumed to be approximately constant from measurement to measurement, but the aerosol loading of the atmosphere will vary, so the aerosol term varies.

The factor of 2 in the exponent argument in equation (2.5.1) is to account for the round trip. For inelastic scattering there will be a different wavelength after the scattering event \((\lambda)\) so the integral accounts for the extinction of the laser light before the scattering, and then the different wavelength light which is scattered (for example equation (2.6.2)).

### 2.6 Applications of the LiDAR equation

Ansmann et al. (1992) uses backscatter and atmospheric extinction coefficients which consider the contributions due to aerosol and molecules separately. For elastic scattering:

\[ P(\lambda_L, h) = P_0(\lambda_L) \int_{\Delta\lambda_X} \xi(\lambda') \frac{d\sigma_X(\lambda', \pi, T)}{d\Omega} \times \frac{O(h)A}{h^2} \left[ \beta_{\text{aer}}(\lambda_L, h) + \beta_{\text{mol}}(\lambda_L, h) \right] \exp \left[ -2 \int_0^h \kappa_{\text{mol}}(\lambda_L, \lambda') + \kappa_{\text{aer}}(\lambda_L, \lambda') d\lambda' \right] \] (2.6.1)

where \(O(h)\) is the overlap function, and for inelastic scattering. Here the integral is taken over the passband of the collection optics (\(\Delta\lambda_X\)) of the LiDAR system, to allow for signal broadening. \(A\) denotes the area of the collection telescope. For elastic scattering:

\[ P_{\lambda_R}(h) = P_0(\lambda_L) \int_{\Delta\lambda_X} \xi(\lambda') \frac{d\sigma_X(\lambda', \pi, T)}{d\Omega} \frac{O(h)A}{h^2} N_R(h) \times \frac{d\sigma_{\lambda_R}(\pi)}{d\Omega} \exp \left[ -\int_0^h \kappa_{\text{mol}}(\lambda_0, \lambda') + \kappa_{\text{aer}}(\lambda_0, \lambda') + \kappa_{\text{mol}}(\lambda_R, \lambda') + \kappa_{\text{aer}}(\lambda_R, \lambda') d\lambda' \right] \] (2.6.2)
where $\lambda_R$ is the Raman-shifted wavelength and $\frac{d\sigma_X(\lambda', \pi, T)}{d\Omega}$ is the Raman backscattering cross-section.

Whiteman (2003a) defines the LiDAR equation as follows:

$$P(h) = P_0(\lambda_L) \frac{O_X(h) A}{h^2} \int_{\Delta \lambda_X} \xi(\lambda') \frac{d\sigma_X(\lambda', \pi, T)}{d\Omega} d\lambda' \exp \left[ - \int_0^h \kappa(\lambda_L, h') + \kappa(\lambda_X, h') dh' \right]$$

(2.6.3)

Note that aerosol backscattering is not considered in equation 2.6.3. Whiteman (2003a) then extends the extinction coefficient by introducing the following:

$$\kappa(\lambda_X, h) = \kappa^{aer} + \left( \sum_i N_i(h) [\sigma_i(\lambda_X) + \eta_i(\lambda_X)] \right)$$

(2.6.4)

Here $\kappa^{aer}$ describes the signal extinction due to atmospheric aerosols (due to both absorption and scattering). The molecular number density of the $i$th scattering species is multiplied by the total scattering cross section $\sigma_i$ and the absorption cross section $\eta_i$ of that species. Note that in this term the total scattering cross section is used rather than the differential backscattering cross section.

The molecular constants $\sigma$ and $\eta$ in equation 2.6.4 can be measured under laboratory conditions, but the aerosol extinction depends on the particle size spectrum, refractive index and shape, and must be derived from the LiDAR profiles themselves.

Drawing together equations 2.5.1, 2.6.1, 2.6.2 and 2.6.3 yields for the total collected signal for a Raman channel ($P(\lambda_L, \Delta \lambda_R, h)$):

$$P(\lambda_L, \Delta \lambda_R, h) = P_0(\lambda_L) \frac{A_0 P_{CE}}{2} \Xi(h) \left( \left\{ \beta^{ae}(\lambda_L, h) + \beta^{mol}(\lambda_L, h) \right\} \xi(\lambda) \exp \left[ - 2 \int_0^h \kappa(\lambda_L, \lambda') d\lambda' \right] \right.$$

$$+ \sum_i \left\{ N_i(h) \left[ \int_{\Delta \lambda_R} \xi(\lambda') d\lambda' \right] \right\} \exp \left[ - \int_0^h \left( \kappa(\lambda_L, \lambda') + \kappa(\lambda, \lambda') \right) d\lambda' \right] \right)$$

(2.6.5)

The first term within the parentheses represents elastic scattering, both from aerosols within the atmosphere (Mie scattering) and from molecular scattering.
\( \beta_{\text{aer}} \) describes the aerosol volume backscatter coefficient for an illuminating wavelength of \( \lambda_L \), at range \( h \), likewise \( \beta_{\text{mol}} \) is the molecular backscatter of the illuminating light.

The second term (from Whiteman (2003a)) of the parentheses represents inelastic (Raman) scattering (hence the two atmospheric extinction coefficients within the exponential term. \( N_i(h) \) is the number density of the \( i^{\text{th}} \) elastic scattering species, at range \( h \) from the receiver optics.

\[
\frac{d\sigma_i(\lambda', \pi, T(h))}{d\Omega} \text{ is the differential scattering cross-sectional area of the } i^{\text{th}} \text{ scattering species at temperature } T \text{ (which itself is a function of altitude and thus linked to the range from the receiver optics the scattering molecule is located). } \xi(\lambda') \text{ is the transmission of the returned signal (wavelength } \lambda' \text{) through the receiver optics (which accounts for spectrally selective optical elements which attenuate the signal by only selectively transmitting specific wavelengths of returned signal).}
\]

This term is of paramount importance to determining atmospheric temperatures because it carries the temperature dependence of the LiDAR equation.

The factors \( \frac{d\sigma_i(\lambda', \pi, T(h))}{d\Omega} \) and \( \xi(\lambda') \) are necessarily integrated over the width of the passband of the receiver optics. These properties must be summed over the full range of the optical system passband (\( \Delta \lambda \)) because different atmospheric species can scatter light within the passband range and must be accounted for separately in the analysis.

### 2.7 Rotational Raman LiDAR equation

By assuming that one can remove extraneous signals through the use of spectrally-selective components the elastic portion of the LiDAR equation (2.6.5) can be removed:

\[
P(\lambda_L, \Delta \lambda_R, h) = P_0(\lambda_L) \frac{A_0}{h^2} \frac{c\tau_E}{2} \Xi(h) \\
\times \exp \left[ - \int_0^h \left( \kappa(\lambda_L, r') + \kappa(\lambda, r') \right) dr' \int \Delta \lambda_R \frac{d\sigma_i(\lambda', \pi, T(h))}{d\Omega} \xi(\lambda') d\lambda' \right] \right) 
\]  

(2.7.1)
The temperature sensitivity of this form of the LiDAR equation is carried by the backscattering cross section shown in equation [2.7.1]. Thus, it is possible to use the rotational Raman scattering from air molecules to determine the temperature of the atmosphere. LiDARs utilising this temperature sensitivity are discussed in chapter 3.

2.8 Error analysis

2.8.1 Random errors

The number of photons counted by the detection optics for any given measurement is characterised by a random error scattered around the ‘true’ value. This error is governed by Poisson statistics, where the error in a count of value $N$ is given by $\sqrt{N}$.

This Poisson error is propagated through the data processing using standard error propagation, using for addition and subtraction relationships:

$$ R = X + Y 
\delta R = \sqrt{[(\delta X)^2 + (\delta Y)^2]} $$

and for products:

$$ S = \frac{A}{B} 
\delta S = \sqrt{\left[\left(\frac{\delta A}{A}\right)^2 + \left(\frac{\delta B}{B}\right)^2\right]} $$

The additive error propagation is used for propagating the uncertainty in each of the BLT channels when making background corrections to the raw data. Additionally, in the case of the Far-field channel - see section 4.3.3 - this correction is used when taking account of any elastic breakthrough into the measured Far-field channel measurements - see section 8.2. The product relationship is used when calculating the ratio between the Near- and Far-field channels used for determining the atmospheric temperature (see Chapters 5 and 7).

This error analysis will be used in the consideration of the random errors for the instrument - see section 8.6. Leblanc et al. (2016) identify the “law of propagation of uncertainty”, which combines the above uncertainty propagation. This concept is carried
Having discussed the rotational Raman technique in this chapter, the following chapter will investigate how previous works have utilised this approach. Starting from the genesis of this concept and advancing through to modern applications in urban environments this chapter outlines the capabilities of rotational Raman LiDARs, as well as drawing a conclusion for some properties of the Manchester Boundary Layer Temperature LiDAR will need.
Chapter 3

Temperature Investigations using Rotational Raman LiDAR

3.1 LiDAR temperature measurements

By assuming that the signals scattered from atmospheric molecules is proportional to molecular density, and using the Ideal Gas Law and hydrostatic equilibrium, a temperature profile can be derived from the scattered intensity profile. Hauchecorne and Chanin (1980) investigated the atmosphere from 35 to 70km with a resolution of 1.2km (gathered over 4-7 hours) by such an approach (the lower limit of their investigation was due to the height to which aerosol scattering affected the returning signals).

Later works improved the resolution and pairing with other scattering regimes allowed for lower-altitude measurements (for example, Keckhut et al. (1990) improved the resolution to 300m for a measurement time of 2-12 hours), still making the assumptions of Ideal Gas Law and hydrostatic equilibrium. However, this method can only be used in regions of the atmosphere where aerosol backscatter is negligible. In the troposphere, and in the boundary layer in particular that is not the case, and a different approach to measuring temperature is needed.

3.2 Rotational Raman LiDAR Atmospheric Temperature measurements

The original proposal to use rotational Raman spectra to measure atmospheric temperatures was made by Cooney (1972). A (giant pulse) ruby laser was used (described
in greater depth in Cooney (1968) - emitting 20 Joules per pulse at a wavelength of 694.3nm. This experiment used the molecular nitrogen and oxygen spectra to directly measure regions of the rotational Raman spectrum (see figure 3.2.1) with opposing temperature dependence using interference filters.

This measurement approach provides a greater sensitivity to the atmospheric temperature than using the overall shape of the rotational Raman spectral envelope, and allows for assumptions of hydrostatic stability or use of the Ideal Gas Law to be removed from the temperature retrieval.

Figure 3.2.1: Locating filters within the rotational Raman spectral envelope. Interference filters $F_1$ and $F_2$ are located in regions of the rotational Raman spectral envelope which carry opposing temperature dependence - as the temperature increases the brightness of the spectral lines close to the lasing line decrease in intensity, while those further increase in brightness. Thus the amount of signal transmitted by filters $F_1$ carries the opposing temperature variation versus the signal transmitted through filter $F_2$.

Taken from Cooney (1972). ©American Meteorological Society. Used with permission.

Figure 3.2.2 reproduces figure 2.4.6 but with two notional rotational Raman channel bandwidths. In the case of 300K the pink filter is located with its centre wavelength at approximately the peak of the Stokes branch of the molecular oxygen and nitrogen spectra, while the black filter is located in a region of significantly less bright spectral lines.
Figure 3.2.2: Rotational Raman spectrum of \( \text{O}_2 \) and \( \text{N}_2 \) at modelled for 300K and 1000K, excited by a frequency-tripled Nd:YAG laser (355nm).

At 1000K the spectral envelope of the rotational Raman spectra has been shifted further from the lasing line, altering the brightness of the spectral lines transmitted by both notional filters. The brightness of the spectral lines transmitted by the pink filter have approximately halved in intensity, while those transmitted by the black filter have increased by a much larger amount. The 1000K spectra have been presented for the purposes of highlighting the temperature-dependence of the spectral line brightness, rather than as a realistic temperature found in the atmosphere.

### 3.2.1 Atmospheric measurement

Gill et al. (1979) took the proposed method of Cooney (1972) (and the extension of this work by Cohen et al. (1976)) and constructed a biaxial LiDAR for measuring atmospheric temperatures. A ruby laser (giant pulse) was again used, lasing at 694.3nm, emitting 20-50ns pulses emitting 4-5J per pulse.
Figure 3.2.3: Atmospheric temperature measurements using Raman LiDAR. Radiosonde temperature data is presented alongside the LiDAR measurements, which have been normalised to the sonde profile at the indicated altitude.

Taken from Gill et al. (1979). ©American Meteorological Society. Used with permission.

Figure 3.2.3 shows data averaged over 75m ranges - this resolution is due to using smoothing techniques on the originally-collected data which had a range resolution of 15m. Open square points show locally-launched radiosonde data, with crosses showing the LiDAR data, which agrees with the sonde measurements to ±0.85°C. Due to the biaxial arrangement of the LiDAR used there is no data collected below 1km - this was selected by the authors’ decision to retrieve data from as great a range as possible.

There is no discussion of the data collection period for this study.
3.2.2 Use of high spectral resolution in the receiver

Following Cooney (1972), Arshinov et al. (1983) argued that breakthrough from the elastic return from a LiDAR must contribute as little as possible to the rotational Raman spectra necessary for temperature measurements - and identified a necessary minimum rejection factor of $10^6$ of elastic return for rotational Raman LiDAR studies. The use of appropriately selected filters as the approach for this rejection was suggested, but double-grating monochromators were highlighted as a preferred method due to the higher rejection factor ($10^8$) of the elastic signal. Such monochromators though, have low throughput, which compromises the signal-noise ratio and hence measurement precision.

A more rapidly pulsing and more powerful laser was used for the work of Arshinov et al. (1983): a copper-vapour laser with output of 510.6nm at 6.7kHz (10ns pulses), delivering a mean power of 5-10W (approximately 1mJ per pulse). A double monochromator was used to isolate single lines in the rotational Raman spectrum in the receiver. The LiDAR achieved temperature measurements in close agreements with locally-launched sondes - with differences from 0.8K at low ranges to slightly over 1.5K at 1km. Calibration of this approach was carried out by measuring the ratio between the LiDAR channels in temperature-controlled nitrogen and oxygen gas. The data collection period for comparison with the sonde data was approximately 10-20 minutes, and the LiDAR could probe as low as approximately 100m.

Problems with this approach

Measuring individual rotational Raman spectral lines for a LiDAR experiment requires high spectral resolution, and total rejection of other signals. This can be especially difficult when the rotational Raman spectral line of an atmospheric species is very close to another species’ Raman spectrum (see for example the lines of molecular Nitrogen and Oxygen at 353.65nm in figure 3.2.2).

This separation can be achieved through the use of monochromators and etalons (Achtert et al., 2013; Arshinov et al., 2005; Baumgarten, 2010; Girolamo and Summa, 2009; Hua et al., 2005), spectral separation approaches which must be very precisely controlled. Minor changes in ambient conditions (most commonly ambient temperature) can alter the calibration, requiring rigorous control over laboratory conditions for their use.

Additionally, because the intensity of individual rotational Raman spectral lines is not very high the telescope and receiver must be as transparent as possible to the spectral lines.
of interest.

Using the ratio between narrow bands of the rotational Raman spectrum

Arshinov et al. (1983) also observed that by taking the ratio of two narrow portions of the rotational Raman spectrum one could derive an atmospheric temperature:

\[
R_T = \frac{\sum {N_2, O_2} \sum_J [I(J, T)]_1}{\sum {N_2, O_2} \sum_J [I(J, T)]_2}
\] (3.2.1)

Here the intensity of the backscattered signal is composed of the rotational Raman lines of both oxygen and nitrogen (whose spectra overlap - see figure 2.4.6) which fall within the acceptance range of the spectral selectors (for example, interference filters).

3.2.3 Broader band filters to accommodate multiple lines

Although LiDARs with very narrow spectral resolution successfully measured atmospheric temperatures, the search for smaller, simpler systems led to a reconsideration of interference filters. By the end of the 1980s filter manufacturers (in particular Barr Inc. - now Materion) could manufacture filters for visible wavelengths with acceptable transmission of the Raman lines while blocking the laser wavelength to better than 1 part in \(10^6\).

In the work of Nedeljkovic et al. (1993) and Vaughan et al. (1993) such interference filters were used to allow rotational Raman LiDAR temperature investigations to reach into the stratosphere (5-20km in the case of Vaughan et al. (1993) and 5-35km for Nedeljkovic et al. (1993)). The lasers used for these investigations were frequency-doubled Neodymium YAG lasers emitting at 532.1nm, at 50Hz (delivering 350mJ per pulse). Vaughan et al. (1993) located their interference filters in the Stokes region of the rotational Raman spectrum (533.3 and 536.1nm) in the case of (widths 0.47nm and 0.77nm, respectively) to take advantage of the brighter spectral lines. Nedeljkovic et al. (1993) located their interference filters in the anti-Stokes region (centred at 529.1nm and 530.4nm, FWHM approx 0.4nm and 0.8nm, respectively), and their work suggests these locations were necessary due to manufacturing constraints on the interference filters.

The benefit of using multiple spectral lines is clear - by increasing the amount of light collected the the range of rotational Raman LiDAR experiments can be increased to
approximately 40km\textsuperscript{1} (Li et al., 2016). A rejection factor of elastically-scattered light of \(10^6\) can now be achieved using a combination of interference filters (Di Girolamo et al., 2004) allowing filters to be located closer to the laser wavelength with a reduced risk of elastic light breakthrough.

Note that greater rejection of laser light is achievable by the use of multiple optical components; for example installing notch filters centred on the lasing wavelength (Hua et al. (2005), for example), utilising gratings (Kim et al. (2006), for example) or etalons (Imaki et al. (2012), for example).

### 3.3 Ratio treatment of rotational Raman signals

One can take the work of Cohen et al. (1976) and simplify the LiDAR equation by allowing a number of factors to cancel, and a calibration constant \(C\) introduced in their place.

The telescope collection area and overlap functions should cancel out when the ratio of signals is considered, and with appropriate filter selection the elastic and aerosol contributions can be removed from the total collected signal.

Further, by using only a single illuminating laser the factors representing the laser pulse length will cancel, and if only one wavelength is emitted then the initial laser power necessarily cancels.

Further to this if one considers the ratio \(R_{\text{LIDAR}}\) of returned signals filtered through filters \((F_1\text{ and } F_2)\) of different passbands \((\Delta \lambda_{R1}\text{ and } \Delta \lambda_{R2}, \text{ respectively})\) one obtains from equation\textsuperscript{2.7.1}

\[
R_{\text{LIDAR}} = \frac{P(\lambda_L, \Delta \lambda_R, h, F_1)}{P(\lambda_L, \Delta \lambda_R, h, F_2)} = \frac{\sum_i \left\{ N_i(h) \left[ \int_{\Delta \lambda_{R1}} d\sigma_i(\lambda', \pi, T(h)) \xi(\lambda') d\lambda' \right] \right\}}{\sum_i \left\{ N_i(h) \left[ \int_{\Delta \lambda_{R2}} d\sigma_i(\lambda', \pi, T(h)) \xi(\lambda') d\lambda' \right] \right\}}
\]

(3.3.1)

Here the LiDAR-specific components of equation\textsuperscript{2.7.1} have cancelled giving the ratio between the signals transferred into each channel. We need to introduce the quantum efficiency of the photodetectors \(Q\) (the ratio between the number of photons striking the photocathode and the amount of electrons liberated - see section\textsuperscript{4.4}) - yielding:

\textsuperscript{1}The increase in available range is that the amount of signals transmitted through each interference filter is greater when multiple spectral lines are allowed.
Note that the variation of the quantum efficiency with wavelength across the filter passbands has been neglected in this treatment.

Equation 3.3.2 gives the ratio between the collected signals for each rotational Raman channel photodetector - the values which are subsequently analysed to determine atmospheric temperatures.

Note that in equation 3.3.2 the measured quantity for each channel is dependent on the backscatter cross sections of the scattering molecules, the ratio of the PMT quantum efficiencies and the spectral transmission of the receiver optics to the rotational Raman spectral lines. Thus this ratio is sensitive to the temperature of the atmosphere.

### 3.4 Calibration

Ratio 3.3.2 can only be adequately used in assessing atmospheric temperatures when it has been calibrated, which can be carried out by characterising the system parameters, but in practice more likely to be achieved by comparison with locally launched balloon measurements (Behrendt, 2005, p.286). Ideally the weather balloon is launched as close temporally and geographically as possible to ensure accuracy (for example a front may have passed over the LiDAR site and not the balloon launch site, thus the temperatures at each location may be different).

Current approaches to calculating atmospheric temperature with rotational Raman LiDAR assumes that each channel only collects light from a single spectral line. This suggests a calibration function \( F(T) \) given by Behrendt (2005, p.287):

\[
F(T) = \exp \left( a - \frac{b}{T} \right)
\]  

(3.4.1)

in which \( a \) and \( b \) represent calibration constants:

- \( a \) is the natural logarithm of the ratio of factors in equation 2.4.11, up to the exponential factor.
- \( b \) represents the difference between the rotational Raman energy of the detected lines divided by \( k \).

\( a \) and \( b \) can be numerically fitted to data for calibration of a LiDAR by comparing the
measured temperature (from inverting equation [3.4.1]) to another measurement - typically a sonde launch.

To appropriately correct this for measuring multiple lines one should extend the number of calibration constants (increasing the degrees of freedom in the calibration) (Behrendt, 2005, p.288):

\[ F(T) = \exp\left( \frac{a'}{T^2} + \frac{b'}{T} + c' \right) \]  

(3.4.2)

with calibration constants \( a', b', \) and \( c' \). This leads to the expression of atmospheric temperature:

\[ T = \frac{-2a'}{m' \pm \sqrt{b'^2 - 4l'(c' - \ln F)}} \]  

(3.4.3)

Other calibration approaches, have been attempted - see Behrendt (2005, p.286-289) for further discussion of the approaches used. However, because this work uses a direct calibration approach (see section [3.4.1]), these approaches will not be discussed.

### 3.4.1 Direct calibration approach

Vaughan et al. (1993) introduced a different approach to calibration by modelling the rotational Raman spectrum excited by a frequency-doubled Neodymium YAG laser emitting 200mJ pulses at 10Hz. By calculating the rotational Raman spectrum for multiple temperatures, as well as the expected intensity of the signals measured in each Raman channel of the LiDAR at these temperatures a calibration curve was calculated. The effectiveness of this approach to calibrating their LiDAR was shown by comparing the LiDAR-derived temperatures with a locally-launched sonde - see figure [3.4.1]

Independently, Nedeljkovic et al. (1993) also developed this approach to calibrating a rotational Raman LiDAR for measuring temperatures using an analytically produced calibration curve. This calibration approach (with minor corrections for polarisation effects and drifts in PMT sensitivity) achieved a temperature accuracy of less than 1K (Vaughan et al., 1993).
Figure 3.4.1: Atmospheric temperature measurements using Raman LiDAR. The LiDAR data has the uncertainty shown by the dashed lines indicated the maximum and minimum temperature based on this uncertainty. Sonde data is presented for comparison.

Taken from Vaughan et al. (1993).

Comparison with locally-launched sondes verified this as an appropriate calibration approach for rotational Raman temperature LiDARs - see figure 3.4.1.

3.5 Other Previous Rotational Raman LiDAR studies

Building on studies previously discussed, Philbrick and Univers (1995) developed a rotational Raman LiDAR which improved previous spatial resolution to 75m and reduced the overlap to a few hundred meters. Calibration of this LiDAR was performed by comparing with sondes, using a quadratic fit (see equation 3.4.2).

Before Behrendt and Reichardt (2000), temperature profiling of the atmospheric using rotational Raman LiDAR had required clear skies - the elastically scattered laser light otherwise overwhelms the Raman signals (breaking through the channel filters). Behrendt and Reichardt (2000) used a series of interference filters (see their figure 2) to reduce elastically scattered light so the Raman signals were not overwhelmed. This allows temperatures to be retrieved, even in the presence of optically-thin clouds, to a range of 40km, with a resolution of 120m. 1K temperature errors were achieved at 20km with 90minute data collection, while tropospheric temperature retrieval with this error were achieved in
a few minutes.

Behrendt and Reichardt (2000) also explored the potential for varying the angle of interference filters in their optics. This serves to not only allow for the rejected light from each filter to be directed onto another filter (and thus to a different channel detector), but also serves to fine-tune the transmission profile as necessary (see section 4.3.9).

By adding in additional vibrational Raman channels, Behrendt et al. (2002) combined temperature detection with water vapour detection. They used a similar system to Behrendt and Reichardt (2000) of using multiple interference filters to reject elastic light and achieve very high spectral selection of returning signals. They used a frequency-doubled Nd:YAG laser, and by using neutral density filters to reduce the collected signal intensity, and subtracting solar returns the Raman signals were retrieved, allowing the first daytime use of a Raman LiDAR.

To simultaneously investigate the temperature and water vapour fields Behrendt et al. (2004) combined temperature measurement with a water vapour channel (using the vibrational Raman spectrum). This technique allows their LiDAR to measure cloud vertical extent and analysis of the LiDAR temperature measurement performance for measurements within clouds.

The work of Di Girolamo et al. (2004) demonstrated the potential of using the third harmonic of the Nd:YAG laser (355nm) for use in a rotational Raman LiDAR. This development allowed the construction of rotational Raman LiDARs using eye-safe lasers - and thus widening their potential use to locations typically not suitable for a LiDAR experiment (for example near a heavy, low altitude, air-traffic area).

Radlach et al. (2008) built on the work of Di Girolamo et al. (2004) by constructing an ultraviolet (frequency-tripled Nd:YAG) rotational Raman LiDAR with scanning capabilities. Their LiDAR used multiple interference filters to very specifically select portions of the returning signals (see their figure 1). Calibration of this LiDAR was performed by comparison with locally-launched sondes using equation 3.4.1

### 3.5.1 Rotational Raman LiDAR Boundary Layer studies

To carry out an investigation of the boundary layer above an urban environment Rotational Raman LiDAR provides a suitable technique due to its high resolution and temporal continuity. Because it is a remote sensing technique no permanent structures need to be constructed above the urban environment (such as the balloon-suspended optical fibre of
Keller et al. (2011). Their work strongly demonstrated the capability of using rotational Raman scattering to examine the boundary layer temperature profile, but highlighted the difficulties of using such measurement structures.

An example of a boundary layer rotational Raman LiDAR is that reported by Mao et al. (2009) at Xi’an University (34°15’N 108°59’E) situated in urban Xi’an. This LiDAR uses a frequency-tripled Nd:YAG (355nm) 300mJ laser operating at 20Hz. This LiDAR instrument was capable of measuring the urban boundary layer:

![Figure 3.5.1: Atmospheric temperature measurements using Raman LiDAR. Radiosonde data is presented for comparison with the LiDAR temperature. Taken from Mao et al. (2009).](image-url)

This temperature profile was collected over a time period of approximately 8 minutes and was collected at 2000 CST (local time) - clearly showing the temperature inversion limiting the boundary layer at an altitude of 2.5km.

Rotational Raman studies of the boundary layer typically do not extend the use of the LiDAR beyond measuring the boundary layer temperature.

By using the third harmonic of their Nd:YAG laser the Xi’an LiDAR is eye-safe at a significantly shorter range than visible lasers used in other studies (see Appendix A for further discussion on eye safety).

Ultraviolet lasers are therefore more suitable for LiDAR investigations over a city with a nearby airport. However some local police forces regularly use helicopters which fly much lower than commercial air traffic so the lasing power needs to be lower than in
the cases of Chen et al. (2011); Hammann et al. (2015); Hua et al. (2007); Imaki et al. (2012); Mao et al. (2009); Radlach et al. (2008); Reichardt et al. (2012); Strauch et al. (1971); Su et al. (2013), amongst others.

The Manchester rotational Raman LiDAR seeks to exploit a diode-pumped neodymium YAG laser with a far higher repetition rate (1kHz) than flash lamp-pumped systems but far less energy per pulse making for improved eye safety for aircraft.

Recent work has shown that the use of rotational Raman LiDAR is not limited to night-time investigations - Imaki et al. (2012) combines a diffraction grating (monochromator) and interference filters, achieving a resolution of 3.75m.

Additional rotational Raman LiDAR work shows that assessment of the structure of the boundary layer by probing for the temperature and identifying regions of largest vertical gradient to locate temperature inversions and thus boundaries between atmospheric layers (Wang et al., 2015) is possible.

### 3.6 Summary of discussed LiDARs

Below is a brief summary of previously-discussed rotational Raman LiDARs in terms of the laser and telescope diameter. Where no specific telescope type is mentioned the telescope was a reflecting telescope. * symbols denote telescopes which focus from the primary mirror onto a fibre.
<table>
<thead>
<tr>
<th>Author(s)</th>
<th>Laser</th>
<th>Wavelength</th>
<th>Pulse energy</th>
<th>Repetition Rate</th>
<th>Telescope</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cooney (1972)</td>
<td>Ruby</td>
<td>694.3 nm</td>
<td>20 J</td>
<td>564 mm</td>
<td></td>
</tr>
<tr>
<td>Gill et al. (1979)</td>
<td>Ruby</td>
<td>694.3 nm</td>
<td>4.5 J</td>
<td>762 mm</td>
<td></td>
</tr>
<tr>
<td>Arshinov et al. (1983)</td>
<td>Copper vapour</td>
<td>510.6 nm</td>
<td>1 mJ</td>
<td>6.7 Hz</td>
<td>Two lens objectives (diameter 300mm)</td>
</tr>
<tr>
<td>Nedeljkovic et al. (1993)</td>
<td>Frequency-doubled Nd:YAG</td>
<td>532 nm</td>
<td>350 mJ</td>
<td>50 Hz</td>
<td>800 mm*</td>
</tr>
<tr>
<td>Vaughan et al. (1993)</td>
<td>Frequency-doubled Nd:YAG</td>
<td>532 nm</td>
<td>200 mJ</td>
<td>10 Hz</td>
<td>600 mm Newton</td>
</tr>
<tr>
<td>Philbrick and Universal (1995)</td>
<td>Frequency-doubled Nd:YAG</td>
<td>532 nm</td>
<td>600 mJ</td>
<td>20 Hz</td>
<td>406.4 mm Cassegrain</td>
</tr>
<tr>
<td></td>
<td>Frequency-tripled Nd:YAG</td>
<td>355 nm</td>
<td>250 mJ</td>
<td>20 Hz</td>
<td></td>
</tr>
<tr>
<td>Behrendt and Reichardt (2000)</td>
<td>Frequency-doubled Nd:YAG</td>
<td>532 nm</td>
<td>200 mJ</td>
<td>50 Hz</td>
<td>900 mm</td>
</tr>
<tr>
<td>Behrendt et al. (2002)</td>
<td>Frequency-doubled Nd:YAG</td>
<td>532 nm</td>
<td>600 mJ</td>
<td>50 Hz</td>
<td>820 mm Cassegrain</td>
</tr>
<tr>
<td>Behrendt et al. (2003)</td>
<td>Frequency-doubled Nd:YAG</td>
<td>532 nm</td>
<td>600 mJ</td>
<td>50 Hz</td>
<td>820 mm Cassegrain</td>
</tr>
<tr>
<td>Di Girolamo et al. (2004)</td>
<td>Frequency-tripled Nd:YAG</td>
<td>354.7 nm</td>
<td>350 mJ</td>
<td>30 Hz</td>
<td>760 mm Dall-Kirkham</td>
</tr>
<tr>
<td>Hua et al. (2005)</td>
<td>Frequency-tripled Nd:YAG</td>
<td>354.7 nm</td>
<td>200 mJ</td>
<td>20 Hz</td>
<td>250 mm*</td>
</tr>
<tr>
<td>Hua et al. (2007)</td>
<td>Frequency-tripled Nd:YAG</td>
<td>354.7 nm</td>
<td>250 mJ</td>
<td>20 Hz</td>
<td>250 mm Schmidt-Cassegrain</td>
</tr>
<tr>
<td>Radlach et al. (2008)</td>
<td>Frequency-tripled Nd:YAG</td>
<td>354.7 nm</td>
<td>300 mJ</td>
<td>30 Hz</td>
<td>400 mm Ritchey-Chretien</td>
</tr>
<tr>
<td>Mao et al. (2009)</td>
<td>Frequency-tripled Nd:YAG</td>
<td>354.7 nm</td>
<td>300 mJ</td>
<td>20 Hz</td>
<td>250 mm Schmidt-Cassegrain</td>
</tr>
<tr>
<td>Chen et al. (2011)</td>
<td>Frequency-doubled Nd:YAG</td>
<td>532 nm</td>
<td>280 mJ</td>
<td>20 Hz</td>
<td>400 mm*</td>
</tr>
<tr>
<td>Imaki et al. (2012)</td>
<td>Frequency-tripled Nd:YAG</td>
<td>354.7 nm</td>
<td>200 mJ</td>
<td>20 Hz</td>
<td>230 mm Schmidt-Cassegrain</td>
</tr>
<tr>
<td>Reichardt et al. (2012)</td>
<td>Nd:YAG (first harmonic)</td>
<td>1064 nm</td>
<td>1600 mJ</td>
<td>30 Hz</td>
<td>200 mm Newton</td>
</tr>
<tr>
<td></td>
<td>Frequency-tripled Nd:YAG</td>
<td>355 nm</td>
<td>450 mJ</td>
<td>30 Hz</td>
<td></td>
</tr>
<tr>
<td>Achert et al. (2013)</td>
<td>Frequency-doubled Nd:YAG</td>
<td>532 nm</td>
<td>350 mJ</td>
<td>20 Hz</td>
<td>508 mm Newton</td>
</tr>
<tr>
<td>Hamann et al. (2015)</td>
<td>Frequency-tripled Nd:YAG</td>
<td>354.7 nm</td>
<td>200 mJ</td>
<td>50 Hz</td>
<td>400 mm Ritchey-Chretien-Cassegrain</td>
</tr>
<tr>
<td>Wang et al. (2015)</td>
<td>Frequency-tripled Nd:YAG</td>
<td>354.7 nm</td>
<td>250 mJ</td>
<td>20 Hz</td>
<td>600 mm Newton</td>
</tr>
</tbody>
</table>

Table 3.6.1: LiDAR system specifications.
3.7 Manchester Temperature LiDAR

This work seeks to modify the LiDAR of Vaughan et al. (1993) to operate with a low power ultraviolet laser, operating at high frequency to allow optical safety at a short enough range to be legally used to investigate Manchester’s nocturnal heat island - particularly with regard to the absolute temperature (and using equation 1.1.3, the potential temperature to assess the stability) of the boundary layer during the course of a night.

Based on the previous works (notably Arshinov et al. (1983), but with a more modern, solid-state laser) which have been discussed in this chapter the temperature LiDAR to be worked with in Manchester will have the following characteristics:

- The LiDAR will utilise the rotational Raman spectrum (utilising an ultraviolet laser) to identify atmospheric temperatures.

- An Neodymium YAG laser will be used in the frequency-tripled mode at low energy per pulse to allow for use without posing a hazard to local air traffic.

- The calibration approach used in Arshinov et al. (1983); Vaughan et al. (1993) will be used with validation by locally-launched radiosondes.

- The LiDAR will operate using interference filters - the advances in the ability of manufacturers to produce high-rejection filters allows for a simpler construction than the monochromators used in Arshinov et al. (1983).

Having identified some of the properties which would be suitable for the Manchester Boundary Layer Temperature LiDAR the following chapter introduces the instrument. Each component of the LiDAR is considered - as is the configuration of the laser and telescope; any changes from the original are reviewed, and a brief discussion of the collection electronics is made.
Chapter 4

Manchester Boundary Layer Temperature LiDAR

4.1 Manchester Boundary Layer Temperature LiDAR

The Manchester Boundary Layer Temperature LiDAR (BLT) has been constructed to monitor the height of the capping temperature inversion of the Manchester nocturnal boundary layer\(^1\) as the first stage of developing a complete nocturnal boundary layer monitoring system. The BLT operates with three channels - two rotational Raman channels for deriving temperature and an elastic channel which is used to monitor the backscattered signals for cloud/aerosol layers, using interference filters for spectral selection and photomultiplier tubes (see section 4.4) used to collect the signals from each channel.

4.1.1 Instrument overview

Figure [4.1.1] shows a schematic of the BLT instrument: the BLT is a biaxial LiDAR instrument utilising a frequency-tripled Neodymium:YAG (Nd:YAG) laser (see section 4.2) emitting a horizontal beam. This beam is expanded using a transmit telescope (see section 4.2.2) before being directed into the atmosphere by a mirror (see section 4.2.3). By using the transmit telescope the signals are eye safe and so do not pose a safety risk to local air traffic (see Appendix A).

The BLE uses a Nasmyth-Cassegrain collecting telescope (see section 4.3.1), using a silica prism to direct the light via collimation lenses (see section 4.3.4) to focus the collected signals on the detection optics. Spectral selection is achieved using interference

\(^1\)The BLT is located in the Simon Building, Brunswick St., 53.465N 2.232W.
filters (see Chapter 5) which are located within the rotational Raman spectral envelope of molecular nitrogen and oxygen. A power beamsplitter (see section 5.3.1) is used to separate the rotational Raman channel signals, which are focused onto photomultiplier tube bialkali photocathodes (see section 4.4) by ‘spatial filters’ (see section 4.3.8). These spatial filters reject signals which are travelling ‘off-axis’ to reduce background noise.

Figure 4.1.1: Manchester Boundary Layer Temperature LiDAR schematic. The intermirror distance indicated is for the final separation of the telescope mirrors following focusing work (see section 4.3.1).

The BLT was developed as a proof-of-concept that a low-power, high repetition laser, coupled with the appropriate optics could be used to monitor the nocturnal boundary layer capping inversion. To this end the BLT was constructed by modifying an existing LiDAR previously used for stratospheric monitoring, replacing the laser and reconfiguring the optics for boundary layer studies. Components of the legacy LiDAR instrument which were not modified during this work include the silica prism, collimation tube and lenses,
the PMTs (see section 4.4), the optics cube (which holds the interference filters) and the channel separation cube.

Because the legacy instrument operated using green laser light the interference filters were changed for filters centred within the rotational Raman spectrum excited by 355nm light. This change preceded this work, and during this project the interference filters were fully calibrated and their performance assessed. See Chapter 5 for further discussion.

Because the LiDAR upon which the BLT was constructed was a stratospheric LiDAR the BLT will be operating within the near-field region of the telescope.

## 4.2 BLT Transmitter

### 4.2.1 Laser properties

![Laser head, expansion telescope and directing mirror.](image)

The laser used for the BLT is a frequency-tripled Neodymium:YAG (Nd:YAG) laser (model WAVE-Y-1000-355 with laser head serial number 09/13/006) from Elforlight. This laser is a diode-pumped solid state laser which outputs low energy but very high repetition pulses (see table 4.2.1).

The laser is mounted in biaxial configuration with the telescope (see section 4.3.1).

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wavelength</td>
<td>354.7nm</td>
</tr>
<tr>
<td>Pulse width</td>
<td>8 ns</td>
</tr>
<tr>
<td>Repetition rate</td>
<td>1000 Hz</td>
</tr>
<tr>
<td>Average pulse energy</td>
<td>240 μJ</td>
</tr>
<tr>
<td>Beam divergence (before transmit telescope)</td>
<td>1 mrad</td>
</tr>
<tr>
<td>Beam waist (before transmit telescope)</td>
<td>3 mm</td>
</tr>
</tbody>
</table>

Table 4.2.1: Laser properties.
These properties of the laser were selected initially with eye safety in mind (see Appendix A). Because of the nearby airport and local helicopter traffic, using a visible laser is too dangerous – hence frequency-tripling the Nd:YAG laser reduces the potential for eye damage by moving the wavelength into the ultraviolet. Frequency tripling is achieved through mixing the fundamental and second laser harmonics in a nonlinear crystal. Two lithium triborate non-linear crystals are used to achieve the third harmonic - the first crystal (type 1) to generate the second harmonic and the second crystal (type 2) to produce the third harmonic.

For a similar reason the laser is operated at low pulse energy - lower energy reduces the number of emitted photons which correspondingly reduces the range before the laser beam is completely eye safe. To ameliorate the reduced number of photons emitted per pulse (and thus reduced number of photons backscattered to the BLT) a high repetition rate was selected for the laser.

Additionally, the low pulse energy ensures that the PMTs will not become saturated from signals scattered from each pulse.

4.2.2 Laser divergence

The energy intensity of a laser beam is distributed in a Gaussian mode with energy density across the laser beam described by:

\[
I = I_0 \exp \left( \frac{-2r^2}{w^2} \right)
\]

Where \(I_0\) describes the intensity at the centre of the laser beam, \(r\), the radial distance of the measurement, and \(w\) the beam radius (determined as the portion of the beam in which 86.5% of the energy is carried (Silfvast, 2003)).

A property of Gaussian beams is that there is a minimum diameter (the distance from the optical axis to the beam edge) of the beam (called the beam waist \(w_0\)) occurring at the focus of the cavity mirrors (or a subsequent lens) (Silfvast, 2003). Following this minimum beam waist, the light rays diverge, leading to beam widening, quantified at a distance \(z\) from the beam waist through a medium of refractive index \(\eta\) (at wavelength \(\lambda\)) by:

\[
w(z) = w_0 \sqrt{1 + \left( \frac{\lambda z}{\eta \pi w_0^2} \right)^2}
\]

(4.2.1)
The increase in the beam waist must be addressed to maximise the useful range of a LiDAR - if laser energy spreads over too large an area then it cannot be brought to focus in the receiver. This can be corrected through the use of a beam expander telescope which collimates the beam and reduces the divergence. In the case of the BLT laser at emission, \( w_0 = 3 \text{mm} \). Additionally, through the use of a beam expander the irradiance of the laser is spread over a greater area (a 10× expansion factor reduces the intensity of the illumination by a factor of 100).

**Expansion telescope**

To minimise the effect of the expansion of the beam waist an expansion telescope (a Thorlabs telescope, component number BE10-UVB) was used - see figure [4.2.3a]. The use of the expansion telescope increases the width of the laser beam Gaussian profile by a factor of 10, but correspondingly also reduces the beam divergence by a factor of 10.

To determine the divergence of a Gaussian laser beam first one must define the Rayleigh range \( z_R \) - the distance over which the cross-sectional area of the beam doubles (Hecht, 2002, p.595):

\[
z_R = \frac{\pi w_0^2}{\lambda}
\]  

(4.2.2)

Figure 4.2.2 shows a sketch of laser beam divergence which is instructive in determining the beam divergence as well as how an expansion telescope affects divergence.

![Beam divergence sketch](image)

Figure 4.2.2: Beam divergence sketch. Minimum beam waist \( w_0 \), Raleigh range \( z_R \), beam divergence \( \Theta \)

By constructing a triangle from \( z_R \) and \( w_0 \), \( \Theta \) can be determined to be:
\[ \Theta = 2 \arcsin \left( \frac{\sqrt{2}}{2} \frac{\lambda}{\pi w_0} \right) \] (4.2.3)

Naturally, as the size of the minimum beam waist increases the argument of the arcsin (and thus the beam divergence) decreases. Correspondingly, following the expansion telescope the laser light has its divergence reduced by the same factor as the increase in the beam width.

4.2.3 Directing the laser into the atmosphere

Following the expansion telescope the laser beam is directed to the vertical and through a roof hatch by a mirror (an Edmund Optics laser line mirror, component number #63-117) designed specifically for reflection at 340-370nm - see figure 4.2.3b.

![Figure 4.2.3: Expansion telescope and transmission mirror.](image)

(a) Transmission expansion telescope (b) Laser transmission mirror

Precise alignment of both the directing mirror and transmit telescope was achieved by mounting them to the optics breadboard on sliding mounts. Following the lateral alignment of these components, the mounts were secured in place, and fine alignments were carried out using the pitch/yaw control screws (visible in figure 4.2.3b). Collimation control for the transmission telescope was performed by rotating the red dial in figure 4.2.3a which varies the separation of the lenses in the telescope. For a discussion of aligning the expansion telescope and laser beam see section 4.3.3.
4.3 Receiver design

4.3.1 Telescope

The telescope used in the BLT is a Nasmyth-Cassegrain\textsuperscript{2} telescope mounted on a secured frame directly underneath the laboratory roof hatch, with mirror properties:

<table>
<thead>
<tr>
<th>Mirror</th>
<th>Shape</th>
<th>Focal length (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Primary</td>
<td>Parabolic</td>
<td>1.8</td>
</tr>
<tr>
<td>Secondary</td>
<td>Hyperbolic</td>
<td>0.33</td>
</tr>
</tbody>
</table>

Table 4.3.1: Telescope mirror properties.

The secondary mirror was matched to the primary mirror to minimise any spherical aberration when focussed onto the aperture allowing a sharp image to be formed on the photomultiplier tube photocathodes (see figure 4.1.1).

The BLT telescope was originally designed for stratospheric work before being repurposed as a boundary layer LiDAR telescope, thus boundary layer investigations would lie within the near-field of the telescope. Correspondingly the telescope focal range was adjusted by raising the secondary mirror (as per the Lensmaker’s equation):

\[
\frac{1}{f} = \frac{1}{s_i} + \frac{1}{s_o}
\]

(4.3.1)

where \( f \) is the focal length of the lens used, \( s_o \) the distance from the lens to the object to be imaged and \( s_i \) is the distance from the lens and the image formed.

\textsuperscript{2}A Cassegrain telescope focusses light behind the primary mirror, while Nasmyth-Cassegrain telescopes still focusses light behind the primary mirror, but uses a tertiary mirror to redirect the light to outside the telescope. Thus the focal plane of the telescope is removed from between the mirrors and therefore observations can be made with only a small amount of shading of the primary mirror by the tertiary mirror.
Figure 4.3.1: Focal points of the telescope. Note that the tertiary mirror is located behind the telescope aperture shown in red.

In case A, the telescope is focussed at infinity or sufficiently large ranges such that the curvature of the wavefronts can be considered negligible (in the Lensmaker’s equation the object distance can be considered infinity). The secondary mirror is positioned such that the focal length of the telescope is at the collection aperture (red points in the figure).

For light originating from the boundary layer the curvature of the wavefront is significant, and the parallel light beam approximation cannot be made (the object distance in the Lensmaker’s becomes finite), and correspondingly the focal plane of the telescope increases in distance from the secondary mirror - see case B.

In case C the secondary mirror has been moved, allowing the light rays of the object to be once again focussed onto the BLT collection aperture.

4.3.2 BLT telescope aperture

The size of the aperture of the BLT telescope is controlled with an iris diaphragm, which can be varied between 1mm and 25mm. Having this variable aperture diameter allows for aligning the laser and telescope field of view (by maximising the returning signal with the minimum aperture ensures that the laser and telescope are aligned).
The diameter of the telescope aperture was set to 20mm because this ensures a combination of the most light accepted from that collected by the telescope, without allowing any to miss the prism located underneath the telescope aperture (see figure 4.3.3), thus losing signals.

### 4.3.3 Focussing the telescope

The optimum position of the secondary mirror above the primary was determined by monitoring the BLT signals on the visualising software and rotating the screw mounting (which traverses the secondary mirror vertically) while monitoring the overlap region.

![Telescope focussing](image.png)

Figure 4.3.2: Effect of focussing the telescope on elastic channel LiDAR signals. Black data shows the collected elastic signal for a telescope not focussed within the boundary layer, with red data showing when the telescope had been refocussed.

The black data was collected with the telescope secondary mirror in its original position - and the red data when it had been moved to adjust the focal plane of the telescope to the BLT aperture.

The black profile shows a significantly higher overlap than the red - only above approximately 1000m does the profile approximately follow the expected approximately linear gradient - the density of atmospheric molecules reduces as an exponential function of height (thus a straight line in logarithmic plots). Additionally, in the left plot signals are much smaller in magnitude, showing that less light was reaching the photomultiplier tubes before focussing.
4.3.4 Collimating tube

Directly below the BLT aperture (red feature to right of figure 4.3.3) is a silican prism (which operates as the tertiary mirror of the Nasmyth-Cassegrain telescope) which redirects the signals collected by the telescope towards the channel separation optics. The prism used is from the original instrument and was not replaced during the course of this work.

Light reflected by the prism is directed along a collimation tube which serves to expand the width of the light column and collimate it into a single beam of parallel light. These lenses were designed so that the primary mirror is imaged onto the photomultiplier tubes to optimise capture of light.

Figure 4.3.3: Optical schematic of the BLT, post telescope. The red aperture on the right (above the prism) corresponds to the red points in figure 4.3.1. Following the prism and collimating lenses the light enters the optics cube where a beamsplitter (red line) separates the signals. Further detail of the optics cube are shown in figure 4.3.5. Spatial filters are located in front of the PMT photocathodes (the brown lines) - see figure 4.3.6 for more.

The collimation tube terminates at the channel separation cube - see figure 4.3.3. A small extension to the tube was manufactured during this project to extend beyond the end of the collimation tube and reduce any light leakage due to incomplete collimation. This extension links to the optics cube (see below) by means of a frictional engagement
with a neoprene rubber collar fitted within a machined bore - see figure 4.3.4.

Figure 4.3.4: Light guide extension fitted into the optics cube.

Collimation was tested by directing light from a halogen lamp into the BLT aperture, having removed the interference filters from the optics cube. A paper screen was placed into the main cube, and moved both within the cube and externally (having removed the PMTs from both Raman channels) to confirm that the illuminated light spot did not vary in size from entering the channel separation cube to beyond the position of the PMT photocathodes.

4.3.5 Optics cube

Channel separation is achieved by the use of a beamsplitter - figure 4.3.5 shows the pathways that the rotational Raman channels are illuminated by either transmission or reflection. The beamsplitter is held in place by a socket located within the top and bottom of a machined aluminium optics cube. Two aluminium blocks are secured to the base of the channel separation optics which hold the optics cube in place - see figure 4.3.4.

The optics cube also holds the interference filters in place and ensures collected signals illuminate the filters such that the light strikes the filters at 90°.

Any signals rejected by the rotational Raman interference filters are reflected and directed by the beamsplitter to illuminate the remaining (elastic) channel - see figure 4.3.5.
Figure 4.3.5: Channel separation and interference filters (interference filters shown as the coloured blocks with a neutral density filter shown as the black block). The beamsplitter is shown by the diagonal red line, with the power split indicated by the annotated percentages. The ‘block-stops’ which keep the optics cube in the proper alignment is shown in purple.

In regard to the interference filters, “Near-field” refers to the channel with the interference filter with the central wavelength closer to the laser wavelength (low-J rotational Raman spectral lines), located in the region of the rotational Raman spectrum which decreases in brightness as temperature increases. “Far-field” refers to the channel with the interference filter further from the lasing line (high-J) where the brightness of the spectral lines increase in brightness as the temperature increases. See figure 6.6.1 for details of calibrations.

4.3.6 Neutral density filter

An absorbing neutral density filter of optical density 0.3 (Edmund Optics stock number #65-811 0.3 OD 50mm Diameter, Absorptive ND Filter) was positioned in front of the elastic filter to reduce the amount of light transmitted into the elastic channel. This serves the dual purpose of ensuring the PMT discriminator of the elastic channel is not saturated (losing detection events in the dead time) and that the light reflected from the interference filter is further reduced in intensity before it hits the near-field channel filter. Breakthrough (see section 5.5) is not expected, but reduction of light (already rejected by a channel) inside the optics cube is advantageous.
4.3.7 Beamsplitter

The beamsplitter used in this work is a fused silica beamsplitter with surface coatings to provide a reflectance of 30% and is held in place at an angle of $45^\circ$ to the collected signals by grooves on the inside of the optics cube. Further information of the beamsplitter is given in section 5.3.

4.3.8 Spatial filters

To reduce the effects of any light leakage within the channel separation cube spatial filters were placed in front of the PMTs. The original spatial filters were hollow cylinders of black acetate with a ‘shelf’ structure to hold a strong lens which is held in place by a split ring washer held in place by frictional engagement. One end of the cylinder is closed (to act as a field stop) with a hole drilled through to allow the passage of light through the centre of the filter field stop - see figure 4.3.6a.

![Figure 4.3.6: Spatial filter schematic.](image)

(a) Spatial filter schematics.  (b) Spatial filter positioning.

These filters transmit light which is incident parallel to the filter axis and a few degrees either side (see figure 4.3.6b) and thus limit the size of the spot formed on the PMT photocathodes. This helps to counter the inherent inhomogeneities in the photocathode sensitivity. The size of the light spot from the telescope changes in size dependent on the range from which the scattering occurs - and correspondingly the size of the light spot on the photocathode varies. To minimise the effects of the inhomogeneities on measured
signals a minimal amount of the photocathode is illuminated - the lens of the spatial filter determining how large the light spot will be.

The acceptance angle of the spatial filters was measured to have a ‘full angle’ of $\approx 18^\circ$ so $\approx 9^\circ$ from the optical axis. Any light entering along an off-axis pathway (such as light scattered from below the laser beam and telescope field of view overlap) will be focussed onto the beam stop and thus prevented from entering the PMTs.

### Altering the spatial filters

Replicas of the black acetate cylinders were made, but with a field stop aperture 1cm in diameter (see figure 4.3.6a,B). An iris diaphragm was fitted across this field stop aperture for dynamic control of the amount of light transmitted by the spatial filter field stop.

The optimum setting for the spatial filter field stop aperture diameter was decided to be 10mm following a series of experiments to determine the aperture effect on collected atmospheric profiles.

### 4.3.9 Interference filters

Interference filters are used to select portions of the rotational Raman spectrum.

The interference filters used in the BLT were manufactured by Materion (previously Barr Associates Inc.) by depositing multiple thin films onto a substrate to reject almost all light falling upon the filter surface while transmitting a narrow-band spectrum. These filters allow for the spectral selection of the regions of the rotational Raman spectrum necessary to derive an atmospheric temperature and thus locate the temperature inversion.

The interference filters are held in place in the optics cube to ensure that they remain exactly perpendicular with the optical axis of the signals incident upon each filter. This positional control is necessary because if interference filters (of effective refractive index $n_E$) rotate by even a small angle ($\Theta$) the centre of the transmission profile is shifted to a shorter wavelength \cite{Carlstrom et al. 1990}:

$$\lambda_{\Theta} = \lambda_0 \sqrt{1 - \frac{\sin^2 \Theta}{n_E^2}}$$ (4.3.2)

Equation 4.3.2 has been used by some LiDAR groups to tune the filter passbands by tilting them \cite{Behrendt and Reichardt 2000, Hua et al. 2007}, for example. Because

$^3$The angle tracing a cone with an apex at the optical component aperture within which light directed at the optical aperture will be transmitted through the component.

$^4$The apex angle of the triangular profile of the acceptance cone.
the BLT was modified from an existing LiDAR instrument and utilises the same channel separation arrangement, notably in the optics cube, the technique of rotating the interference filters to 'tune' the BLT channel passbands was not used. Additionally, because this approach shifts the central wavelength of the interference filter to lower wavelengths, tuning the BLT filters would bring the passbands closer to the laser line.

The interference filters and their calibration are discussed in greater detail in Chapter 5.

4.4 Signal detection

4.4.1 Photomultiplier tubes

Photomultiplier tubes detect light using the photoelectric effect which liberates electrons from the surface of the photocathode. These electrons are then accelerated through a series of dynodes with voltage steps. The accelerated electrons pass on energy to the next dynode in the chain and liberate further electrons so that by the anode of the PMT many thousands of electrons have been liberated per electron liberated from the photocathode. This electron cascade produces a small electric signal which must be amplified before being of practical use. Not every photon incident on the photocathode results in a liberated electron - only approximately 25% of UV photons liberate an electron (Wandinger, 2005b, p.255) - a proportion known as the quantum efficiency.

**BLT Photodetectors** The BLT uses EMI 9902 photomultipliers with bialkali cathodes, operated in photon-counting mode for optimum sensitivity (Wandinger, 2005b). This sensitivity does lead to limitations, in the form of a maximum incident light before potentially overloading the detector - limiting the BLT to nocturnal operation. Similarly, strong returns (for example elastic scattering from clouds) can saturate the PMTs.

Because the interference filters have such narrow passbands (see Chapter 5), the assumption made when discussing the rotational Raman channel signal ratio (equation 3.3.2) can be supported.

4.4.2 Discriminator

A discriminator is used to reduce the effects of thermal noise events - random signals from the PMTs. The random signals are caused by electrons being thermally liberated
from a dynode within the PMT. These electrons follow the same electron cascade to the photoelectrons from the photocathode, but because the cascade begins at a dynode rather than the photocathode fewer electrons will strike the anode.

A discriminator rejects signals (current pulses) which are too small - as determined by a user-set threshold - while allowing the signals which are sufficiently strong.

![Figure 4.4.1: Example discriminator trace. $i_d$ shows the threshold strength for signals; any weaker signals are rejected by the discriminator. $\tau$ is the discriminator dead time during which further signals cannot be processed by the discriminator.](image)

Figure 4.4.1 shows an example input to a discriminator, with the threshold level indicated by the grey line. The signals which do not exceed the threshold signal $i_d$ will be rejected, while those which exceed it will be passed further through the collection electronics circuit.

Once a sufficiently strong signal pulse has been received the discriminator very briefly ceases detecting input signals to pass on the accepted signal pulse. The time for which the discriminator (and thus the detection electronics) cannot detect any signals is known as the discriminator dead time $\tau$.

Considering figure 4.4.1 the first detection event exceeding the threshold level has no signals arriving before the discriminator dead time has elapsed so there is no lost signal. However the second detection exceeding the threshold level does have another signal pulse arriving before the dead time has elapsed but the discriminator would have rejected this signal anyway as it is too weak.

The third detection event which exceeds the threshold level is followed by another signal that exceeds the threshold level, but because the dead time of the discriminator has not elapsed this signal is lost. This is one limiting factor of using discriminators - if sufficient signals exceed the threshold level in a short period of time the dead time of the discriminator can ‘saturate’ and lose a significant portion of the signal.
A correction to the measured signal must be applied to the measured count rate \( C_{\text{meas}} \) (Evans 1955, p.785-788), (assuming Poisson statistics in the received pulses) as defined by:

\[
C = \frac{C_{\text{meas}}}{1 - \tau C_{\text{meas}}}
\]  

(4.4.1)

It should be noted that with a very high count rate (measured) the maximum observed counting rate asymptotes to \( \frac{1}{\tau} \). This is why LiDAR experiments using photon counting data collection methods need to ensure that the expected range of signal intensity does not saturate the detectors. Neutral density filters can be used to reduce strong signals to manageable levels. For LiDARs operating with small collected signals compared with solar background (such as the BLT) using neutral density filters may not transmit sufficiently strong LiDAR returns, restricting such experiments to nocturnal investigations.

In the BLT \( \tau \) was set to 10ns; equation 4.4.1 then provides an accurate correction to \( C_{\text{meas}} \) up to around \( C_{\text{meas}} = 20 \text{MHz} \)

**Setting the discriminator level**

The discriminators for the BLT are located on the data acquisition cards used to convert the analogue signals into a binary data file. The cards used are multi-channel scalar cards and were supplied by Ortec, the signals from which are processed by a LabView script - see section 4.4.3.

The levels for the discriminators on each card (one for each PMT) were set when the BLT was used for its original stratospheric investigations by David Wareing (see Vaughan et al. (1993)), using the following method.

By setting the discriminators to zero and observing the output of the PMTs on an oscilloscope all signals are allowed, including those arising from thermal noise along the dynode chain as well as any electronic reflections (from the end of each cable). By increasing the threshold for the discriminator the spurious signals are rejected, until only the signals passing along the entire dynode chain are sufficiently strong (they have been amplified through the dynode chain cascade) to pass through the discriminator. The optimum setting of the discriminators were determined by adjusting the threshold while monitoring the output on an oscilloscope triggered by the emission of the test pulse.

Spurious signals can arise at the ends of the coaxial cable from electronic reflection which are addressed through the use of series and parallel termination in the cable.
4.4.3 Real-time data visualisation

Data from the data acquisition cards is compiled into a series of files by a LabView script written originally by David Wareing which bins the data dependent on the range from which the signals were scattered. Each range bin contains the total number of photons collected by a channel during each time window, and a bin is constructed for each channel.

Additional features of this software is that the signals are displayed in real time, as well as an option for displaying the ratio between the two Raman channels, and options for background corrections and high count rate corrections.

4.4.4 Data recording

Data is recorded into 2048 range bins, the width of which are set by the user using equation 2.2.1 Further the user can select the time window for the collection - the time over which signals are collected. Using narrower time windows allows for finer temporal resolution, but at the cost of fewer photons counted during each run. Similarly, an increased spatial resolution reduces the counted photons in each range bin.

Each range bin is saved as .mcs (binary) file at the end of each time window (see below).

4.4.5 Signal Processing

Once the signals are saved as .mcs files they can be read into IDL (Harris Corporation) for data analysis - see section 8.1 for more.

In this chapter each component of the BLT has been identified and any changes made from the original instrument to create an instrument capable of monitoring nocturnal urban boundary layer temperature. The next chapter discussed the approach used to calibrate the instrument to this end.
Chapter 5

Spectral Calibration

5.1 Interference filters

The interference filters are used in the BLT to spectrally select very narrow portions of the collected light corresponding to sections of the rotational Raman spectrum excited by the laser. The spectral lines in the rotational Raman spectrum follow opposing temperature-dependence in their brightness, so a ratio of intensity from lines of opposing dependence provides the optimum sensitivity as first suggested by Cooney (1972) - see figure 3.2.1.

The interference filters must be accurately calibrated because of the strong difference in the brightness of the rotational Raman spectral lines (see figure 2.4.6). The temperature measurement of the BLT is detailed in Chapter 7 which requires exact knowledge of the interference filters and the rotational Raman spectral lines.

Interference filter degradation  Interference filters formed of thin films deposited onto the surface of a substrate can be degraded by the intrusion of water vapour between the layers over time. As such to increase the lifetime of an interference filter they need to be stored in a dry environment. In the case of the BLT interference filters the cube in which they (and the beamsplitter) were mounted was removed from the BLT optics when not in use and placed into a humidity-controlled environment.
5.2 Calibration equipment and method

5.2.1 Monochromator

Monochromators are widely used to select narrow wavelength ranges for calibration purposes by using a diffraction grating to separate individual wavelengths. Many of the wavelengths of the diffraction pattern are directed into a beam dump but a slit in the beam dump allows the desired wavelength to be used.

Varying the angle at which light strikes the diffraction grating allows for controlled selection of which wavelength light is directed towards the slit in the beam dump (see figure 5.2.1). Controlling this angle using a stepper motor allows monochromators to scan across a range of wavelengths. The spectral resolution of the spectrometer is determined by the size of the entrance and exit slits (by calibrating the monochromator using a mercury lamp the separation of the 365nm doublet was resolved).

The monochromator used for this work was a Hilger Analytical Monospek 1000 Scanning Monochromator, controlled by a Hilger Analytical Programmable Monochromator Controller A430. This monochromator uses two mirrors, one to collimate the light from the slit to illuminate the diffraction grating and one to focus the light from the diffraction grating onto the monochromator exit slit (the beam dump for this monochromator is inside the casing). This monochromator model is supplied with variable width entrance and exit slits and a shutter to close off the entrance slit.

Figure 5.2.1: Monospek monochromator schematic. Light enters via the entrance slit and is focussed onto a diffraction grating to separate the light by wavelength. The scattered light is focussed on the monochromator exit hatch.

Taken from the user manual.

To calibrate the monochromator a mercury lamp was used - the lamp light was fo-
cussed onto the entrance slit with a PMT located after the exit slit and a scan made of the 365nm (365.015nm and 365.484nm) doublet. A light screen was constructed to shield the PMT from stray light.

For all further calibrations using the monochromator a halogen lamp was used for its stable output and broad, smooth spectral profile. The focussing optics were left in place for all future calibration work to ensure the halogen lamp output was focussed onto the monochromator entrance slit.

### 5.2.2 In situ. calibrations

To scan the interference filters *in situ* the monochromator output needs to be transferred to the BLT optics. To this end a liquid light pipe (Edmund Optics part number #53-691) was used - see figure 5.2.2.

![Coupling the monochromator to the BLT optics](image)

Figure 5.2.2: Coupling the monochromator to the BLT optics. The liquid light pipe is shown by the green line and the light is focussed onto the BLT aperture using a lens.

To ensure that the light from the light pipe travels into the BLT optics at an appropriate angle to simulate signals collected by the telescope the ‘divergence cone’ of light leaving the light pipe needs to be matched to the *f* number of the receiver using a lens. Figure 5.2.3 shows the light leaving the light pipe (red rays) and spreading out before a lens focusses the light onto the BLT aperture.
The position and power of the lens was determined by considering the cone constructed between the secondary mirror (upper curve in figure 5.2.3) and the BLT aperture. This cone has a shallower apex angle than the grey ray cone which serves to limit the size of the light spot passing through the collimating tube and into the optics cube. A light screen was positioned around the end of the light pipe, secured to the BLT aperture.

![Diagram of lens position and power determination](image)

Figure 5.2.3: Matching divergence and acceptance cones.

**Monochromators and polarisation**

Breckinridge (1971) identified that monochromators may impart some polarisation onto the output light. However, by passing light through a light pipe or fiber-optic cable it is possible to remove the polarisation from a light source, which is examined in section 5.3.

### 5.2.3 Calibration procedure

To calibrate the receiver the laboratory required blacking out and light screens were constructed around the halogen lamp mount and the interface between the light pipe and the monochromator exit hatch.

A time period was required to allow the PMT dark current to equilibrate - the output for which (under no illumination) was monitored using ORTEC MCS-32 software Version 2.11. When the dark currents for each PMT had equilibrated (approximately 40
minutes) the monochromator entrance slit shutter was opened and the receiver scanned from 352.5000nm to 358.2000nm at a rate of 0.5nm min\(^{-1}\). To make a background measurement the shutter was closed again after the scan had completed. These background measurements include signals arising from dark current, as well as any ambient light present in the BLT optics.

5.3 Polarisation calibration

Rotational Raman spectra carry a polarisation which is 57% parallel to the laser polarisation [Behrendt, 2005, p.284] so any calibrations performed using unpolarised light are not representative of atmospheric signals. To address this, calibrations were performed using light polarised parallel and perpendicular to the laser light by mounting a polarisation filter (Comar Optics component number 01 WL 50) across the optics cube.

The orientation of the polarisation plane of the laser was determined by running the LiDAR with a polarising filter fixed in a rotating graduated mount and averaging data over 3 minutes for 10° rotational steps in the polariser orientation. The elastic LiDAR return is almost 100% polarised parallel to the laser, so this provided a reference for the calibration; a sharp minimum in signal was observed when the polariser was orientated at 90 degrees to the laser polarisation.

The calibrations using light polarised parallel and perpendicular to the laser light were then combined in a weighted ratio following:

\[
R(T) = \frac{fS_{N,\parallel}(T) + (1 - f)S_{N,\perp}(T)}{fS_{F,\parallel}(T) + (1 - f)S_{F,\perp}(T)}
\]  

(5.3.1)

where \(f = 0.57\) for the component of the rotational Raman spectrum polarised parallel to the laser light. \(S_N\) and \(S_F\) are the channel sensitivities of the near- and far- field channels, respectively. Naturally if the light source used to calibrate the rotational Raman channel filters is not unpolarised a bias will be introduced to the calibration.

5.3.1 Relative PMT sensitivities

By comparing the sensitivities of the rotational Raman channel PMTs it is possible to deduce whether the monochromator output light carries any polarisation following passage through the light pipe. By making a calculation of the beamsplitter ratio for the ‘normal’
arrangement, as well as the swapped arrangement, the relative photosensitivity (see section 4.4) of the PMTs can be deduced. The measured signal in each channel is determined by the beamsplitter function \( B^R \) for reflection, \( B^T = 1 - B^R \) for transmission, the response function of the interference filter for that channel \( T^{\text{Filt}X} \) and the quantum efficiency of that channel PMT \( Q_X \), thus:

\[
\text{Ratio}^{\text{Norm}} = \frac{S^\text{Norm}_N}{S^\text{Norm}_F} = \frac{T^{\text{Filt}2} B^R Q_2}{T^{\text{Filt}1} B^T Q_1},
\]
\[
\text{Ratio}^{\text{Swap}} = \frac{S^{\text{Swap}}_N}{S^{\text{Swap}}_F} = \frac{T^{\text{Filt}2} B^R Q_1}{T^{\text{Filt}1} B^T Q_2}.
\]

The beamsplitter function was examined and found to be polarisation-independent. Thus, because the interference filter and beamsplitter terms cancel:

\[
\frac{\text{Ratio}^{\text{Norm}}}{\text{Ratio}^{\text{Swap}}} = \left( \frac{Q_2}{Q_1} \right)^2 \tag{5.3.2}
\]

To make this calculation, the BLT was run during a night. Data was collected for each of the PMT arrangements and the ratios for equation 5.3.2 calculated using data from 1170-1230m. From this data it was determined:

\[ Q_2 = (1.095 \pm 0.001) \times Q_1 \]

By modifying the calculation of the beamsplitter ratio \( B^R \) to incorporate this PMT sensitivity the following relationship was determined:

\[ B'^R = B^R \times 1.095 \tag{5.3.3} \]

Where \( B'^R \) is the ‘adjusted beamsplitter ratio’.

**Light pipe output polarisation**

Using this adjusted beamsplitter ratio, the hypothesis that the output of the light pipe (while coupled to the monochromator as a light source - see figure 5.2.2) is composed of light polarised crossed with and parallel to the laser emission and weighted by weighting factor, \( \chi \). Thus the total signal reflected from the beamsplitter \( B^R \) is a linear combination of the reflected light polarised crossed with the laser \( B^R_\perp \) and the reflected light polarised parallel with the laser \( B^R_\parallel \):

\[ B^R = \chi B^R_\perp + (1 - \chi) B^R_\parallel \tag{5.3.4} \]
Where $R$ is the beamsplitter ratio as calculated from light passed from the light pipe and then through a polarising filter (fixed across the BLT aperture).\footnote{Note that for this experiment no interference filters were present in the optics cube.}

This value was compared to the beamsplitter ratio as measured with no polarising filter, see table 5.3.1:

<table>
<thead>
<tr>
<th>$B^R_\perp$</th>
<th>$B^R_\parallel$</th>
<th>$B^R_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.425</td>
<td>0.143</td>
<td>0.2845</td>
</tr>
</tbody>
</table>

Table 5.3.1: Beamsplitter ratios for different polarisations.

The value of $\chi$ which agrees the manufacturer’s data according to equation 5.3.4 is $\chi = 0.5018$, which to within measurement errors concludes that the light from the light pipe, which is used to calibrate the BLT receiver, is unpolarised.

5.4 Spectral profiles of the rotational Raman channels

Initially, the rotational Raman channel filters were both positioned in the Stokes branch of the rotational Raman spectrum. For this work they will be identified as the ‘near-field filter’ for the filter whose peak transmission is located closest to the lasing line, and the ‘far-field filter’ for the filter with its peak transmission further from the lasing line. The Stokes region of the rotational Raman spectrum was chosen for the superior brightness of the Stokes spectral lines over the anti-Stokes region (see the height of the grey and red spectral lines in figure 5.4.1).

5.4.1 Response function

The profiles shown in figure 5.4.1 (and throughout this work) represent a combination of several factors of the optics system. Firstly, the transmission profiles of the interference filters is the strongest contributor to the displayed traces. Secondly, any contributions from the beamsplitter, for example any variation of the reflection properties with wavelength. Thirdly, the spectral dependence of the PMTs, and fourthly the spectral dependence of the illuminating halogen lamp.

These calibrations ensure that any variation in beamsplitter reflectivity and PMT spectral sensitivity is incorporated into the response function, while the lamp spectral function
Initial calibrations of the BLT interference filters are shown in figure 5.4.1.

Figure 5.4.1 shows the background-corrected photon count for each channel (averaged over six profiles).

The difference in the sizes of the response functions is to ensure the total signal collected by each channel is of the same order of magnitude (see, for example figure 5.5.1 for comparative LiDAR signals).

### 5.5 Signal breakthrough

At the beginning of this work the BLT rotational Raman channel already had interference filters fitted into the system. Early work with the BLT highlighted that there was signal breakthrough of laser light into the near-field channel - see figure 5.5.1, which shows a LiDAR profile of both Raman channels and the elastic channel taken in the presence of...
Clearly there is a correlation between the features in the elastic and near-field Raman channels at approximately 500m, and to a lesser degree, at 1500m. This is indicative of some of the elastically-scattered light being accepted into the near-field Raman channel - the Raman filter does not reject enough of the returning elastic signal. Because the temperature determination of this experiment depends entirely on the ratio between the two rotational Raman channels (see, for example Ricketts and Vaughan (2012)) this breakthrough must be removed.

Figure 5.5.1: Breakthrough from the elastic channel and the near-field channel. Elastic signals are shown as the solid line, near-field channel in dashed line and far-field channel in dotted lines. Data presented from 20 October 2015.

The breakthrough seen between 500m and 600m indicates that the original near-field filter of the BLT transmits some laser light (see figure 5.5.2).
Rotational Raman spectral lines

Figure 5.5.2: Figure 5.4.1 with magnified region showing laser line transmission for near-field filter. Rotational Raman spectral lines are shown, modelled at 300K for molecular nitrogen and oxygen and are presented to show the relative brightness of the spectral lines at the same wavelengths of the channel response functions.

To address the breakthrough into the near-field channel by elastic scattering a replacement filter was designed. Chapter 6 discusses the approach taken to identify the necessary properties of the replacement filter, and introduces the modelling approach used to identify these properties. This model is compared with the work of Hammann et al. (2015), who have performed similar modelling work, before concluding that there are manufacturing limitations which must be considered.
Chapter 6

Replacement Filter Design

6.1 Spectral positioning of the replacement filter

Instead of replacing the original near-field interference filter with another near identical filter (without the degradation leading to the breakthrough), it was decided to move the near filter to the anti-Stokes side of the laser line. This region was chosen because as a thin-film interference filter degrades the tendency is for the lower-wavelength edge of the transmission profile to begin extending towards shorter wavelengths. By designing the replacement interference filter in the anti-Stokes region any degradation will not allow the filter transmission to extend to the laser line.

To achieve this the approach of Hammann et al. (2015) (after Radlach et al. (2008) - outlined in greater detail in (Radlach 2009, Appendix 1)) was taken. Atmospheric LiDAR returns were modelled (section 6.2) and the response of the BLT receiver system with a cosine-shaped filter (see section 6.2.2). The performance of this modelling work was compared with that of Hammann et al. (2015) before being used to identify a replacement interference filter for the BLT.

6.2 Modelling LiDAR signals

To identify the optimum characteristics of a replacement filter the return from the atmosphere must first be calculated - including the effects of the BLT collection settings (for example the spatial resolution and the time over which collected signals are accumulated).
6.2.1 Modelling photon arrival rate

To identify the response of a LiDAR optical system one must initially identify the number of photons arriving into the system, starting with the LiDAR equation (see equation 2.6.2).

The number of photons per unit time measured at the receiver (scattered from height \( h \)) - \( P_X(h) \) - is given by

\[
P_X(h) = P_0 E_X O(h) \frac{A}{h^2} \Delta R N_R(h) \int_{\Delta \lambda_X} \xi(\lambda') \frac{d\sigma_X(\lambda', \pi, T)}{d\Omega} \tau(\lambda', h) d\lambda'
\]

(6.2.1)

where \( P_0 \) is the number of photons per unit time emitted into the atmosphere from the laser - given by the number of photons emitted per pulse multiplied by the pulse repetition frequency. \( O(h) \) is the overlap function of the LiDAR instrument, \( A \) is the area of the telescope mirror, \( E_X \) indicates the efficiency of detector channel \( X \) and \( \Delta R \) is the range resolution of the LiDAR instrument.

\( \xi_X(\lambda') \) is the filter transmission at \( \lambda' \) for channel \( X \) and \( \tau(\lambda', h) \) indicates the atmospheric transmission of the atmosphere for the two-way trip of the scattered light (at altitude \( h \) and wavelength \( \lambda' \)). The integral over \( \lambda' \) is over the range of the interference filter of channel \( X \).

\( N_R(h) \) is the atmospheric number density of the atmosphere at altitude \( h \) above the instrument, taken from a standard atmospheric model.

\[
\frac{d\sigma_X(\lambda', \pi, T)}{d\Omega}
\]

denotes the rotational Raman backscatter cross section at wavelength \( \lambda' \).

Because the boundary layer capping inversion is typically about 1km, the LiDAR return from that altitude is modelled. Making the estimates that \( \tau = 1 \) and \( O(h) = 1 \) (assuming that the LiDAR is completely overlapped at a range of 1km) and that an altitude of 1km the pressure is 900hPa and invoking the Ideal Gas Law \( P_X(h) \) becomes:

\[
P_{X,1km} = \left\{ P_0 \Delta R \frac{A \cdot 900hPa}{k_B T} \right\} E_X \int_{\Delta \lambda_X} \xi(\lambda') \frac{d\sigma_X(\lambda', \pi, T)}{d\Omega} d\lambda'
\]

(6.2.2)

The bracketed terms are wavelength-independent so for the purposes of modelling the LiDAR signal from 1km they can be treated as a single constant \( Y \).

\[
P_{X,1km} = Y E_X \int_{\Delta \lambda_X} \xi(\lambda') \frac{d\sigma_X(\lambda', \pi, T)}{d\Omega} d\lambda'
\]

(6.2.3)

Note that this treatment assumes that the efficiency of the optics \( (E_X) \) is unity for simplicity.
6.2.2 Modelling filter profiles

A cosine-shaped filter profile (as opposed to the Gaussian profiles used by Radlach et al. (2008)) was modelled using the following:

\[
T_{\text{filter,}X}(\lambda) = \begin{cases} 
T_{\text{max},X} \left[ \cos \left( \frac{2\pi(\lambda - \lambda_{\text{filter,}X,\text{centre}})}{3\lambda_{\text{filter,}X,\text{FWHM}}} \right) \right] & \text{when } |\lambda - \lambda_{\text{filter,}X,\text{centre}}| < 0.75\lambda_{\text{filter,}X,\text{FWHM}} \\
0 & \text{when } |\lambda - \lambda_{\text{filter,}X,\text{centre}}| \geq 0.75\lambda_{\text{filter,}X,\text{FWHM}}
\end{cases}
\]

- \(T_{\text{filter,}X}(\lambda)\) Filter X transmission at wavelength \(\lambda\)
- \(T_{\text{max},X}\) Maximum transmission of filter X
- \(\lambda_{\text{filter,}X,\text{centre}}\) Central wavelength of filter X
- \(\lambda_{\text{filter,}X,\text{FWHM}}\) FWHM of filter X
- \(\lambda\) Wavelength of rotational Raman spectral line

For the purpose of modelling the transmission of the filter was considered to be 30%. A cosine shape was selected for the steeper increase from zero and flatter top of the profile better matching the shape of the existing BLT interference filter response functions.

6.3 Modelling LiDAR response to rotational Raman spectral lines

By modelling the response of the BLT to different portions of the rotational Raman spectrum of molecular nitrogen and oxygen possible changes to the interference filters can be identified, modelled and the effects of such changes can be quantified. This allows modelling an optimum replacement for the original near-field filter to remove the elastic breakthrough.

To calculate the signal in each of the channels \((S_X)\) the backscatter cross section of each the rotational Raman spectral line is multiplied by the filter transmission at that wavelength and the photon arrival rate from the area of interest:

\[
S_{\text{channel,}X} = \sum_{\lambda} \frac{d\sigma}{d\Omega_{\text{Raman line}}} (\lambda) \xi_{\text{filter,}X}(\lambda) Y
\]

This sum is performed over the first 50 spectral lines (for both the Stokes and anti-Stokes regions of the rotational Raman spectrum) excited by the illuminating laser, and
for a number of different temperatures, extending beyond those expected in the nocturnal boundary layer above Manchester.

The ratio between the channel signals (near-field to far-field channels) is calculated, which is used to produce a lookup function for calculating the temperature (see chapter\[7\] for details).

### 6.3.1 Temperature error

Photons arriving at the photocathode are assumed to be statistically independent so the arrival rate follows Poisson statistics. In this case, if $S_X$ photons are counted in channel X then the standard error for that channel count is given by $\sqrt{S_X}$. As the intensity of the Raman spectral lines are temperature dependent then so are the signals measured in each channel.

The standard error in the measured ratio ($R$) is therefore:

$$\Delta R(T) = R(T) \sqrt{\frac{1}{S_{\text{near-field}}(T)} + \frac{1}{S_{\text{far-field}}(T)}}$$  \hspace{1cm} (6.3.1)

This error treatment gives the error in the ratio between the signals, which is converted to a temperature uncertainty by approximating the shape of the ratio between the Raman signals as linear over small ranges.

Thus the error in the calculated temperature is given by equation\[6.3.2\]:

$$E_T(T) = R(T) \sqrt{\frac{1}{S_{\text{near-field}}(T)} + \frac{1}{S_{\text{far-field}}(T)}} \frac{dR}{dT}$$  \hspace{1cm} (6.3.2)

### 6.3.2 Validating this approach

The model was verified against the work of Hammann et al. (2015) - repeating their analysis of locating the minimum temperature error for their LiDAR using the filter profiles supplied in their table 1:

<table>
<thead>
<tr>
<th>Filter Type</th>
<th>Peak Transmission</th>
<th>FWHM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Low-J filter</td>
<td>0.53</td>
<td>0.3nm</td>
</tr>
<tr>
<td>High-J filter</td>
<td>0.52</td>
<td>0.5nm</td>
</tr>
</tbody>
</table>

Table 6.3.1: Initial filter properties of Hammann et al. (2015).
By modelling the LiDAR response with these filters the following temperature errors were calculated:

![Image](image.png)

(a) Hammann et al. (2015) filter identification (see their figure 5). Colours indicate the magnitude of error associated with using this temperature measurement technique (K).

(b) Modelled filter identification of this work.

Figure 6.3.1: Comparison of the model and the work of Hammann et al. (2015). The disagreement between the depths of the minima is because our model does not temporally average the modelled LiDAR signals (thus the Poisson noise is greater and the temperature uncertainty correspondingly greater).

The data for figure 6.3.1 was produced by holding the FWHM of the filters constant at 0.3nm for the near-field filter and 0.5nm for the far-field filter, to replicate the work of Hammann et al. (2015) (see their table 1). The model subsequently varies the filter central wavelengths calculating for each the temperature error to identify the temperature error minimum. This model finds the minimum at (352.7,354.3) [far-field filter centred at 352.6nm, and near-field filter centred at 354.3nm], compared to (352.95,354.4) from the previous work. The difference between the near-field filter central wavelength is attributed to the difference in the filter profile shapes: the idealised filters used in our model follow a cosine profile, instead of measured profiles of Hammann et al. (2015).

Note that this analysis did not temporally average the signals, although this would not change the position of the temperature minimum, only the depth of the minimum. The improvement in temperature error arises from an increase in the modelled number of
photons arriving at the PMT photocathode, and thus a decrease in the Poisson error in the signal.

Having verified that our model accurately reproduces the calculations of similar instruments (Hammann et al., 2015) it was adapted to calculate the optimum properties of the replacement near-field filter for the Manchester BLT.

6.4 Optimum position of the near-field filter

To identify a replacement near-field filter the model was initialised using a principal central wavelength and FWHM for the modelled filter as described in section 6.2.2 (the far-field filter was described by the calibration data for the response function). The model calculates a modelled signal ratio as well as a modelled temperature error as per equation 6.3.2.

The modelled near-field filter was varied by iteratively varying the FWHM across a small range. After the ratio and temperature error were calculated for each step of the FWHM variation the central wavelength was varied by a small step and the FWHM variation (with ratio and temperature error calculations performed) repeated. This process was repeated until the desired range of central wavelengths and FWHM had been modelled, the data for which are presented in figure 6.4.1.
Figure 6.4.1: Locating the temperature error minimum for a LiDAR using the existing far-field filter and a cosine-shaped new near-field filter located in the anti-Stokes region of the rotational Raman spectrum. The diagonal lines shows combinations of FWHM and CWL which transmit elastically-scattered light.

From this calculation the minimum in temperature error of 1K using these interference filters requires a near-field filter located at 354.3nm with a FWHM of 0.5nm - shown in figure [6.4.2]. Note that the diagonal line in figure [6.4.1] is indicative of when the near-field filter overlaps the lasing line and exhibits elastic signal breakthrough so data is not presented for this region. These data are for a LiDAR operating with an averaging time of 90s, and averaging over an atmospheric cylinder of 30m length.

This modelled near-field filter for the BLT optical system is shown below.
6.5 **Comparison of modelled, old and replacement filters**

Materion were requested to produce a filter based on the properties identified by the model, but could not guarantee sufficient rejection of the filter that close to the lasing line of the LiDAR. Instead the suggested closest that could be produced is summarised in table 6.5.1:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Materion best match filter</th>
<th>Modelled filter</th>
</tr>
</thead>
<tbody>
<tr>
<td>CWL</td>
<td>354.0 ± 0.1 nm</td>
<td>354.3 nm</td>
</tr>
<tr>
<td>FWHM</td>
<td>0.3 ± 0.05 nm</td>
<td>0.5 nm</td>
</tr>
<tr>
<td>Peak transmission</td>
<td>≥ 30%</td>
<td>30%</td>
</tr>
</tbody>
</table>

Table 6.5.1: Manufacturer's closest match to modelled replacement filter.

Following the procedure to calculate the temperature error (see section 6.3.1) using a filter with the above properties will allow measurements to be made with a 2.1K temperature error.
Figure 6.5.1: Multiple runs of model to identify temperature errors for a number of LiDAR settings and filters.

Here we can see that increasing the temporal period over which the LiDAR signals are collected or increasing the spatial range reduces the temperature error in the calculated temperature. By averaging over 60s and 30m the modelled BLT temperature calculation can be reduced to less than 1K.

Note that these signals were modelled to arrive from a range of 1km (assuming an atmospheric pressure of 900hPa), with an atmospheric temperature of 280K, a complete overlap of the BLT telescope field of view and the laser spot, and no atmospheric extinction. See section 6.2.1 for a more complete discussion.

6.6 Characterising the replacement filter

The response function of the replacement filter was characterised using the calibration approach used previously:
The replacement filter has a central wavelength of 354.05nm and a FWHM of 0.35nm, corresponding to a temperature error of 2.1K - see figure 6.4.2.

Following the design and installation of the replacement filter the BLT receiver was calibrated with this filter in place. Modelling work was carried out to determine the rotational Raman signals collected by each channel, and thus the ratio between the channels. By controlling the temperature of the modelled atmosphere the calculated ratio carries such temperature information - see Chapter 7 for details.
Chapter 7

Lookup Curve

7.1 Lookup Curve

The BLT calibration curve was calculated by modelling the rotational Raman spectrum excited by a laser of wavelength 354.7nm (see figure 6.6.1) at a specified temperature, similar to the approach used by Vaughan et al. (1993).

The backscatter cross-section \( \beta(J, T) \) of each of the rotational Raman spectral lines shown in figure 6.6.1 is multiplied by the spectral response functions of the near and far BLT channels. This follows the approach of equations 2.4.11 and 3.3.2, but with the filter function \( \xi \) replaced by the channel response function \( S \):

\[
\text{Ratio}(T) = \frac{\sum_j \beta(J, T) S_{N,j}}{\sum_j \beta(J, T) S_{F,j}} \quad (7.1.1)
\]

where \( S_{N,j} \) and \( S_{F,j} \) are the sensitivities of the near and far channels evaluated at wavelength \( \lambda_j \).

Because the rotational Raman spectrum is thermally-varying, this calculation is repeated for a temperature range expected to be observed overnight above Manchester. Based on this model, a lookup curve can be constructed, linking the model temperature to the expected signal ratio from the rotational Raman channels. First, however, allowance must be made for polarisation of the rotational Raman spectrum and the spectral profile of the halogen lamp.
7.2 Lookup curve polarisation breakdown

Having ascertained that the light passing through the light pipe from the monochromator is unpolarised as it enters the BLT receiver (see section 5.3), the signals measured in each channel when a polariser is fitted to the aperture may be taken as a measure of the relative sensitivity of that channel to the corresponding polarisation ($S_N$ and $S_F$). From equation 5.3.1 the expected ratio for light scattered from the atmosphere is:

$$\text{Ratio} = \frac{S_N}{S_F} = \frac{\mu I_{N,\perp} + (1 - \mu)I_{N,\parallel}}{\mu I_{F,\parallel} + (1 - \mu)I_{F,\perp}}$$

Where $I_{Y,XX} = \sum \beta_j S_{Y,XX,j}$ denotes the expected signal in channel Y with polarisation XX relative to the laser. $\mu$ is the fraction of the Raman-scattered light polarised parallel to the laser (57%) (Behrendt, 2005, p.284).

Because the polarising filter attenuates the incident light substantially, the signal to noise ratio of the calibration scans used to determine $S_\perp$ and $S_\parallel$ for each channel was significantly lower than for unpolarised light (2-5, compared with >10). As the rotational Raman spectrum is a series of discrete lines, noise in the measured spectrum can introduce errors in the lookup curve. To mitigate this, the scans using polarised light were smoothed by fitting to the curve measured using unpolarised light, as polarisation will not affect the spectral shape:

$$I_{N,\perp} = I_{N,Un} \frac{\int I_{N,\perp}d\lambda}{\int I_{N,Un}d\lambda}$$

$$I_{N,\parallel} = I_{N,Un} \frac{\int I_{N,\parallel}d\lambda}{\int I_{N,Un}d\lambda}$$

(7.2.1)

7.3 Planck correction

Because the ratio between the near and far channels is used, an additional correction must be made to the wavelength calibrations to account for the Planck function in the output of the halogen lamp used to illuminate the monochromator. This accounts for the variation of the intensity of output light due to the blackbody radiation of the lamp. This radiation function is determined by:

$$B = \frac{2hc^2}{\lambda^5} \exp\left[\frac{hc}{k_BT\lambda}\right] - 1$$

(7.3.1)
Here $B$ refers to the spectral radiance of the blackbody energy emission at wavelength $\lambda$, $c$ is the speed of light, $h$ is the Planck constant and $k_B$ the Boltzmann constant. $T$ is the temperature of the black body, which in the case of the halogen lamp is the temperature required for a black body emitter to emit a peak wavelength intensity at the same wavelength as the halogen lamp (given by the manufacturer as 3100K).

Assuming the halogen lamp is a black body emitter the spectral radiance of its output at the wavelengths of interest for this calibration is shown below:

![Blackbody radiance variation](image)

**Figure 7.3.1: Black body intensity variation with wavelength in relative units.**

Clearly the variation in the black body radiance over the region of interest for calibrating the response function of the Raman channels is small, but necessary to factor into the calibration. In figure 7.3.1 the intensity of black body spectral radiance has been scaled for plotting purposes. The inset shows the spectral radiance of the halogen lamp over a wider range of wavelengths.

### 7.3.1 Lookup curve with all corrections made

By incorporating the Planck correction the effects of the different polarisations of light (and polarisation weightings) the following lookup curves are produced.
The unpolarised light curve (green) was obtained by evenly weighting the contributions of the perpendicular- and parallel-to the laser polarisation curves. Similarly, the Raman polarisation curve is produced by adding together the parallel and perpendicular curves, but weighting 47:53 them as per Behrendt (2005, p.284).

The broad shape of the lookup curves in figure 7.3.2 can be explained by considering the response functions of each rotational Raman channel (shown in figure 6.6.1). At lower temperatures the near-field channel will measure a larger signal than at higher temperatures because of the dimming of the spectral lines in that region of the rotational Raman spectrum (see figure 2.4.6). Similarly, as the atmospheric temperature increases the signal measured by the far-field channel increases. Thus lower temperatures produce a larger ratio between the measured signals of the near and far channels.

7.3.2 Lookup curve uncertainty

Because the PMTs were operated in photon counting mode to calibrate the response function of the rotational Raman channels and this data is propagated to determine the lookup curve, the lookup curve uncertainty is determined by the Poisson noise of the calibration data.

By standard error propagation of these errors through the calculation of the lookup curve the following uncertainty was calculated:
7.4 Problems with the approach

7.4.1 Cube positioning

Comparison of BLT-derived temperatures with locally-launched sondes (see section 8.3.1) highlighted that the calibrations were much less accurate than expected from the calculations above. Further investigation of this erroneous calibration indicated that such calibrations were highly sensitive to the position of the channel separation cube. Each time the cube was removed and replaced in the BLT optics the angle it sat within the optics could vary slightly.

Correspondingly the exact locations which were illuminated on the near-field channel PMT photocathode varied slightly - causing changes in the response function calibration. To address this the cube was placed in the BLT optics, the response function was calibrated and the cube was not moved again. The risk of interference filter degradation was deemed to be too small to affect the calibration over the time period over which data was collected for this project.

7.4.2 Shading of the primary mirror

The shadowing of the primary mirror by the collimation tube (see figure 7.4.1) was not included in the calibration of the response functions.
Figure 7.4.1: Shadowing of the primary mirror. Visible are the support arms for the secondary mirror, the laser head and directing mirror support platform and the collimating tube.

Figure 7.4.1 shows the view of the secondary mirror from the BLT aperture. Clearly visible are the support arms for the secondary mirror (diagonal features), the laser head support platform (to the left of the image) and the collimation tube (right of the image). These act to shade the primary mirror from atmospheric signals. Since the receiver telescope focusses the mirror surface onto the photocathode the same pattern of masking propagates to the PMTs when the BLT is used for atmospheric investigations - but is absent when the system is calibrated. Therefore an ‘adjustment factor’ was needed to ameliorate this shortfall - see section 8.3.3.
Chapter 8

Data processing and error analysis

8.1 Data processing approach

Data saved into .mcs files by the LabView script were processed in one main IDL script, which is outlined in figure 8.1.1.

The data arrays contain counts both from backscattered laser light and background signals, including PMT noise unrelated to incoming photons. Fortunately, the background signals are constant in time and can therefore be quantified and subtracted from the gross signal. Here, the mean count in each channel over the final 200 range bins (ranges of 27.7 - 3.07 km) was taken as a measure of the background signal (and PMT noise) and subtracted from the gross signal, leaving only the atmospheric backscatter.

This script corrects for the breakthrough from laser light into the far-field Raman channel (see section 8.2).

An adjustment factor to correct for the shading of the primary mirror (which was not accounted for in the calibration (see section 7.4.2)) is made - see section 8.3.3 for details.

The ratio between the two rotational Raman channels is calculated, both as a whole night mean and for each range bin of each data file (to allow for evolution of the temperature structure to be identified).

An overlap correction is needed below 1 km to allow for the incomplete overlap of the laser light and the telescope field of view. Locally-launched sondes are used to quantify this correction (see section 8.4), which is then applied to the low-altitude data.

The corrected rotational Raman signal ratio is passed through the lookup curve to yield an absolute temperature for the atmosphere and displayed as both a whole night mean value (for clear skies) and a time and height varying temperature plot (see section 9.4). The absolute temperature data is converted to potential temperature data using equation 317.
1.1.3 to produce a the whole night mean stability profile.

The LiDAR backscatter ratio is used as a measure of the aerosol distribution of the boundary layer. This is achieved by taking the ratio between the elastic (which uses a far broader interference filter than the rotational Raman channels) and near-field channels (see section 8.9) of the BLT. A separate overlap correction is used for the backscatter ratio (outlined in section 8.9.2).
Figure 8.1.1: Flowchart outlining the main analysis script.
8.2 Breakthrough into far-field

Following the calibration work some breakthrough into the far-field channel was diagnosed - most clearly in the regions of low clouds. Because of the much smaller degree of breakthrough into the far-field channel compared to the near-field channel (with the original interference filter), and the time required for the replacement filter production and delivery, the far-field interference filter was not replaced during this work.

By modelling the breakthrough of elastic signals into the far-field channel as a linear combination of the true far-field signal and the elastic signal the degree of breakthrough can be determined:

\[
\text{Far signal}_{\text{true}} = \text{Far signal}_{\text{Measured}} - \epsilon \text{Elastic signal}_{\text{Measured}} \quad (8.2.1)
\]

Here \(\epsilon\) indicates the degree to which the breakthrough occurs. A linear correction is appropriate because of the small amount of breakthrough in clear air.

To identify the severity of breakthrough into the far-field channel we must examine data in which there is a readily recognisable feature visible in the elastic channel - such as a cloud layer. Because elastic scattering has a significantly higher scattering cross section than rotational Raman scattering, the signals on the elastic channel saturate in low cloud regions. Therefore the cloud layer used to quantify the breakthrough needs to be high enough that the elastic channel is not saturated. By considering this cloud layer and the breakthrough seen in the far-field Raman channel and subtracting a small percentage of the elastic channel counts (0.14%±0.01%) the breakthrough feature can be removed.

Note that this correction is limited to clear skies because in regions of cloud the elastic return is greatly brighter than in clear skies, whereas the far-field return is not substantially affected.

8.3 Sonde corrections

Because the calibration of the response functions was very sensitive to the position of the optics cube (and thus filter locations) the spectral calibrations could not be used directly to derive temperature profiles. Further calibration was accomplished by comparing the BLT temperature measurements to radiosondes launched next to the BLT when it was running. This allows identification of any systematic offset and also allows the overlap function of the instrument to be determined without recourse to highly involved modelling (as in
The use of locally-launched radiosondes has been a common approach to calibrating LiDAR instruments; see Behrendt and Reichardt (2000); Cooney (1983); Li et al. (2013); Nedeljkovic et al. (1993); Su et al. (2013), for some examples.

### 8.3.1 Sondes for data validation

The locally-launched sondes were supplied by Windsond (owned by Sparv Embedded AB) and each sonde launched was calibrated to ambient conditions using laboratory barometer and thermometer, prior to launch. These sondes are comprised of a motherboard with attached temperature, pressure, humidity and GPS sensors, small enough to fit inside a polystyrene drinking cup - see figure 8.3.1.

The sondes measure at a rate of 1Hz, transmitting to the receiver in real time. The intended ascent rate for the sondes was 2ms⁻¹, although in practice this differed slightly for each launch due to small variations in the amount of helium in the balloons used.

The temperature resolution of the sondes is greater than 0.35°C with operating temperature range of 233K - 353K, which is appropriate for local boundary layer temperatures. Two varieties of sondes were used, during the course of this work - summarised in table 8.3.1.

<table>
<thead>
<tr>
<th>Model</th>
<th>Operating temperature range (°C)</th>
<th>Resolution (°C)</th>
<th>Accuracy (°C)</th>
<th>Temperature sensor</th>
</tr>
</thead>
<tbody>
<tr>
<td>S1B</td>
<td>-40 - 80</td>
<td>0.1-0.35</td>
<td>0.3-0.7</td>
<td>Thermistor</td>
</tr>
<tr>
<td>S1H2</td>
<td>-40 - 80</td>
<td>0.01</td>
<td>0.3</td>
<td>Band gap</td>
</tr>
</tbody>
</table>

Table 8.3.1: Summary of the sonde sensors.

The radio antenna is visible as the white wire extending from the bottom of the cup in figure 8.3.1 with the humidity and temperature sensors protruding from the cup close to the lid.
By launching very small sondes no risk is posed to local air traffic due to the small party balloons (30cm diameter) needed to launch the sondes. Additional control is achieved using the user-controlled severing of the cord linking the sonde to the balloon\(^1\) so if the sondes were to be carried near to the airport they could be aborted and drop to the ground (the balloon ascent rate correspondingly increases to pass over the airspace of the airport at a safe altitude). Additionally, by considering the local weather forecast and using on-line tools allowed for predictions of where the balloons would drift and no launches were carried out if these predictions took them close to local airports.

### 8.3.2 Comparison experiments

Comparisons of the BLT temperature data against locally-launched sondes were carried out on four separate nights.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Observation date</th>
<th>Sonde model launched</th>
<th>Sondes launched</th>
</tr>
</thead>
<tbody>
<tr>
<td>IOP1</td>
<td>24-25 November 2016</td>
<td>5 sondes launched</td>
<td>S1B</td>
</tr>
<tr>
<td>IOP2</td>
<td>04-05 January 2017</td>
<td>2 sondes launched</td>
<td>S1H2</td>
</tr>
<tr>
<td>IOP3</td>
<td>13 January 2017</td>
<td>1 sonde launched</td>
<td>S1H2</td>
</tr>
<tr>
<td>IOP4</td>
<td>26-27 January 2017</td>
<td>5 sondes launched</td>
<td>S1H2</td>
</tr>
</tbody>
</table>

Table 8.3.2: Dates of comparison experiments.

Note that the second sonde launched during IOP1 has not been used in later analysis because it swiftly entered cloud thick enough to block the BLT signals. For the night

\(^1\)The radio link allows the user to monitor the sonde data as well as send a command to activate a heating wire to sever the thin cotton cord holding the sonde to its balloon.
of IOP3 approaching showers necessitated terminating the experiment early so only one sonde was launched.

8.3.3 Adjustment Factor

By passing the temperature measured by locally-launched sondes (see section 8.3.1) through the lookup table an expected Raman channel ratio is calculated, which may be compared to the measured channel ratio. If these ratios (expected and measured) are the same then there is no necessary adjustment required; however, in this case there is a discrepancy - a factor of 1.443 - see figure 8.3.2.

![Image](image.png)

Figure 8.3.2: Determining the adjustment factor. Presented is the ratio between the measured BLT ratio and the necessary ratio to agree with the sonde-measured temperatures. Four adjustment factor profiles are shown corresponding to sonde launches throughout the night of 24 November 2016 with the mean of these adjustment profiles shown in orange.

The data for figure 8.3.2 was collected during the night of 24th November 2016 (IOP1), compared to sondes launched during the night. The BLT data compared to the sonde-expected signal ratios has been averaged over a 20 minute window, centred on the time of sonde launch and has been smoothed over a moving boxcar of five range gates (spread over 75m). The sonde data was interpolated to ensure the comparison between
the sonde and BLT data are for the same range bins. The mean value of this ratio is shown in red. Clearly visible is that above an altitude of 2000m there is good agreement with the straight line fitted at 1.443. Visible at low altitudes (below approximately 1500m) the structure of the profile is indicative of a LiDAR profile not yet fully overlapped (see figure 2.2.2).

By this consideration making an adjustment to the lookup curve of a factor 1.443 brings the BLT-derived temperature into line with the sonde-measured temperature. The adjusted lookup table is shown in figure 8.3.3:

![Comparison of lookup curves](image)

Figure 8.3.3: Comparison of the lookup curve and the adjusted lookup curve.

This adjustment factor corrects for the effect of shading of the primary mirror that was not captured by the calibration procedure.

### 8.4 Overlap correction

The ratio in figure 8.3.2 increasingly departs from the far-field value below around 1700m. This is caused by the incomplete overlap between the laser emission and the telescope field of view.

A height-dependent correction factor \( X(h) \) was determined by considering the expected ratio as determined using the sonde profile (with the adjusted lookup curve) \( S_R(h) \) and the measured Raman channel ratio of the near-field channel \( N(h) \) and far-field channel \( F(h) \):

\[
X(h) = S_R(h) \frac{F(h)}{N(h)} \tag{8.4.1}
\]
This overlap correction factor was calculated for a single sonde launch (at 06:13) during the night of IOP4 (see table 8.3.2 for date) - see figure 8.4.1. This data has been averaged over the course of a 20-minute period centred on the time of the sonde launch, and vertically smoothed using a moving boxcar average of width 75m.

![Figure 8.4.1: Overlap factor. Data collected on night of 28 November 2016.](image)

Factoring in this overlap correction factor adjusts the discrepancy between the BLT-derived temperature (coloured profiles of figure 8.4.2) and the sonde-measured temperatures (black profiles). Figure 8.4.2a shows the comparison between the temperature determined from unadjusted BLT signals. Figure 8.4.2b shows the comparison between the sonde profiles and the temperatures determined from the overlap-corrected BLT data.
Figure 8.4.2: Effect of overlap correction factor on temperature comparison. Black profiles show the measured sonde temperature profiles, with the BLT temperatures shown in orange. The red and blue profiles show the maximum and minimum temperatures based on the Poisson noise of the BLT signals.

8.4.2a: uncorrected signals, 8.4.2b: corrected to IOP4 06:13 launch.

The blue and red colours of the plotted BLT-derived temperatures indicate the possible spread of measured temperatures based on the Poisson noise (see section 2.8.1) of each of the rotational Raman channels (blue for coolest possible temperature, red for warmest). Clearly with no correction applied to the ratio before the lookup table is consulted there is almost no agreement between the BLT temperature profiles and the sonde-measured temperature.

The agreement between the BLT temperature data and the sonde profiles is not perfect - indicating that there is a drift in the overlap correction function during the night, improving in agreement as the night progresses. This is to be expected because the method of producing the overlap correction function fits the BLT data to the 5th sonde profile of the night of 26-27 January 2017 (IOP4), by which time the BLT collimation tube had been exposed to cold air for an entire night (compared with the 19:16 launch of the same night where the collimation tube started at laboratory temperature of 22°C). Further, because
the 06:13 sonde profile from IOP4 will be a poor representation of the boundary layer temperature of other nights, the overlap correction function was calculated for each night a sonde was launched.

Note that at low altitude (below 500m) there is always a disagreement between the BLT data and the measured sonde temperature. This is because at very low altitudes the BLT struggles to resolve signals. The structure of the overlap correction factor profile in figure 8.4.1 varies very strongly at lower altitudes (below approximately 500m) showing that the overlap correction approach taken cannot fully address the restrictions of operating the BLT within the telescope near-field region. Thus, data collected from below 500m will not be presented.

8.5 Data averaging

By increasing the number of files over which the data is averaged the random error in the signals is reduced, at the expense of how representative the data is of the atmosphere (for example rapid temperature changes will be smoothed out by averaging).
Figure 8.5.1: Difference between sonde temperature and BLT-derived temperature for different averaging windows. The BLT data is averaged across the indicated time periods, centred on the time of sonde launch (03:10 of the night of 26 January 2017).

Data smoothed using 75m moving boxcar average.
Figure 8.5.1 is constructed by taking the mean of each range bin from a collection period window, centred at the time of sonde launch (03:10 during IOP4 - 26-27 January 2017). This value is subtracted from the sonde-measured temperature, with the darker shading indicating a disagreement of 1K or less between the sonde-measured temperature and the BLT-derived temperature - the lighter shading indicates a temperature discrepancy of ±1.5K. The percentages printed in the plots indicate the amount of measurements within the darker shaded area (upper value) and within the lighter shading (lower value). This calculation is performed for a number of different collection period windows ranging from 20 - 90 minutes.

By increasing the time averaging window to 90 minutes the proportion of the BLT measured temperatures for which disagreement between the sonde and BLT temperature is ≤1K reaches 59%. At the same time, the proportion of BLT measurements within 1.5K of the sonde measurements increases to 74.0%.

Because increasing the averaging time period above 40 minutes does not significantly reduce the 1.5K disagreement between the sondes and the BLT-determined temperature the data averaging time for later analysis was set to 40 minutes.

It needs to be noted that this work establishes the smallest bias between the BLT and sonde data sets. The uncertainty in the BLT temperature is determined by the (random) Poisson noise in the collection electronics as well as the systematic uncertainty of the near-field filter.

### 8.6 Error analysis

**Background error**

Note that the uncertainty in the background calculation is not included in the error analysis because the total photon count for each rotational Raman channel is significantly larger (typically by a factor of 330 for signals below 5000m) than the background count. The background is a combination of the true background ultraviolet light present in the atmosphere and the dark currents of the PMTs. The background for each channel is eleven orders of magnitude smaller than the signals, thus for the purposes of error analysis have been discounted.

By propagating through the errors of the photon count arrays the error in the rotational
Raman channel for a night’s worth of data\textsuperscript{2} is calculated, and hence an error on the temperature calculation. The error bars were produced by propagating the Poisson errors on the BLT rotational Raman channel signals.

Figure 8.6.1: Comparison of the BLT temperature data and the associated error for 28 November 2016. The error bars shown are random noise error bars based on the Poisson error of the collected signals. BLT data smoothed using 75m moving boxcar average and collected over 8.75 hours.

The temperature profile displayed in figure 8.6.1 has been averaged over the course of the night of 24 November 2016, excluding data from cloudy periods (averaging over 1049 files, corresponding to a little under 8 hours 45 minutes). Further, the temperature data has been spatially smoothed using a moving boxcar average of width 75m (equivalent to 5 range bins); the temperature error has not been smoothed.

At a height of 1km (1005m) the total width of the temperature error bar is 0.31K. Note that this is less than the 2.1K systematic error obtained using the lookup curve approach with the replacement filter, which must be considered the minimum obtainable uncertainty when operating the BLT with the calibration curve approach for temperature retrieval.

\textsuperscript{2}The whole night data was produced by calculating the mean ratio between the rotational Raman signals corresponding to each height bin before applying the lookup function to provide a whole-night mean temperature. This effective reduces the Poisson noise and thus uncertainty of the measurement because the errors are summed and divided by the number of data collection files (1 every 30s of data collection).
8.6.1 Systematic errors

By comparing how the overlap correction factor varies from night to night a measure of the stability of this correction factor can be made. Figure 8.6.2 shows uncorrected BLT data and the sondes launched for comparison. This data is presented for each IOP, with the exception of the final launch of IOP4.

Figure 8.6.2: Comparison of uncorrected BLT-derived temperatures and individual sonde launches. Data averaged over a 40-minute window, centred on the sonde launch.

By applying the correction factor shown in figure 8.4.1 on the temperature profiles shown in figure 8.6.2 the profiles shown in figure 8.6.3 are determined.
Figure 8.6.3: Comparison of BLT-derived temperatures, corrected to IOP4 06:13 sonde launch and individual sonde launches. Data averaged over a 40-minute window, centred on the sonde launch.

Figure 8.6.3 shows the comparison of the BLT-derived temperature and the sonde temperatures, but this does not show how closely the datasets agree. By subtracting the BLT-determined temperature from the measured sonde temperature (interpolated to the same height as the BLT data, where necessary) a direct comparison can be drawn - see figure 8.6.4.
Figure 8.6.4: Comparison of sonde and BLT temperatures. BLT data overlap corrected with IOP4 06:13 sonde launch data. Data averaged over a 40-minute window, centred on the sonde launch.

As with figure 8.5.1, the lighter shading denotes a discrepancy of 1.5K, and the lighter shading shows a 1K difference. Note that the data in figures 8.6.4 and ?? have not been smoothed.

Immediately clear is that the temperature difference between the interpolated sonde measured and BLT-determined temperatures is that correcting using the 06:13 sonde launch from 26 January 2017 (IOP4) is appropriate for the other profiles of IOP4. However, data for the other IOPs have been adjusted such that they overestimate the temperature by several degrees (3K-5K) at below 1000m, although further aloft the temperature difference is lower.
Because correcting to the final launch of IOP4 brings the temperature determined during IOP3 into good agreement with the sonde measurement above approximately 600m, we will investigate whether using a reference sonde from another night to correct the BLT data produces a better agreement with sonde measurements than not using any sonde-determined corrections. Thus, data from nights when no sondes were launched will be corrected using the overlap correction was taken from the closest sonde launch under similar atmospheric conditions available, but care must be taken in drawing detailed conclusions.

By using a sonde from each night to calculate the overlap correction factor, an the difference between the measured sonde profiles and the BLT-determined temperatures is significantly reduced - see figures 8.6.5 and ??.
Figure 8.6.5: Comparison of BLT-derived temperatures, corrected to the final sonde launched during each IOP. Data averaged over a 40-minute window, centred on the sonde launch.
There is an intriguing structure in the temperature retrieved by the BLT above altitudes of approximately 1500m - the temperature structures show a strong variability not seen in the sonde profiles. Within the uncertainty of the retrieved temperatures (the red and blue lines) the BLT temperature still agrees with the sonde profiles, but the increasing uncertainty is attributed to the reduction in signal strength with height, and the correspondingly increased relative magnitude of the Poisson error compared with the signal strength.

By using a sonde for each IOP experiment to determine an overlap correction for each night the BLT temperature retrievals are brought into much closer agreement with the locally-launched sondes. Figure ?? shows this more quantitatively.
Figure 8.6.6: Comparison of sonde and BLT temperatures. BLT data overlap corrected with the temperature profile obtained by the final sonde profile launched that night. Data averaged over a 40-minute window, centred on the sonde launch.
These data show that the sonde and BLT-derived temperature measurements generally agree to 2K, especially below 1500m. There is a good agreement between the sonde measurements and the BLT-derived atmospheric temperatures, especially below 1500m (see figure 8.6.7 for a scatter comparison).

Figure 8.6.7: Comparison of sonde and BLT temperatures from 540m to 1200m. Black data are for 24 November 2016, blue data are for 04 January 2017 and red data are for 26 January 2016. The 1:1 line is shown in solid black, with the ±1K and ±2K spread shown in the dotted and dashed lines, respectively. Clearly visible is the positive bias of the BLT-derived temperature compared with the sonde measured temperatures.

The data presented above clearly shows that the agreement between the BLT-derived temperature data and the sonde measurements is typically less than 2K for measurements taken under 1500m. Also shown is the overestimation of the temperature by the BLT. The BLT clearly performs better at determining the atmospheric temperature under high pressure synoptic conditions compared with the southerly flow conditions (shown in the orange data).

Similarly, the comparison with the first sonde launched during IOP2 shows an overestimation of temperature, although this does not often exceed a 1.5K difference (light shading in figure ??) until an altitude of approximately 1600m, indicating that below the temperature inversion temperature retrieval is good, with increasing disagreement (underestimation) above the inversion.

This is sufficient to identify the temperature inversion for the IOP experiments (see tables 9.3.1 and 9.5.1).
8.7  BLT temperature retrieval

As discussed previously the ratio between the rotational Raman channels is used to determine the temperature using the lookup table shown in figure 8.3.3.

Data from the night of 24 November 2016 (figure 8.7.1) show that the BLT is capable of determining temperatures with the expected lapse rate (7K km\(^{-1}\), shown in blue lines\(^3\) in figure 8.7.1) both above and below the boundary layer capping temperature inversion.

These data are averaged over the course of the night, but files for which cloudy-skies obscured higher-altitude signals were excluded from this averaging. This is because the minor breakthrough into the far-field channel in the cloudy regions breaks the cloud-free skies assumption in the analytical correction made to the collected far-field signals (see section 8.2). Figure 9.4.2 shows all of the data for the night, displayed in a curtain plot. The overlap correction factor for this data was determined using the fifth launch of the night of IOP1.

Also plotted is the temperature profile as measured by the fifth balloon ascent of the night (05:56am on 25 November 2016) which shows the boundary layer capping temperature inversion at the same altitude (1km). However because the presented data is the mean for the whole night, rather than for the same time as the sonde launch the sonde data

\(^3\)Correspondingly to a lapse rate of 0.525K per range gate.
is not necessarily representative of the whole night temperature average. What is shown, however, is that the sonde-measured lapse rate for the night of 24 November 2016 is 7 K km$^{-1}$, and agrees well with the whole-night mean of the BLT data.

This agreement indicates that the BLT is capable of determining the lapse rate of the atmosphere accurately, as well as locating the boundary layer capping inversion when a overlap correction is made.

**8.8 Potential temperature**

The absolute temperature derived from the rotational Raman channel ratio and lookup curve can be entered into equation 1.1.3 to produce the potential temperature. Figure 8.8.1 shows the comparison of the 24 November 2016 temperature data with the calculated potential temperature.

Passing the absolute temperature derived from the rotational Raman channel ratio and lookup curve through equation 1.1.3 produces the potential temperature. Figure 8.8.1 shows the comparison of the 24 November 2016 temperature data with the calculated potential temperature.

**Figure 8.8.1: Whole night mean absolute temperature (blue) and potential temperature (red) for the night of 24 November 2016.**

Data smoothed using 75m moving boxcar average.
The potential temperature profile at lower altitudes shows a slightly increasing temperature with height (above the hump structure below 300m), which is indicative of a non-convective boundary layer - see figure 1.1.1ii. At the same altitude as the inversion shown in the absolute temperature (blue trace) the potential temperature begins strongly increasing with height - indicating a region of strong stability, and thus a strong indicator of the boundary layer capping temperature inversion. Further, figure 9.4.2 indicates the air aloft of this inversion is clean (see section 8.9 for further) compared with the more aerosol-rich air below, indicating an inversion.

While the potential temperature in this case is not necessary to identify the capping inversion (the absolute temperature shows a strong increase in temperature from approximately 1500 - 1800m), in the case of 04 January 2017 the use of the potential temperature shows stronger evidence of the boundary layer capping inversion - see figure 8.8.2.

![Figure 8.8.2: Whole night mean absolute temperature (blue) and potential temperature (red) for the night of 04 January 2017. Data presented are for cloud-free skies. Data smoothed using 75m moving boxcar average.](image)

More visible in the potential temperature (red) profile is that at approximately 1400m the atmospheric stability increases, which in the absolute temperature (blue) profile is not so clear. The potential temperature for the observations made is therefore presented in Chapter 9 to clarify the trends shown in the absolute temperature data.
8.9 LiDAR backscatter ratio

8.9.1 BLT elastic channel data

It is not only the rotational Raman channels which can be used to probe the boundary layer capping inversion. By monitoring the elastic channel of the BLT it is possible to build a picture of overnight cloud cover and aerosol layers, monitored by using the LiDAR backscatter ratio ($R(z)$):

$$R(z) = \frac{\beta_{\text{aer}}(z) + \beta_{\text{mol}}(z)}{\beta_{\text{mol}}(z)} \quad (8.9.1)$$

where $\beta_X$ refers to the aerosol and molecular contribution to the backscattered light.

The molecular component of backscattered light can be approximated by the near-field measured signal.

However, because the temperature of the atmosphere varies with height, so does the backscatter cross section of light which can be detected by the near-field filter. Thus the molecular term can be cast as:

$$\beta_{\text{mol}}(z) = \frac{S_N(z)}{I_N(T(z))} \quad (8.9.2)$$

where $I_N(T(z))$ is the modelled response of the near-field filter to varying temperature.

Bringing together equations 8.9.1 and 8.9.2 the expression for the LiDAR backscatter ratio is obtained:

$$R(z) = \frac{S_E(z)}{S_N(z)} I_N(T(z)) \quad (8.9.3)$$

This value can be calculated for all range gates for each file, and have a separately calculated normalisation factor, using clear air above the boundary layer, to scale the calculated backscatter appropriately. $S_E$ is the signal retrieved by the elastic channel of the BLT, which uses a filter significantly broader than that of either of the rotational Raman channels. See figure 8.9.1 for an example of the LiDAR backscatter profile measured on the night of 24 November 2016.

Because the method of calculating the overlap correction (see section 8.4) provides a correction to the Near/Far channel ratio - not to individual channels - no overlap correction
can be made to the LiDAR backscatter ratio calculations using sonde profiles. Section 8.9.2 outlines the approach taken to partially correct for the overlap function.

**Temperature profile and LiDAR backscatter ratio**

Because the boundary layer capping temperature inversion limits the dispersion of the boundary layer aerosol, the temperature inversion should be located at approximately the same height as the normalised backscatter ratio drops to a ‘clean air’ value. Figure 8.9.1 shows the LiDAR backscatter ratio for the night of 24 November 2016 for clear-sky data (the LiDAR backscatter ratio cannot be calculated in regions of clouds due to the different sensitivity to attenuation and scattering of each of the elastic and near-field rotational Raman channels).

![Figure 8.9.1: BLT temperature and LiDAR backscatter ratio for clear skies on 24 November 2016.](image)

The backscatter ratio does show a strong change between the ‘humped’ structure and the curved profile above, but the expected abrupt change indicative of the top of the boundary layer produces a backscatter ratio which remains stable aloft of the boundary layer (in clean air). The curve in the backscatter ratio at higher altitudes than the temperature inversion layer indicates that an overlap correction needs to be made to this data before
meaningful conclusions can be made.

Section 8.9.2 discusses the approach taken to ameliorate this shortcoming in the Li-DAR backscatter ratio calculation.

### 8.9.2 Overlap correction

By fitting a quadratic function (see figure 8.9.2) to a portion of the backscatter profile in clear air (above the aerosol present in the boundary layer) an estimation of the overlap function can be made. Figure 8.9.1 shows an example of a quadratic overlap correction factor (shown in red).

![Correcting for overlap](image)

Figure 8.9.2: Fitting a quadratic curve to correct for backscatter overlap.

By making the assumption that this quadratic fit is a reasonable fit for lower altitude (above 600m - delineated by the blue line) clear air, this quadratic function can be used to normalise to clear air below the complete overlap height. This approach in effect calculates the necessary correction from equation 8.9.3 but also normalises the backscatter ratio to the clean air to which the quadratic curve is fitted. By doing so, the profile in figure 8.9.3 is obtained.
Figure 8.9.3: BLT temperature and overlap corrected LiDAR backscatter ratio for clear skies on 24 November 2016.

This LiDAR backscatter ratio clearly shows the aerosol ‘shelf’ at the top of the boundary layer with the greatest change in the ratio (dropping from the ratio peak) is located approximately 100m below the temperature inversion.

Because the overlap function for the LiDAR backscatter is not stable until approximately 600m, any observations from lower than this height will not be presented.

This overlap correction approach is dependent on the height of the temperature inversion because clean air is needed to identify the quadratic function, so this correction approach is calculated for each night the BLT was run (see the case studies in section 9.4).

Having concluded that the BLT is capable of making temperature measurements which, working with the whole-night average (figure 8.7.1), agrees with the expected lapse rate, case studies will be presented. These case studies use the correction and overlap factors determined earlier in this chapter, and present the evolution of the BLT determined temperatures. A LiDAR backscatter ratio and overlap correction approach has been in-
roduced to support the conclusions drawn from the temperature data. Comparisons are draw
with a forecasting model, presenting BLT data for the model time step alongside both the locally-launched sonde profile and the BLT data.
Chapter 9

Observations

This chapter seeks to address the third and fourth questions posed in chapter 1; whether the nocturnal boundary over Manchester is observed to become stably stratified according to the BLT temperature retrieval and whether the inversion is adequately represented in weather forecasting models.

This chapter will present six case studies investigating the nocturnal boundary layer over Manchester during winter under different synoptic regimes (see section 9.1). The maximum precision of the BLT temperature retrievals will be presented in section 9.2 before the data for the case studies will be presented in section 9.4.

By considering not only the temperature retrieval, but the LiDAR backscatter ratio (see section 8.9) too, the boundary layer capping inversion will be examined with regards to the temperature and aerosol profiles.

The BLT data is supported by a local monitoring station operated by the University of Manchester. The Whitworth Observatory is located on top of the George Kenyon Building (approximately 160m from the BLT), and is supported by a number of street-level temperature sensors, which record temperature data in 60s intervals. The data presented in figures 9.4.5 and 9.4.13 is from a Rotronic Hygroclip S3 mounted in a passive radiation shield and located on the George Kenyon Building.

Following the comparison with sondes the BLT capping inversion height is compared with a model (WRF version 3.4.1) output for the night in question (see section 9.5). Because only limited data is available this comparison is presented to identify model short-
comings, rather than to comprehensively quantify them\(^2\). To identify the ability of the model to resolve the nocturnal boundary layer over Manchester is assessed, with regards to the height, strength (defined by the temperature difference between the base of the inversion and when the temperature again begins falling with altitude), and depth of the inversion layer.

### 9.1 Case study synoptic regimes

The case studies took place under four distinct synoptic regimes - three in high pressure regimes, one under westerly flow, another under north-westerly flow and the final one under southerly flow. Table 9.1.1 summarises the conditions for each of the case studies presented.

<table>
<thead>
<tr>
<th>High pressure</th>
<th>Westerly flow</th>
<th>North-westerly flow</th>
<th>Southerly flow</th>
</tr>
</thead>
<tbody>
<tr>
<td>24 November 2016†</td>
<td>21 December 2016</td>
<td>13 January 2017*</td>
<td>26 January 2017**</td>
</tr>
<tr>
<td>28 November 2016</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>04 January 2017‡</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 9.1.1: Synoptic conditions of case studies. Dates suffixed with †, ‡, * and ** are those for which sonde data is used alongside the BLT data to quantify the performance of the BLT.

Table 9.1.2 lists the nights for which sonde data is used to support the BLT data and the figure which displays the synoptic chart for those nights.

<table>
<thead>
<tr>
<th>Night of observation</th>
<th>IOP</th>
<th>Synoptic chart</th>
</tr>
</thead>
<tbody>
<tr>
<td>24 November 2016†</td>
<td>IOP1</td>
<td>Figure 9.4.1</td>
</tr>
<tr>
<td>04 January 2017‡</td>
<td>IOP2</td>
<td>Figure 9.4.9</td>
</tr>
<tr>
<td>13 January 2017*</td>
<td>IOP3</td>
<td>Figure 9.4.19</td>
</tr>
<tr>
<td>26 January 2017**</td>
<td>IOP4</td>
<td>Figure 9.4.22</td>
</tr>
</tbody>
</table>

Table 9.1.2: Nights of sonde launches. The synoptic chart for each of the nights are shown in the figures listed.

\(^2\)Such comparisons could form the basis for further works, investigating not only the WRF model examined in this work, but a wider range of models.
9.2 Precision of temperature data

9.2.1 Whole night temperature averages

By taking the whole night mean (mean value of each range bin over the course of a data collection period) of the rotational Raman channel signals (for example, see figure 8.7.1) the effects of Poisson noise (see section 2.8.1) can be reduced. Taking the average removes any information about the evolution of the structure of the boundary layer capping inversion, in effect smoothing out any temporal information.

This smoothing out of temporal information is of particular significance when there are short-lived structures within the data. As such, presenting the mean temperature profile is of strong benefit during nights when there is little change in the temperature profile, or for short periods (see figures 8.6.5 and 9.4.21 for example), but in general the natural variability in the temperature structure of the boundary layer is lost.

Figure 9.2.1 presents BLT data showing the whole night temperature average from three IOPs 1, 2 and 4. All of the data in figure 9.2.1 have been vertically smoothed using a moving boxcar average of width 75m.

Note that the data for cloudy conditions during the night of 24 November 2016 have been excluded from the data plotted in figure 9.2.1. This is because the correction for elastic breakthrough into the far-field channel is not valid in regions of cloud, where the elastic return is much brighter.
Figure 9.2.1: Average overnight absolute temperatures for IOPs 1, 2 and 4. Error bars indicate the 1 σ random temperature error due to Poisson errors.

The temperature error (arising from Poisson noise) in the determined temperature retrieval at a height of 1000m is 0.31K for the night of 24-25 November 2016, 0.31K for the night of 04-05 January 2017 and 0.36K for the night of 26-27 January 2017.

The inversion depth is defined as the atmospheric region where the temperature is not falling with height. In the cases presented in figure 9.2.1 the inversions can be summarised as:

<table>
<thead>
<tr>
<th>Night</th>
<th>Inversion base</th>
<th>Inversion Strength</th>
<th>Inversion depth</th>
</tr>
</thead>
<tbody>
<tr>
<td>24 November 2016 (IOP1)</td>
<td>900 ± 45m</td>
<td>14.8 ± 2.1K</td>
<td>765 ± 90m</td>
</tr>
<tr>
<td>04 January 2017 (IOP2)</td>
<td>1500 ± 200m†</td>
<td>5.7 ± 2.1K †</td>
<td>495 ± 300m†</td>
</tr>
<tr>
<td>26 January 2017 (IOP4)</td>
<td>165±(?m ‡</td>
<td>5.7 ± 2.1K</td>
<td>405±(?m</td>
</tr>
</tbody>
</table>

Table 9.2.1: Inversion statistics for whole night averaged temperature data.

†The temperature inversion for the night of 04 January 2017 was considered to be from the lowest temperature measured by the BLT which in the profile is the higher of the two inversions. The magnitude of the uncertainty of this value reflects the inability of the data to differentiate between the inversions shown to conclude which indicates the base of the boundary layer temperature inversion. Similarly, the uncertainty of the inversion depth is also large. See tables 9.3.1 and 9.5.1 and their discussion for further discussion of temperature inversions found by the BLT and how they compare with sonde
measurements and a forecasting model output.

The inversion located by the BLT data is below the 500m limit identified in section 8.4 thus this value must be treated with caution (and why the error in the measurement has not been estimated). The discussion of the data from 26 January 2017 in section 9.4 outlines the approach taken to draw conclusions from this case study.

The uncertainties in the inversion base and depth presented in table 9.2.1 were made by considering how abruptly the temperature profile changes direction at the inversion base.

Because local minima are used to determine the inversion base, noise spikes in the near-field channel data can produce an erroneously low temperature value. By considering other points near to the inversion the effects of such noise spikes can be ameliorated. Thus the uncertainty in the inversion base is a measure of how many data points need to be considered to be confident that the inversion base is not caused by a random noise spike. The uncertainty of the inversion depth is a combination of the uncertainty in the inversion base and when the temperature begins falling again with height. This height is similarly affected by noise spikes so a number of data points around this height are considered, hence the larger uncertainty in inversion depth.

Because the strength of the temperature inversions has a large uncertainty for weaker inversions (notably the inversion from the night of 04 January 2017) caution must be used when drawing conclusions regarding inversion strength - see table 9.3.1 for more.

### 9.3 Comparison with locally launched sondes

To draw comparisons between the BLT and sonde data, the BLT data for the night was divided into times corresponding to the time of launch of the sonde. These time periods were 40 minutes in duration, centred on the time of sonde launch, over which the BLT data was averaged.

The temperature inversion was identified by considering when the absolute temperature profile began rising with height (ie the temperature lapse rate trend became positive). The depth of the temperature inversion is a combination of the uncertainty of the height of the inversion base, combined with the uncertainty of the top of the inversion (where the temperature stopped rising with height). Considering the data in figure 8.6.5 yields the following temperature inversion statistics:
<table>
<thead>
<tr>
<th>Synoptic/flow conditions</th>
<th>Investigation</th>
<th>BLT Base</th>
<th>BLT Strength</th>
<th>BLT Depth</th>
<th>Sonde Base</th>
<th>Sonde Strength*</th>
<th>Sonde Depth</th>
</tr>
</thead>
<tbody>
<tr>
<td>High pressure</td>
<td>IOP1 launch 1</td>
<td>720 ± 100m</td>
<td>9.9 ± 2.1K</td>
<td>195 ± 150m</td>
<td>‡ 845 ± 2m</td>
<td>6.7 ± 1.4K</td>
<td>443 ± 4m</td>
</tr>
<tr>
<td></td>
<td>IOP1 launch 3</td>
<td>690 ± 60m</td>
<td>7.6 ± 2.1K</td>
<td>405 ± 80m</td>
<td>‡ 686 ± 9m</td>
<td>5.9 ± 1.4K</td>
<td>398 ± 9m</td>
</tr>
<tr>
<td></td>
<td>IOP1 launch 4</td>
<td>960 ± 50m</td>
<td>14.3 ± 2.1K</td>
<td>495 ± 100m</td>
<td>912 ± 9m</td>
<td>9.8 ± 1.4K</td>
<td>423 ± 11m</td>
</tr>
<tr>
<td></td>
<td>28 November 2016</td>
<td>900 ± 100m</td>
<td>10.49±2.1K</td>
<td>495 ± 150m</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>IOP2 launch 1</td>
<td>1500 ± 100m</td>
<td>8.9 ± 2.1K</td>
<td>240 ± 200m</td>
<td>1421 ± 4m</td>
<td>6.4 ± 0.6K</td>
<td>317 ± 6m</td>
</tr>
<tr>
<td>Westerly</td>
<td>21 December 2016</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>North-westerly</td>
<td>IOP3 launch 1</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>Southerly</td>
<td>IOP4 launch 1</td>
<td>510 ± 45m</td>
<td>7.8 ± 2.1K</td>
<td>330 ± 90m</td>
<td>521 ± 3m</td>
<td>8.9 ± 0.6K</td>
<td>423 ± 4m</td>
</tr>
<tr>
<td></td>
<td>IOP4 launch 2</td>
<td>†</td>
<td></td>
<td></td>
<td>183 ± 3m</td>
<td>5.2 ± 0.6K</td>
<td>506 ± 4m</td>
</tr>
<tr>
<td></td>
<td>IOP4 launch 3</td>
<td>†</td>
<td></td>
<td></td>
<td>180 ± 13m</td>
<td>6.6 ± 0.6K</td>
<td>642 ± 14m</td>
</tr>
<tr>
<td></td>
<td>IOP4 launch 4</td>
<td>†</td>
<td></td>
<td></td>
<td>121 ± 2m</td>
<td>4.8 ± 0.6K</td>
<td>214 ± 4m</td>
</tr>
</tbody>
</table>

Table 9.3.1: IOP temperature inversion data.

* The uncertainty in the strength of the temperature inversion as seen by the sondes is calculated as twice the temperature accuracy for the type of sonde launched.

†These sonde profiles contain multiple temperature inversions. The data presented in table 9.3.1 is for the lowest of these inversions. The lowest temperature inversion in each case is also the strongest temperature inversion, which is most significant to boundary layer dynamics.

‡While the BLT data has identified a temperature inversion at these altitudes, data obtained by the BLT for altitudes lower than approximately 500m is well within the telescope overlap region. Correspondingly, such measurements cannot be used to draw meaningful conclusions (see section 8.4 for further details).
The data for 28 November 2016 and 21 December 2016 are whole night averages and, because no sondes were launched no sonde data is presented.

Any table entry of N/A indicates that no temperature inversion was identified, and correspondingly no data can be plotted in the comparison plots (see below). The data for IOP3 shows that in the case where no temperature inversion is located by the sonde the BLT data does not show a temperature inversion.

Figure 9.3.1 draws direct comparison between the inversion statistics for the BLT and sonde data (for inversions identified at heights greater than 500m).

Figure 9.3.1: Scatter plot comparing inversion statistics from BLT and sonde data. Black data indicate high pressure synoptic regimes, while orange data is from the southerly flow synoptic regime. Dashes show the 1:1 line. Dotted lines show ±100m for the inversion base and depth plots (panels i and iii), and ±3K for the inversion strength plot (panel ii). The BLT error bars presented show the 1σ error range.

Considering panel i, to within experimental uncertainty the BLT and sonde measurements of the data agree for all sonde launches for which an inversion was identified. Because of the high-frequency of the sonde measurements (1Hz) the error bars regarding sonde altitude are very small, correspondingly the identification of the inversion base from the sonde data carries little uncertainty. The BLT data, having been determined through 15m range bins as well as the uncertainties introduced through the use of the lookup function technique, overlap and adjustment corrections are substantially larger. However, because in each case the error bars reach the 1:1 line the data can be considered to agree with the sonde data.

Further the BLT yielded no false results regarding the presence of an inversion - the night of IOP3 (13 January 2017) showed no temperature inversion in either the BLT data
or the sonde data.

Panel ii of figure 9.3.1 shows the comparison of the inversion strength from the sonde and BLT data. By this metric the BLT performs less well - with a difference of around 3K between the BLT and sonde inversion strength data. Although the points are within 2 sigma measurement uncertainty, the points are not evenly distributed about the 1:1 line. The BLT data under a high pressure regime appear to overestimate the strength of the inversion, while the single data point from the southerly flow regime agrees much better.

Panel iii of figure 9.3.1 shows the inversion depth and highlights the weakness in the BLT’s ability to precisely resolve this parameter. While the BLT data (to within measurement uncertainty) all lies within 100m of the sonde data, the size of the error bars are often comparable to the determined value itself. Correspondingly, more work needs to be performed to constrain the temperature profile aloft of the inversion to capture the low tropospheric temperature profile, although that is beyond the scope of this work.

While there is some disagreement between the BLT data and the sonde profiles the values obtained agree sufficiently to allow an examination of the nocturnal boundary layer to determine whether a temperature inversion is present, as well as the evolution of the inversion base throughout the night.

9.4 Boundary layer profiles

Curtain plots  Curtain plots show data which varies both temporally and spatially within time/height space. They are very useful for monitoring temperatures retrieved by LiDAR instruments because they show both the spatial and temporal evolution of atmospheric parameters.

The temperature data in the curtain plots shown in this chapter were collected using 15m range bins and 30s collection time per file, and have been temporally and spatially smoothed using a moving boxcar average of width and height 40 minutes and 75m. Because the signal retrieval of the BLT is compromised below altitudes of 500m due to the operation in the near-field region of the telescope (see section 8.4) no data is presented for these regions.

The potential temperature of the atmosphere is calculated using equation 1.1.3 to high-
light the stability of the boundary layer. Because the temperature data is used in the calculation of potential temperature the smoothing is the same as that of the temperature curtain data.

Because clean air is needed to normalise the LiDAR backscatter ratio (see section 8.9) there are some times where it cannot be calculated (similarly there is no data for altitudes lower than 600m). The lidar backscatter ratio data presented in curtain plots was calculated from elastic and near-field data smoothed using the same boxcar averaging at the temperature data.

**High pressure regimes**

**24 November 2016 (IOP1)** The synoptic conditions on this night were characterised by high pressure centred over the United Kingdom, which persisted throughout the night. These conditions had formed the previous day, from an extending ridge off the Azores high following the north-eastwards migration of a low pressure centre from over the North Sea. This high pressure ridge was subsequently cut off from the Azores high, forming a high pressure centre over the UK. Figure [9.4.1](#) shows the surface pressure plot for the beginning of the observation period.

![Synoptic conditions on 25 November 2016](https://example.com/synoptic_plot)

**Figure 9.4.1**: Synoptic conditions at 0000 UTC on 25 November 2016.

During the night a layer of cloud formed at an altitude of approximately 800m, visible

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3From the UK Met. Office, accessed through [www1.wetter3.de](http://www1.wetter3.de).
in both the temperature and aerosol curtain plots as high-signal events. The increase in the BLT-retrieved temperature is due to clouds reflecting more elastic light than clear-sky, thus the breakthrough correction for the far-field channel is not sufficient (an increase in the far-field channel signal decreases the Raman channel signal ratio and thus the temperature appears larger - see figure 7.3.3). This cloud layer formed at 1900, before dissipating by 2145, following which the night sky remained cloud-free, barring a short-lived cloud layer again between 2230-2330.
Figure 9.4.2: Temperature and aerosol data for the night of 24 November 2016.

The vertical temperature profile during the course of the night shows the temperature dropping with increasing altitude (see figure 8.7.1), passing through an inversion before returning to a reduction with height. The boundary layer capping inversion at 1000m, descends slightly to approximately 900m by 0000 before rising to 1100m by 0500. This is approximately the shape of the absolute temperature profile in case D in figure 1.1.1i.
Because this relationship extends throughout the night we can conclude that the boundary layer remains unstable below the temperature inversion.

Further to the change in the capping inversion height, the lower atmosphere appears to warm during the course of the night (changing from a turquoise colour to a more yellow tone) at approximately 500m. Similarly aloft of the temperature inversion the atmosphere warms (changing from a more orange colour to red).

Visible in the LiDAR backscatter ratio data in figure 9.4.2 is a gradient from the higher-ratio data in the boundary layer to the cleaner air above. This evolution of the ‘aerosol inversion’ broadly mirrors the temperature inversion capping the boundary layer, although it is located approximately 100m lower, in line with the behaviour of figure 8.9.1. In part this arises from the different definitions used for temperature and aerosol inversions (Seibert et al., 2000), and the fact that the aerosol profile does not show a step change. While this finding is in line with the work of Hennemuth and Lammert (2006) who show that LiDAR measurements of boundary layer height agrees to within ±200m with sonde measurements, further work is recommended to understand fully the source of this discrepancy.

Note that the lowest 600m of LiDAR backscatter ratio data has not been plotted due to the overlap concerns outlined in section 8.9.2.

By considering the potential temperature, the inversion visible in figure 9.4.2 is clearly shown at the boundary between the blue and green colours. This boundary between the blue and green colours matches the evolution shown in the absolute temperature plot (figure 9.4.2).
Figure 9.4.3: Potential temperature curtain plot for 24 November 2016.

Considering individual profiles for separate times in the curtain plots provides a slightly clearer picture:
Figure 9.4.4: Temperature profiles for the night of 24 November 2016.

Note that the profile for 06:00 has less averaging than the other profiles because the data collection period ended before 06:20, not allowing the 40 minute averaging period recommended in section 8.5 to be completed.

Immediately visible in the above temperature profiles is the cloud layer from 700-900m in the 2000 profile. Additionally, the temperature inversion can be seen to change from the initial altitude of approximately 800m (at 1800), rising to 1km (2200) before falling to 900m for the rest of the night.

Discounting the profile for cloudy skies in figure 9.4.4 (second panel) there is strong evidence of a strengthening temperature inversion during the course of the night.

Because the BLT returns for under 500m cannot necessarily be considered accurate low-level temperature probing is not possible. Considering the temperature evolution at urban canopy level\(^4\) (figure 9.4.5) it can be seen that is little change during the night supporting the curtain plot in the conclusion that the inversion strengthening is due to

\(^4\)Using the Whitworth Observatory temperature sensor on the George Kenyon Building.
warmer air advecting over the site above the inversion.

![Temperature graph](image)

**Figure 9.4.5: Urban canopy level temperature for the night of 24 November 2016.**

**28 November 2016**  The high pressure persisted over the UK for several days before moving northwards in the days before 28 November 2016. It merged with another high pressure system centred over Greenland, although during this time the winds experienced by the UK remained weak westerlies. The Greenland high pressure system moved south-eastwards into the North Sea on 28 November 2016, still imposing anticyclonic conditions on the UK for the next few days.

Because this synoptic regime had persisted since the 24 November data collected for this case study used the overlap correction from the final sonde launch from IOP1.

![Synoptic map](image)

**Figure 9.4.6: Synoptic conditions at 0000 UTC on 29 November 2016.**
The temperature inversion for this night is stable at a height of 1000m which strengthens during the course of the night, with lower altitude air warming slower than air further aloft; as for 24 November 2016. However, the LiDAR backscatter ratio shows a different evolution in the aerosol layers within the boundary layer. The night begins with little visible in the LiDAR backscatter ratio, but develops a strong gradient at about 1900. This gradient strengthens significantly (the LiDAR backscatter ratio difference across the boundary increases) from 1900-2000, indicative that the boundary layer aerosol loading increases during this time. This gradient weakens slightly, before restrengthening between 2230-2300.
Figure 9.4.7: Temperature and aerosol data for the night of 28 November 2016.

Following 2300 the aerosol boundary drops rapidly to 900m, and weakens, almost decaying entirely by the end of the night.

The strengthening of the boundary layer capping inversion shown in the absolute temperature plotted in figure 9.4.7 is visible in the potential temperature profile, with the boundary between the deeper and lighter blue colours becoming more clearly defined.
during the night.

Figure 9.4.8: Potential temperature curtain plot for 28 November 2016.

04 January 2017 (IOP2) The high pressure during the night of 4 January 2017 formed following the passage of a cold front across the UK, and is a migration of the Azores high centre, initially into the mid-Atlantic, but then moving eastwards to just off the west coast of Ireland and merging with a high pressure in northern France to form a large high pressure system. This was prevented from dominating the UK conditions by a deep low pressure over the Baltic Sea, which slowly moved eastwards, allowing the high pressure system to move southwards and settle over the UK during 4 January.
During the night of IOP2 a layer of cloud formed at an altitude of 1300-1400m, persisting from 2145-0215. During this time the BLT was incapable of making temperature retrievals at altitudes above the cloud base due to the breakthrough of elastic signals into the far-field channel (see section 8.2 for details).
Figure 9.4.10: Temperature and aerosol data for the night of 04 January 2017.

The lower boundary layer appears to rise slightly in temperature with height during the night by a few degrees before the much stronger temperature rise shown in figure 9.4.10 at approximately 1600m. This temperature rise remains at approximately the same height during the night, which weakens during the cloudy period, before strengthening for the rest of the night. The inversion descends slightly as it strengthens between 0400
As indicated in section 8.9 the LiDAR backscatter ratio has not been calculated for data representative of cloudy skies. The LiDAR backscatter ratio shows a boundary descending from 1500m and strengthening as the cloud layer develops. Following the clearing of the skies, the LiDAR backscatter weakens, but remains at the same height, supporting the conclusion that the temperature inversion does not significantly change in height during the night.

The inversion height more clearly remains constant during the night when the potential temperature is considered (see figure 9.4.11). Further, the descent of the capping inversion between 04:00 and 05:00 is clearly visible.

By considering individual temperature profiles the evolution of the structure of the temperature inversion can be identified:
Very visible in the overnight temperature profiles in figure 9.4.12 is the cloud layer at the top of the boundary layer. This obscures the exact location of the temperature inversion because the reduced signals which penetrate the clouds twice are so noisy accurate temperature retrieval is not possible. However, because boundary layer clouds typically form with cloud top at the temperature inversion it is possible to make a judgment of where the boundary layer capping inversion is through the clouds of this night.

The profile for 1800 shows an inversion at 1500m, which corresponds to the top of the detected cloud layer - suggesting that the temperature inversion does not change in height significantly during the cloudy period. Once the cloud layer cleared it appears that the temperature inversion falls to 1400m at 0200 before rising again to 1500m by 0600. The ‘double inversion’ structure (at 1200m-1500m) at 0400 is intriguing, but without a corresponding sonde launch for this time validation of this feature it is not possible.

The BLT data for this night (figure 9.4.10) shows a stable stratification of the Manch-
ester nocturnal boundary layer, supported by the broadly unchanging potential temperature with height (see figure 9.4.11). These profiles are reminiscent of cases B and C of figure 1.1.1i, and supports the work of (for example) Kolev et al. (2000) in observing a stable boundary layer in an urban environment.

Low-altitude temperature retrievals of the BLT cannot be used to diagnose temperature because they are under the overlap correction limit. By considering the Whitworth Observatory data (figure 9.4.13) low-level cooling is shown, which is not identified by the BLT data above the overlap correction limit.

Figure 9.4.13: Urban canopy level temperature for the night of 04 January 2017.

The lack of temperature evolution in figure 9.4.12 despite the data shown in figure 9.4.13 indicates boundary layer stability within measurable range for the BLT is already present before data collection began. Considering figure 1.1.1i, this would indicate that the evolution between times B and C where low level cooling continues, but further aloft the temperature profile does not change.

**Westerly flow regime**

**21 December 2016** The westerly flow conditions were produced by a deep low pressure system centred over Iceland which, coupled with the Azores high pressure had maintained these conditions for nearly two days. Frontal passages during the day brought heavy rain, leaving mostly clear skies for the rest of the day and well into the following day.
Because there were no locally-launched sondes for this case study the overlap correction from IOP4 was used. See figure 9.4.15 for how the IOP overlap correction factors affect the agreement between the BLT data to sonde data from the Watnall atmospheric sounding station. This sonde was launched at 0000 22 December 2016, and the data retrieved from http://weather.uwyo.edu/upperair/sounding.html

The Watnall sonde data was not used to identify the overlap because of the low spatial resolution within the boundary layer, but it serves a good comparison to identify which IOP overlap correction factor to use.

5Located at (53.006N 1.251W); the closest station to the University of Manchester.
Identifying the appropriate overlap correction factor

Figure 9.4.15: Identifying which overlap correction factor is appropriate for 21 December 2016 data. Shown in red is the Watnall upper air sounding, the BLT data has been corrected using different correction factors and shown in the coloured and black traces.

Figure 9.4.15 shows the sonde profiles which have been used in constructing the correction factors for each IOP night, compared with the Watnall sounding for the night of 21 December 2016. It is apparent that the closest agreement between the Watnall sonde and the sondes launched to constrain the overlap correction factor is the sonde launched to constrain the IOP4 data, despite locating the temperature inversion at different locations. Thus, the overlap correction factor from IOP4 is the most appropriate to use (see figure 9.4.16).

There does not appear to be a temperature inversion during this night of 21 December (see figure 9.4.16). Instead the temperature profile for this night seems to be particularly consistent over time, justifying using a whole night average to diagnose the boundary layer (see figure 9.4.17).
Figure 9.4.16: Temperature and aerosol data from the night of 21 December 2016.

The LiDAR backscatter ratio has not been plotted for the period at the beginning of the night with the short-lived broken clouds before 20:00. While the temperature profile does not show any temperature inversion, the LiDAR backscatter ratio shows strong evidence for a series of aerosol-intensifying events throughout the post-cloud night.

There appears to be a wave-like structure at the top of the aerosol layers indicating
that the height of the aerosol ‘shelf’ changes during the night, but without evidence of a
temperature inversion little can be concluded other than raising the possibility of advected
aerosol-rich air from upwind. Due to the westerly flow this aerosol-rich air may carry ma-
rine aerosols, but this is impossible to diagnose using this instrument.

Because the thermal structure of the boundary layer observed overnight is unchanging,
a whole-night temperature average can be constructed to reduce random errors, without
smoothing out the changes in the temperature inversion height (see figure 9.4.17). Further,
because the temperature retrieval aloft shows good agreement with the Watnall sonde data
this data can be considered representative of a large-scale weather system, extending at
least from Manchester to Watnall.
Figure 9.4.17: Temperature data from the night of 21 December 2016. Black data is BLT-derived absolute temperature, red profile is the Watnall radiosonde temperature sounding.

The potential temperature profile (red in figure 9.4.18) similarly shows the stability of
the boundary layer - increasing with height above 800m\textsuperscript{6}. The presented data is the whole night mean of the potential temperature, which, due to the unchanging absolute temperature profile during the night is a good representation of the stability of the atmosphere for the whole night.

![Figure 9.4.18: Absolute (blue) and potential (red) temperature data from 21 December 2016.](image)

Considering these data in light of figure\textsuperscript{1.1.1ii} the absolute and potential temperature profiles above 800m closely resemble those of time B.

Below 800m the absolute and potential temperatures fall (before the potential temperature begins rising with height), suggesting a low-altitude behaviour more reminiscent of case A in figure\textsuperscript{1.1.1i} (absolute temperature falling with height and potential temperature showing a change in vertical gradient). Because the observations took place shortly after nightfall, this is attributed to the ground-level heating present in urban areas in the form of sensible heat from central heating, extending the lifetime of convective motions.

\textsuperscript{6}The decrease at low altitude is attributed to an overlap issue.
North-westerly flow regime

13 January 2017 (IOP3) The synoptic conditions were characterised by a high pressure centred in the mid-Atlantic and a series of low pressure centres in central Europe. Prior to the showers which forced the aborting of this observation period visibility was good, with north-westerly winds characterising the path taken by the sonde.

![Synoptic chart](image)

Figure 9.4.19: Synoptic conditions at 1800 UTC on 13 January 2017.

There does not appear to be a temperature inversion on the night of 13 January; further there is very little aerosol in evidence in figure 9.4.20. This might be expected from the synoptic conditions for this night. North-westerly flows typically bring clean air from over the north Atlantic, although in this case a similar LiDAR backscatter ratio to the night of 21 December 2016 might have been expected due to flow over the ocean.
Figure 9.4.20: Temperature and aerosol data from the night of 13 January 2017.

Because data was collected for a short period for this night the data in figure 9.4.21 is a good representation of the absolute (blue) and potential (red) temperature for this night of 13 January 2016.
Immediately visible is the stability of the boundary layer - identified by the rising potential temperature with height. This persists for the window during which observations were made. Considering the theoretical temperature profiles presented in figure 1.1.1 the data above strongly suggest that the atmosphere was still convective when the BLT measurements were taken (see temperature profiles in A of figure 1.1.1i).

The data for this night and for the night of 21 December 2016 pose some evidence towards answering the third question posed in chapter 1, regarding the stable stratification of the Manchester nocturnal boundary layer. However, more observations are needed to conclusively answer this question.

It should be noted that the shape of the temperature profile shown in figure 9.4.21 does not agree exactly with the profile shown in figure 8.6.3 because a different sonde launch...
Southerly flow regime

26 January 2017 (IOP4)  The synoptic conditions for the night of 26 January 2017 were defined by a strong high pressure over central Europe, with a low pressure centre located off the south coast of Iceland. There had been high pressure systems over continental Europe since 15 January, often extending their influence over the UK. The movement of a deep low pressure system north-eastwards across the Atlantic moving into the Arctic Ocean brought the southerly winds which characterised the data collection night.

Because the temperature inversion for 26 January 2017 is so low (see figure 9.4.24 for sonde profiles) the BLT is operating very close to the limit of the overlap correction. Considering the sonde profiles instead of the BLT data initially, we see the evolution of the temperature inversion in discrete steps:

The inversion begins the night (1917) at an altitude of 521m and a strength of $8.9 \pm 0.4$K. The inversion rapidly drops to an altitude of 183m by 2217 where it remains for much of the night. Between 0056 and 03:10 the inversion drops again, to 121m and rises slightly by the final sonde ascent at 0613.

---

7The data for figure 9.4.21 uses the sonde launch from this night of 13-14 January 2017 to constrain the data whereas the data shown in figure 8.6.3 used the final sonde launch to constrain the temperature profile.
The strength of the boundary layer inversion during the course of the night is striking; there is a sudden drop in strength between the first two soundings, followed by a restrengthening period between 2217 and 0056. Following this the inversion strength weakens until the final sonde launch at 0613 (where it reaches a minimum value of 3K). This degradation of the inversion strength is mostly due to low-level warming, rather than cooling aloft (the data for the 2217, 0056, 0310 and 0613 soundings showing a stable temperature at a height of 800m).

Having examined the evolution of the temperature inversion through the sonde data some analysis of the BLT data will be attempted. Figure ?? shows a good agreement between the BLT-determined temperatures and the corresponding sonde measurements down to approximately 300m, so the curtain plot of the BLT temperature data for this case study will be extended down to this limit.

![Figure 9.4.23: Temperature data from the night of 26 January 2017.](image)

The data for IOP4 shows the strengthening of a temperature inversion during the night, from a very weak inversion located at approximately 700m at 2100, which slowly strengthens and descends to 500m by 2300. At 0120 the temperature inversion begins strengthening and descending, passing below the limit of the overlap correction by 0200.

Comparing the BLT data to the sonde profiles, the temperature inversion evolution is not particularly well captured - typically overestimating the inversion height by approximately 100m (see table [9.3.1]). However, considering the size of the overlap correction
which must be applied (and the fact the BLT is operating very near to its overlap correction limit), achieving these measurements which capture the broad trends in the inversion statistics, if not the exact values, is encouraging for this approach to boundary layer investigation.

Figure 9.4.24: Sonde temperature profiles for the night of 26 January 2016.

9.5 Comparison with WRF model

To answer the fourth of the questions posed in chapter 1 a forecast model to compare with is needed (similar to the work of Banks and Baldasano (2016); Gan et al. (2011) who compared LiDAR data with WRF-based models to assess boundary layer properties. Gan et al. (2011) identified that for daytime (convective) measurements the WRF model chosen for testing against a LiDAR instrument reliably identified the height of the New York City boundary layer. Similarly, Banks and Baldasano (2016) found that the
daytime boundary layer was well-captured by the WRF model they chose to compare with a LiDAR instrument.

The model selected for comparison in this work is the ManUniCast model (Schultz et al., 2015) and combines the functionality of two modelling systems, Advanced Research Weather Research and Forecasting (WRF-ARW) and Weather Research and Forecast Model with Chemistry (WRF-Chem).

Further details of the model regarding the domains, boundary conditions and parameterisations can be found at http://manunicast.seaes.manchester.ac.uk/model.html.

This model was chosen principally because of the accessibility of the model output data, but also because atmospheric parameters are calculated for the Whitworth Observatory it provides a nearly direct comparison for the BLT data.

Figure 9.5.1 shows a direct comparison between the WRF model output temperatures, the BLT-determined temperatures and the locally launched sondes.

---

8WRF 3.4.1, operating at a 4km-grid spacing.
Figure 9.5.1: BLT temperature profiles (red) with locally-launched sonde profiles (black) and ManUniCast model output (light blue).
As with figure [8.6.5], these data have been corrected to the final sonde launch of each IOP experiment.

A summary of the performance of the model against the BLT-determined temperature profile is presented in table [9.5.1]. The IOP3 data is presented to identify whether the model produces a temperature inversion for a night when one did not develop.

To determine the strength of the inversion ($\Delta T$) shown in the model data the difference between the inversion base and top was taken:

$$\Delta T = T_{top} - T_{base}$$

Where the inversion base is determined as the range bin above which temperature increases with height, and the inversion top by the range bin above which the temperature begins falling with height. The difference between the temperatures of these range bins ($T_{top}$ and $T_{base}$, respectively) is the inversion strength.

### 9.5.1 Model uncertainty

Because the spatial resolution was inconsistent (successive range bins were of differing depths) the following calculation was performed to estimate the spatial uncertainty:

$$\Delta R_i = \sqrt{\left(\frac{R_b - R_{b-1}}{2}\right)^2 + \left(\frac{R_{b+1} - R_b}{2}\right)^2} \quad (9.5.1)$$

Where $R_b$ is the height of the range bin at which the temperature begins increasing with height and $R_{b\pm1}$ are the adjacent range bins.

The uncertainty in the boundary layer depth was calculated by:

$$\Delta R_t = \sqrt{\left(\frac{R_b - R_{b-1}}{2}\right)^2 + \left(\frac{R_{b+1} - R_b}{2}\right)^2 + \left(\frac{R_t - R_{t-1}}{2}\right)^2 + \left(\frac{R_{t+1} - R_t}{2}\right)^2} \quad (9.5.2)$$

Where $R_t$ is the height of the range bin at which the temperature ceases increasing with height and $R_{t\pm1}$ are the adjacent range bins.

---

9The model temperature data was read directly from the model output files.
Model output was available at each model gridpoint at 1-hour intervals, and the temperature uncertainty was estimated using the difference in temperature between consecutive timesteps. The standard deviations for each model level were calculated for the lowest 3km of the atmosphere and are presented in figure 9.5.2.

Figure 9.5.2: Standard variation of model output temperatures. Data presented are for sets of three consecutive hours (as indicated by caption). Vertical dashed line shown at a temperature of 0.4K

This figure suggests that the standard deviation in the lowest range bins of the model is around 0.4K over a time period of 1 hour. This is essentially a measure of the representativity error in a model profile.

Correspondingly, the temperature error of the model output is estimated at 0.4K (thus a conservative estimate of the representativity error in the inversion strength is 0.8K. To improve on this estimate would require a more rigorous in-depth study of the model, which is beyond the scope of this work.

---

\[10\] This analysis used the gridpoint located at the Whitworth Observatory.
<table>
<thead>
<tr>
<th>Synoptic/flow conditions</th>
<th>Investigation</th>
<th>BLT Base</th>
<th>BLT Strength</th>
<th>BLT Depth</th>
<th>Model Base</th>
<th>Model Strength</th>
<th>Model Depth</th>
</tr>
</thead>
<tbody>
<tr>
<td>High pressure</td>
<td>IOP1 launch 1</td>
<td>720 ± 100m</td>
<td>9.9 ± 2.1K</td>
<td>195 ± 150m</td>
<td>691 ± 104m</td>
<td>3.77 ± 0.8K</td>
<td>474 ± 113m</td>
</tr>
<tr>
<td></td>
<td>IOP1 launch 3</td>
<td>690 ± 60m</td>
<td>7.6 ± 2.1K</td>
<td>405 ± 80m</td>
<td>505 ± 83m</td>
<td>3.89 ± 0.8K</td>
<td>1420 ± 125m</td>
</tr>
<tr>
<td></td>
<td>IOP1 launch 4</td>
<td>960 ± 50m</td>
<td>14.3 ± 2.1K</td>
<td>495 ± 100m</td>
<td>505 ± 83m</td>
<td>4.22 ± 0.8K</td>
<td>1420 ± 125m</td>
</tr>
<tr>
<td>28 November 2016</td>
<td></td>
<td>900 ± 100m</td>
<td>10.49 ± 2.1K</td>
<td>495 ± 150m</td>
<td>153 ± 77m</td>
<td>1.95 ± 0.8K</td>
<td>206 ± 179m</td>
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<tr>
<td>IOP2 launch 1</td>
<td></td>
<td>1500 ± 100m</td>
<td>8.9 ± 2.1K</td>
<td>240 ± 200m</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>Westerly</td>
<td>21 December 2016</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>87 ± 43m</td>
<td>2.83 ± 0.8K</td>
<td>274 ± 152m</td>
</tr>
<tr>
<td>North-westerly</td>
<td>IOP3 launch 1</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>Southerly</td>
<td>IOP4 launch 1</td>
<td>510 ± 50m</td>
<td>7.8 ± 3.2K</td>
<td>330 ± 90m</td>
<td>359 ± 65m</td>
<td>6.85 ± 0.8K</td>
<td>1050 ± 100m</td>
</tr>
<tr>
<td></td>
<td>IOP4 launch 2</td>
<td>†</td>
<td>N/A</td>
<td>N/A</td>
<td>359 ± 65m</td>
<td>5.36 ± 0.8K</td>
<td>810 ± 90m</td>
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<tr>
<td></td>
<td>IOP4 launch 3</td>
<td>†</td>
<td>N/A</td>
<td>N/A</td>
<td>244 ± 52m</td>
<td>4.71 ± 0.8K</td>
<td>680 ± 90m</td>
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<tr>
<td></td>
<td>IOP4 launch 4</td>
<td>†</td>
<td>N/A</td>
<td>N/A</td>
<td>242 ± 51m</td>
<td>3.33 ± 0.8K</td>
<td>450 ± 80m</td>
</tr>
</tbody>
</table>

Table 9.5.1: Comparison of retrieved and modelled inversion data.

†As with table 9.3.1 determining temperature inversions at such a low altitude is impossible, but for completeness of this table have been presented anyway. N/A entries in the table indicate that no temperature inversion was identified.
As with figure 9.3.1, figure 9.5.3 displays the direct comparison between the inversion statistics from the BLT and model data.

Figure 9.5.3: Scatter plot comparing inversion statistics from BLT and model data. Black data indicate high pressure synoptic regimes, while orange data is from the southerly flow synoptic regime. Dashes show the 1:1 line. Dotted lines show ±100m for the inversion base and depth plots, and ±3K for the inversion strength plot for the BLT-sonde comparison data.

The WRF modelled data clearly disagree with the BLT-determined data regarding all of the parameters displayed in figure 9.5.3.

The model typically locates the temperature inversion at a lower altitude than the BLT data, as well as poorly capturing the strength and depth of the inversion. The poor capturing of the inversion strength and depth, is attributed to the poor spatial resolution in the model (there are only 13 model levels in the lowest 3km of the atmosphere, corresponding to the large spatial uncertainties in table 9.5.1). This is in line with the finding of Banks and Baldasano (2016) who found in their comparison with LiDAR data that and WRF model output systematically underestimates the height of the boundary layer capping inversion - in the four boundary layer schemes they investigated.

The depth of the inversion layer in the modelled data disagrees with the measured temperature inversion layer, typically overestimating the depth of the layer by several hundred meters.

The strength of the temperature inversion captured by the model is weaker than that shown in the BLT data, and in the case of the night of IOP2 the model does not resolve
any temperature inversion within the lowest 3km of the atmosphere.

However, for the night of 21 December 2016 where no temperature inversion was measured by the BLT the model resolved a rising temperature at low altitudes which peaks and begins falling at a height of 381m. Because the lowest model height data is output the base of this inversion is considered to be the lowest model level (87m) . This rising temperature at low altitudes is recorded as an inversion in table 9.5.1.

The model data found no temperature inversion during the night of IOP3, which is in line with the observed lack of temperature inversion.

Model performance for the periods with very low temperature inversions was assessed using the sonde launches for IOP4. Table 9.5.2 shows the temperature inversion statistics from tables 9.3.1 and 9.5.1 collated into a single table (see table 9.5.2) and presented as scatter plots (see figure 9.5.4) for comparison with the BLT and sonde data.

Immediately clear is that the model poorly captures the boundary layer capping inversion by all of the parameters presented, compared with the sonde data.

The model underestimates the height of the boundary layer inversion compared with both the BLT and sonde data. This underestimation is more pronounced under anticyclonic conditions where it typically underestimated the temperature inversion height by several hundred meters. On the night of IOP2 a temperature inversion was detected by the BLT and sondes launched but the model failed to resolve such an inversion.

Conversely, the model overestimates the thickness of the boundary layer capping inversion in most instances, by several hundred meters.

The uncertainty in the inversion strength (arising from large uncertainty in the temperature data) identifies that the model is incapable of identifying the inversion strength in a high pressure system, although under southerly flow the inversion strength was captured to within the model uncertainty.

These conclusions need to be considered in light of the limited comparisons available. Further observations with the BLT are needed to conclusively examine the model performance and clarify whether these comparisons are representative of the model performance over a larger number of observations.
<table>
<thead>
<tr>
<th>Synoptic/flow conditions</th>
<th>Investigation</th>
<th>BLT Base</th>
<th>BLT Strength</th>
<th>BLT Depth</th>
<th>Sonde Base</th>
<th>Sonde Strength</th>
<th>Sonde Depth</th>
<th>Model Base</th>
<th>Model Strength</th>
<th>Model Depth</th>
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<tbody>
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<td>High pressure</td>
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<td>720 ± 100m</td>
<td>9.9 ± 2.4K</td>
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<td>‡ 845 ± 2m</td>
<td>6.7 ± 1.4K</td>
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<td>3.77 ± 0.8K</td>
<td>474 ± 113m</td>
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<tr>
<td></td>
<td>IOP1 launch 3</td>
<td>690 ± 60m</td>
<td>7.6 ± 2.4K</td>
<td>405 ± 80m</td>
<td>‡ 680 ± 9m</td>
<td>6.9 ± 1.4K</td>
<td>439 ± 9m</td>
<td>505 ± 83m</td>
<td>3.89 ± 0.8K</td>
<td>1420 ± 125m</td>
</tr>
<tr>
<td></td>
<td>IOP1 launch 4</td>
<td>960 ± 50m</td>
<td>14.3 ± 2.4K</td>
<td>495 ± 100m</td>
<td>912 ± 9m</td>
<td>9.8 ± 1.4K</td>
<td>423 ± 11m</td>
<td>505 ± 83m</td>
<td>4.22 ± 0.8K</td>
<td>1420 ± 125m</td>
</tr>
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<td>28 November 2016</td>
<td></td>
<td></td>
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<td></td>
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</tr>
<tr>
<td></td>
<td>IOP2 launch 1</td>
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<td>8.9 ± 2.4K</td>
<td>240 ± 200m</td>
<td>1421 ± 4m</td>
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<td>Westerly</td>
<td>21 December 2016</td>
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<td></td>
<td>87 ± 43m</td>
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<td></td>
<td></td>
<td></td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>Southerly</td>
<td>IOP4 launch 1</td>
<td>510 ± 50m</td>
<td>7.8 ± 2.1K</td>
<td>330 ± 90m</td>
<td>521 ± 3m</td>
<td>8.9 ± 0.6K</td>
<td>423 ± 4m</td>
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<td>6.85 ± 0.8K</td>
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</tr>
<tr>
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<td></td>
<td></td>
<td>183 ± 3m</td>
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<td>5.36 ± 0.8K</td>
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</tr>
<tr>
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<td>IOP4 launch 3</td>
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<td></td>
<td></td>
<td>180 ± 13m</td>
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<td>4.71 ± 0.8K</td>
<td>680 ± 90m</td>
</tr>
<tr>
<td></td>
<td>IOP4 launch 4</td>
<td>†</td>
<td></td>
<td></td>
<td>121 ± 2m</td>
<td>4.8 ± 0.6K</td>
<td>214 ± 4m</td>
<td>242 ± 51m</td>
<td>3.33 ± 0.8K</td>
<td>450 ± 80m</td>
</tr>
</tbody>
</table>

Table 9.5.2: Temperature inversion data.

†While the BLT data has identified a temperature inversion at these altitudes, data obtained by the BLT for altitudes lower than approximately 500m is well within the telescope near-field region and so is not presented in this table.

‡These sonde profiles contain multiple temperature inversions. The data presented in table 9.5.2 is for the lowest of these inversions.
As with previous comparisons between the BLT and sonde data, and BLT and model data, direct comparisons of the inversion statistics are shown below in figure 9.5.4.

Figure 9.5.4: Scatter plot comparing inversion statistics from BLT, sonde and model data. Black data indicate high pressure synoptic regimes, while orange data is from the southerly flow synoptic regime. Dashes show the 1:1 line. Dotted lines show ±100m for the inversion base and depth plots, and ±3K for the inversion strength plot for the BLT-sonde comparison data.

In conclusion, the model chosen to compare with the BLT data (and, where necessary, the sonde data) does not perform well at resolving the boundary layer capping temperature inversion overnight.

Having presented the project from its conception to this stage, and having answered the questions posed in Chapter 1, the final chapter of this work discusses the possible future modifications to be made to the instrument.
Chapter 10

Project conclusions

This work has presented the development of a rotational Raman LiDAR instrument to monitor the capping temperature inversion of the nocturnal boundary layer over Manchester. The first of the questions of the BLT laid out in chapter 1 has been answered - a low pulse energy, high repetition laser can be used as the illumination source for a LiDAR instrument. Further the second question has also been answered; boundary layer temperatures can be retrieved using a LiDAR instrument with such a laser (see figure 8.7.1), so long as the variations in temperature are greater than 3.5K.

The third of the posed questions in chapter 1, regarding whether the nocturnal boundary layer over Manchester becomes stably stratified during the course of a night, has only been partially answered. There is a small amount of evidence from the night of 04 January 2017 showing a gently rising temperature with height (see figure 9.4.11 and 9.4.12). Further observations are necessary to fully address this question. Future observations using this instrument, in conjunction with locally-launched sondes will allow this question to be answered more completely.

The fourth question from chapter 1, regarding whether models can capture the boundary layer capping inversion at night has been preliminarily investigated. To achieve this, a WRF model output was compared with the BLT and locally-launched sonde data and the performance rated by comparison with three boundary layer inversion parameters. This work has highlighted a possible failure of the model chosen to capture the nocturnal boundary layer temperature profile and further work is needed to conclusively quantify this failure. Additionally, other models should be tested regarding their capture of the nocturnal boundary layer over Manchester.
10.1 Project Overview

The BLT instrument was developed from a legacy biaxial LiDAR designed for stratospheric work to measure the nocturnal boundary layer capping temperature inversion, utilising rotational Raman scattering from molecular nitrogen and oxygen excited by a laser at 355nm. This development included the replacement of an interference filter, for which the response of the instrument to atmospheric signals was modelled, allowing optimum filter parameters to be identified (see Chapter 6).

Following the installation of the replacement interference filter the received system was calibrated for light with polarisations parallel to and perpendicular to the laser light (Chapter 5). These calibrations allowed a lookup curve to be constructed (Chapter 7) to allow atmospheric temperature retrieval.

A correction factor (see section 8.3.3) has been determined to account for the shading of the BLT primary mirror by the collimation tube, as well as the laser platform and secondary mirror, using sonde launches to derive this correction factor. Similarly, sonde launches have been used to constrain the overlap correction (see section 8.4) necessary in using the receiver system of the original instrument, which is operating in its near-field region. These investigations have identified that sonde launches are necessary for each night of operation to fully constrain this overlap correction factor, although making a correction using another night’s correction factor is always significantly better than using no correction.

The LiDAR backscatter ratio (see section 8.9) is calculated to support the diagnosis of the boundary layer capping temperature inversion. A quadratic fit to low altitude, clear-air backscatter ratio data has been used to estimate a correction factor for the overlap function of the BLT for this ratio. While the approach taken in this work is not as rigorous as other studies it serves only to support the temperature analysis, not to act as a stand-alone aerosol-investigation instrument.

10.2 Instrument performance

After these calibrations and identification of the correction factors the BLT was shown to be capable of determining the height of the boundary layer capping inversion in good agreement (less than 100m) with the locally-launched sondes (see sections 8.5 and 8.7). This is within the experimental uncertainty of the BLT measurement and is observed
under strikingly different synoptic conditions.

Similarly, to within experimental uncertainty, the BLT captures the inversion depth to within 100m, and the inversion strength to within 3K. This is categorised to determine the temperature inversions shown in table 9.5.2 which shows the smallest temperature inversion strength as $7.6 \pm 2K$.

The contribution to the BLT temperature uncertainty measurements from Poisson noise (at a height of 1000m) was shown to be less than 1K when the data was averaged over the whole duration of a night (section 9.2).

Because the major source of uncertainty in the BLT signals arises from signal noise and the lookup curve is not very temperature sensitive (see figure 8.3.3) the uncertainty of the instrument is limited to 2.1K (see figure 6.4.1). Correspondingly temperature variations of less than this cannot be measured by the BLT - however all of the temperature inversions identified were measured to have a strength greater than 2.1K (see figure 9.5.4).

To increase the signal received (and thus less error) a brighter laser could be used, or lasing pulse frequency could be increased. Alternatively, by using more efficient receiver optics (for example PMTs optimised for UV light, ), weaker signals could be measured.

In order to accurately map the temperature of the boundary layer overnight a time resolution of approximately 1 hour is necessary. By reducing the averaging period from a whole night collection (approximately 8 hours) to one hour, the contribution from Poisson noise increases to approximately 2.8K. In the context of the inversions observed using the BLT, this increase in uncertainty would not increase the uncertainty of greater than the inversion strength. However, decreasing the averaging period further would begin impacting the inversion strength calculations with uncertainties of the same order as the observed inversion strength.

In addition to increasing the averaging period, increasing the width of the range gates reduces the impact of the Poisson noise at the expense of spatial resolution. Because a primary goal of the BLT was to monitor the temperature inversion base this is unsuitable for use to reduce this noise.

This is a fundamental issue limiting the capabilities of LiDAR instruments, where a compromise between the spatial resolution, the temporal resolution and the signal to noise

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1Both options increase the amount of output photons, and thus the number of scattering events measured.
The boundary layer thermal profiles during 6 nights showed (section 9.4) that the BLT is capable of identifying the height of the temperature inversion in the nocturnal boundary layer to within 100m of that given by sonde measurements. The measured strength of such inversions agrees with sonde measurements, to within experimental uncertainty, performing better under the southerly wind regime compared with the high pressure regime when compared with the sonde data.

The BLT data shows that for the nights of 24 November 2016 and 28 November 2016 the temperature falls with height before reaching the capping inversion (see figures 9.4.2 and 9.4.7). For the night of 04 January 2017 instead what is seen is a gently rising temperature with height before a strong increase in temperature at the capping inversion (see figure 9.4.10).

Under Westerly flow conditions (see the night of 21 December 2016) the BLT temperature retrieval (see figure 9.4.16) was observed to fall with height for the whole of the range of the BLT measurement. By comparing with the sonde launch from Watnall (figure 9.4.17) this profile can be concluded to be representative of a large-scale feature, extending from Manchester to Watnall (84km).

The night of 26 January 2017 (Southerly flow conditions) showed an evolution in the boundary layer temperature profile. Beginning the night with a falling temperature with height, an inversion develops by 2100 and descends during the course of the night. This inversion falls below the minimum range the BLT can retrieve temperatures.

Because of approaching rainfall the data collection for the night of 13 January 2017 had to be abandoned early, but showed a strong decrease of temperature with height, indicating the boundary layer was convective during the observation.

Shortcomings in the agreement between the sonde data and the BLT-determined temperature data has suggested that an improvement in signal strength is needed - achievable by either modifying the receiver optics or increasing the brightness of the laser output. This increase in laser output intensity increases the distance over which the laser is not eye-safe (see Appendix A) and thus such changes might not be appropriate for use in Manchester.

\[^2\] In the case of the BLT the signal to noise ratio correlates to the temperature uncertainty.
Alternatively by increasing the time period over which data is collected, improvements in data quality can be made (by improving the signal to random noise ratio). For example, the data-files used in this work were constructed over 30s before being read into the analysis scripts, which could be increased to five minutes to reduce the effects of random noise to the collected signals. This is still a fast enough sampling to observe the evolution of the boundary layer capping inversion structure without compromising temporal accuracy.

Of the four questions posed at the outset of this work, two have been answered (regarding the capability of the instrument to measure boundary layer temperatures over Manchester) - a caveat to this is that locally-launched sondes are needed to properly constrain the overlap correction factor.

The third question, regarding whether the boundary layer becomes stably stratified has not been conclusively answered due to the limited evidence showing this stability. Further observations supporting the findings of the night of 04 January 2017 are needed, to be measured with a sonde launch for each night to constrain the correction factor.

The fourth question, regarding the suitability of the chosen WRF model to capture the boundary layer temperature profile has not been satisfactorily answered and further nights of data collection and comparison are needed to quantify the performance of the model. However, preliminary findings suggest that the model poorly captures the boundary layer.

### 10.3 Instrument future

Possible routes to advance the functionality of the BLT would be to redesign the receiver optics - primarily to replace the telescope to use one with a lower f number so that the BLT is not operating in the near-field region of its telescope.

Additional work is required to replace the far-field filter; updating the original filter to address the laser light breakthrough and optimising the pairing of the near-field and far-field filters to minimise the uncertainty in temperature measurements at 1km. Using the approach outlined in see Chapter 6, figure 10.3.1 is obtained:
Figure 10.3.1: Identifying a possible replacement far-field interference filter using the current near-field filter and a cosine-shaped new far-field filter located in the Stokes region of the rotational Raman spectrum, as per section 6.4.

By replacing the far-field filter with (cosine-shaped) filter centred at 356.9nm with a FWHM of 1.2nm, the systematic error arising from using the lookup curve to determine atmospheric temperature would be reduced to 0.26K from 1K (see section 6.4). Similarly to the replacement near-field filter, manufacturing a filter to this specification may be challenging, so similar work will need to be carried out to the near-field filter analysis following consultation with a filter manufacturer.

Replacing the PMTs would potentially reduce the effects of inhomogeneity and thus the significance of off-axis signals to the temperature-sensitivity at different heights. UV-optimised PMTs would increase the signal strength, extending the operational range of the BLT, and allowing for observations through cloud layers.

Further, a narrow wavelength notch filter can be installed across the beam guide exten-
sion to block elastically-scattered light. This filter would need total suppression of elastic signals no further than 0.1 nm from the laser line to ensure no elastic signals are captured by the Rotational Raman channels (see figure 6.6.1). Commercially-available notch filters appear to have too wide a notch (see for example Edmund Optics component number #67-1006), so manufacturers would need to be consulted whether this is an appropriate method for rejecting elastically scattered light.

10.3.1 Telescope redesign

Beyond simply changing the telescope to one with a smaller f number, introducing a tertiary mirror into the telescope, located between the telescope mirrors would allow the light to be focussed at a point perpendicular to the telescope axis. This allows the removal of the collimation tube from between the telescope mirrors - see figure 10.3.2 for a schematic.

Figure 10.3.2: Possible future design of BLT telescope allowing the removal of the collimation tube from between the mirrors and reducing the amount of the primary mirror shading.

This would remove a significant portion of the primary mirror shading - completely removing the shading from the collimation tube. However, alignment of the collimation tube with the optical axis following the directing tertiary mirror needs to be extremely well-controlled. Further, by removing the collimation tube from under the laboratory roof hatch, the effects of thermal contraction due to cold air intrusion through the roof hatch will be reduced.

Alternatively, instead of using a tertiary mirror to direct light into the collimation tube, a fibre optic cable could be used. This requires precise focusing of captured signals onto one end of the fibre, but the shading of the primary mirror from a fibre would be almost
zero. Further, smaller components could be used for filtering and detection, allowing the detection optics to be substantially reduced in size.

### 10.3.2 Optics redesign

By arranging reflecting filters tuned to the appropriate regions of the rotational Raman spectrum of molecular nitrogen and oxygen, as well as the vibrational Raman spectrum of water vapour shown in figure 10.3.3, the BLT optics can be redesigned to allow fine spectral control of the light reaching the PMTs by using equation 4.3.2 to tune the transmission windows of the interference filters (see, for example the work of Behrendt and Reichardt (2000); Hua et al. (2007)), reducing some of the manufacturing constraints for the interference filters. Further, this arrangement could be made modular, allowing for the introduction of further channels in the instrument in future - and a testing of replacement channels against current channels based on simultaneous measurements.

![Possible future design of BLT optics](image)

**Figure 10.3.3:** Possible future design of BLT optics. Green and purple components represent reflecting filters tuned to the rotational Raman spectrum of molecular nitrogen and oxygen, and vibrational (red) Raman spectrum of water vapour.

**Proposed laboratory redesign** By installing further heaters and fans in the laboratory, slaved to the climate control, the effects of cold air flowing across the collimation tube can be addressed. Directing warm air across and vertically upwards through the roof hatch would remove (or ameliorate) the effects of cold air flowing over the telescope and collimation tube.
While the cold-air intrusion into the laboratory could be addressed by installing a window. Such a window would need to be constructed from fused silica which, if it were to span the width of the roof hatch, would cost too much to be practicable.

Such a window constructed from fused silica, spanning the width of the roof hatch, would cost too much to be practicable. Alternatively, using BK7 glass could be suitable such a glass panel were sufficiently thin, although a design study would need to be undertaken to confirm this.

10.3.3 Future instruments

Because this work has demonstrated that it is possible to probe the urban nocturnal boundary layer temperature structure the BLT might form the inspiration for other LiDAR instruments using low pulse energy, but high repetition ultraviolet lasers. Because of the short-range nature of the safety risk this would allow the development of instruments to monitor the nocturnal boundary layers of other urban environments. These instruments (and the BLT if the receiver optics are updated) would allow air quality forecasting models to more accurately constrain the boundary layer schemes, thus improve their ability to make accurate forecasts within urban regions.

By using LiDARs similar to the BLT it is possible to construct small instruments capable of monitoring boundary layer temperature profiles. Such instruments could be used in projects similar to the Clean Air for London (ClearfLo, see Bohnenstengel et al. (2015)) to more accurately constrain the temperature profiles of major urban areas to potentially inform air quality models.

By mounting the BLT (or similar instruments) on an observation tower (or tall building) and rotating the BLT telescope and laser head to the horizontal, observations of the size of the Manchester urban heat island could be measured. Because of the eye-safety of the laser the risk to local air traffic would be minimal. This would have an advantage over the work of Pal et al. (2012), who measured vertical temperature profiles using multiple LiDARs, needing intercomparisons to be performed to calibrate the instruments relative to each other.

The eye safety of the laser allows for remote operation, allowing for the possibility of a network of such instruments to be constructed over an extended area (similar to the

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3For example Thorlabs component number WG12012.
European Aerosol Research Lidar Network (EARLINET) - see [Ansmann et al. (2010)]. Such a network could allow the measurements of the temperature profiles at multiple locations across an urban-rural boundary to be made, opening the door for three-dimensional modelling of the urban-rural boundary layer interface.

Finally, because of the low power laser not requiring a large power supply, miniaturising the BLT would allow for a highly portable instrument similar to the instrument developed by [Althausen et al. (2009)]. Such mobility would allow for rapid deployment of instruments suitable for boundary layer profiling in response to evolving demand.

In conclusion, the using a high-repetition, low power laser for a LiDAR instrument has been shown to be possible, and temperature retrievals have been made. That such principles have been shown by modifying an existing instrument demonstrates the viability of this technique for instruments designed and implemented following this principle.
Appendix A

Laser Safety

A.1 Basic safety

Eye safety is an important consideration regarding the use of lasers - which takes into consideration the energy emitted per pulse, the pulse repetition frequency and the wavelength of the lasing light. Due to the small divergence of laser emissions a very large flux of energy is delivered onto a small area - from which arises the risk to health.

The highest risk of damage from laser light arises from laser light entering the eye (Reidenbach, 2007). This is because the human eye is optimised to focus visible light, effectively focussing the already intense radiation flux onto the retina. This delivery of high energy flux raises the temperature of the retinal tissue potentially leading to enormous damage in the form of a photoacoustic shock (Reidenbach, 2007, p.1256) where tissue is heated to sufficiently high temperatures to become plasma.

Ultraviolet wavelengths are significantly less dangerous to eye safety because the eye is significantly more opaque to these wavelengths, as well as the lens not acting to further focus the laser emission onto a small spot on the retina.

Photoacoustic shocks are not the only risk of damage - indeed they are the extreme cases of tissue heating which can arise from energy being delivered to a small area of the human body.

Because this work uses a frequency-tripled Nd:YAG laser the UV-A (315nm-400nm) (Reidenbach, 2007, p.1257) region of the electromagnetic spectrum will be the focus of this eye safety discussion. The associated risks from lasers operating within this region are outlined in table A.1.1.
UV-A Eye health risk | Skin health risk
---|---
Cataract formation (lens is principal absorber) | Acute pigmentation | Skin burns | Carcinoma (skin cancer)

Table A.1.1: UV-A health risks.
Reproduced from [Reidenbach 2007](#), p.1256).

### A.2 Maximum Permissible Exposure

The limits of safe exposure are set by calculating the maximum permissible exposure (MPE). The University of Manchester laser safety manual was consulted to determine the eye safety of the BLT, which outlines the following steps to determining the MPE:

1. Calculate $\text{MPE}_{\text{single}}$ for a single pulse using the pulse-length as the duration time.

2. Calculate $\text{MPE}_{\text{train}}$ for a train of pulses using the formula: $\text{MPE}_{\text{train}} = \text{MPE}_{\text{single}} \times N^{-0.25}$

3. Calculate $\text{MPE}_{\text{average}}$ using the formula: $\text{MPE}_{\text{average}} = \frac{(\text{MPE}_{\text{duration}})}{N}$

Where $N$ is the number of pulses in the duration

The maximum permissible exposure for the BLT laser firing a single pulse is determined using:

$$\text{MPE}_{\text{single}} = 5.6 \times 10^2 t^{0.25} \quad \text{(A.2.1)}$$

where $t$ is the pulse length of 8nm (see table 4.2.1) yielding a $\text{MPE}_{\text{single}}$ of 537 Jm$^{-2}$.

$\text{MPE}_{\text{train}}$ is calculated for an accidental exposure, presuming that the exposure is for the entire duration of the train of pulses. The University of Manchester Laser Safety Manual stipulates that for invisible wavelengths this corresponds to a 10s exposure. The BLT laser operates at 1kHz (thus $N=10000$), yielding $\text{MPE}_{\text{train}} = 5.3 \text{ Jm}^2$.

$\text{MPE}_{\text{average}}$ is also calculated for an accidental exposure, using equation A.2.1 but using $t=10$s. Further, this exposure is averaged over the number of pulses contained within
the train of pulses \( N = 10000 \), yielding a MPE_{average} of 1 \( \text{Jm}^{-2} \).

The most restrictive of these MPEs is the MPE_{average} at 1 \( \text{Jm}^{-2} \).

A.2.1 Laser output intensity

The BLT laser outputs an average pulse energy of 240\( \mu \text{J} \) which, following the transmission telescope is spread over an area of 3cm. This produces an irradiance of 0.3 \( \text{Jm}^{-2} \) - lower than the most restrictive of the MPEs calculated above.

A.3 Laboratory safety measures

A.3.1 Passive protection

To ensure that laboratory users are not at risk from the laser beam while within the laboratory the laser head was mounted at the top of the BLT telescope telescope scaffold - see figure 4.1.1. Because the laser head is 129cm above the ground and directed horizontally through the expansion telescope at the directing mirror it is impossible to accidentally expose oneself to the radiation.

A.3.2 Personal Protection Equipment

During the adjustment of the expansion telescope and directing mirror (following their installation) laser safety goggles were worn to ensure that no reflections could pose a health risk.

A.3.3 Unattended Operation

During unattended data collection signs are placed on the laboratory door, identifying the appropriate person to be contacted in the even of needing to access the laboratory. The roof access point (for the roof of the laboratory through which the laser beam passes) also carries signage indicating that when the roof hatch is open the laser is in use.

The roof hatch itself carries safety warnings that when it is open UV laser light is being emitted to ensure that anybody with rooftop access is aware of the risk posed by the BLT.
Finally, the laboratory door has a layer of black neoprene rubber secured around its perimeter to ensure that no laser light can be scattered out of the laboratory during any adjustments to the laser or its directing mirror.
Bibliography


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