Instrument Trade Studies for Satellite Remote Sensing of Ammonia

A thesis submitted to the College of Graduate and Postdoctoral Studies in partial fulfillment of the requirements for the degree of Master of Science in the Department of Physics and Engineering Physics University of Saskatchewan Saskatoon

By Cara Remai

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Abstract

Atmospheric ammonia (NH$_3$) has effects on air quality and water quality, but due to its short lifetime and high spatial variability, obtaining global measurements is a challenge. Advances in radiative transfer modelling and radiometric instrument sensitivity have allowed for satellite NH$_3$ observations to be performed by instruments such as NASA’s Tropospheric Emission Spectrometer and NASA’s Cross-track Infrared Sounder, but these instruments, and others like them, were not designed specifically to measure ammonia. This thesis pursues the development of an optimized instrument to measure ammonia with daily Canadian coverage, good ground spatial resolution (around 1 km), and a high signal-to-noise ratio. The work presented here shows an investigation into the optimized satellite remote sensing system by combining forward modelling, sensor design, and data retrieval algorithms.

An imaging Fourier Transform Spectrometer (IFTS) is chosen for the instrument for its wide spectral range and high throughput. A software model of the instrument is used to generate interferograms for each pixel, average four neighbouring interferograms, and recover a spectrum. A secondary model convolves the theoretical instrument lineshape for an off-axis square pixel with the high-resolution radiance. The Rodgers-based retrieval algorithm takes in the spectrum from the full instrument model, and iterates (using the convolution model) to retrieve a surface temperature value and an ammonia profile. These three pieces working together allow for an exploration of different instrument configurations. The investigation of the instrument parameters resulted in two configurations that were selected for further study. These two configurations differed in the number of samples taken of the interferogram and the time required to obtain an interferogram, having undersampling factors of 2 and 3, respectively. In a large-scale run of microwindowed retrievals using high-resolution model fields of NH$_3$, both sets of specifications were able to perform ammonia retrievals. Due to the use of microwindowing, the retrieved surface temperature values had errors large enough to impact the ammonia retrievals. Small tests using a full spectrum retrieval resulted in better performance for both the surface temperature and ammonia retrievals. Both sets of instrument specification meet the requirements for the project, though the case with an undersampling factor of 2 has a lower brightness noise level than the other case.
Acknowledgements

I would like to thank my supervisors, Dr. Adam Bourassa and Dr. Doug Degenstein, for their feedback and guidance during the last two years. I would also like to thank Chris McLinden and Mark Shephard, from Environment and Climate Change Canada, for their ideas and support, as well as Frédéric Grandmont and Stéphane Lantagne, from ABB Ltd, for their help with the optical design. Thank you as well to the Natural Sciences and Engineering Research Council, for providing funding to make this project possible.

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<td>ADC</td>
<td>Analog-to-Digital Converter</td>
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<tr>
<td>AIRS</td>
<td>Atmospheric Infrared Sounder</td>
</tr>
<tr>
<td>CEDS</td>
<td>Community Emission Data System</td>
</tr>
<tr>
<td>CrIS</td>
<td>Cross-track Infrared Sounder</td>
</tr>
<tr>
<td>DoD</td>
<td>Department of Defense</td>
</tr>
<tr>
<td>DOFS</td>
<td>Degree(s) of Freedom for Signal</td>
</tr>
<tr>
<td>ECCC</td>
<td>Environment and Climate Change Canada</td>
</tr>
<tr>
<td>EOS</td>
<td>Earth Observing System</td>
</tr>
<tr>
<td>ESA</td>
<td>European Space Agency</td>
</tr>
<tr>
<td>EUMETSAT</td>
<td>European Organisation for the Exploitation of Meteorological Satellites</td>
</tr>
<tr>
<td>FOV</td>
<td>Field of View</td>
</tr>
<tr>
<td>FTS</td>
<td>Fourier Transform Spectrometer</td>
</tr>
<tr>
<td>GEM-MACH</td>
<td>Global Environmental Multi-scale – Modelling Air-quality and CHemistry</td>
</tr>
<tr>
<td>GEOS</td>
<td>Goddard Earth Observing System</td>
</tr>
<tr>
<td>GHGsat</td>
<td>Greenhouse Gas Satellite</td>
</tr>
<tr>
<td>HITRAN</td>
<td>High-Resolution Transmission</td>
</tr>
<tr>
<td>HyTES</td>
<td>Hyperspectral Thermal Emission Spectrometer</td>
</tr>
<tr>
<td>IASI</td>
<td>Infrared Atmospheric Sounding Interferometer</td>
</tr>
<tr>
<td>IFTS</td>
<td>Imaging Fourier Transform Spectrometer</td>
</tr>
<tr>
<td>ILS</td>
<td>Instrument Lineshape</td>
</tr>
<tr>
<td>JPSS</td>
<td>Joint Polar Satellite System</td>
</tr>
<tr>
<td>LEO</td>
<td>Low Earth Orbit</td>
</tr>
<tr>
<td>MOPD</td>
<td>Maximum Optical Path Difference</td>
</tr>
<tr>
<td>NASA</td>
<td>National Aeronautics and Space Administration</td>
</tr>
<tr>
<td>NEdT</td>
<td>Noise Equivalent Differential Temperature</td>
</tr>
<tr>
<td>NOAA</td>
<td>National Oceanic and Atmospheric Administration</td>
</tr>
<tr>
<td>NPP</td>
<td>National Polar-orbiting Partnership</td>
</tr>
<tr>
<td>Acronym</td>
<td>Definition</td>
</tr>
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<td>---------</td>
<td>------------</td>
</tr>
<tr>
<td>OPD</td>
<td>Optical Path Difference</td>
</tr>
<tr>
<td>RVMR</td>
<td>Representative Volume Mixing Ratio</td>
</tr>
<tr>
<td>SNR</td>
<td>Signal-to-Noise Ratio</td>
</tr>
<tr>
<td>SRAK</td>
<td>Sum of the rows of the averaging kernel</td>
</tr>
<tr>
<td>TES</td>
<td>Tropospheric Emission Spectrometer</td>
</tr>
<tr>
<td>TIR</td>
<td>Thermal Infrared</td>
</tr>
<tr>
<td>VMR</td>
<td>Volume Mixing Ratio</td>
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<td>ZPD</td>
<td>Zero Path Difference</td>
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## Radiative Transfer

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<tr>
<td>$h$</td>
<td>Planck constant</td>
</tr>
<tr>
<td>$\nu$</td>
<td>Wavenumber</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>Wavelength</td>
</tr>
<tr>
<td>$I$</td>
<td>Spectral radiance</td>
</tr>
<tr>
<td>$E$</td>
<td>Energy</td>
</tr>
<tr>
<td>$\Omega$</td>
<td>Solid angle</td>
</tr>
<tr>
<td>$t$</td>
<td>Time</td>
</tr>
<tr>
<td>$\theta$</td>
<td>Angle</td>
</tr>
<tr>
<td>$s$</td>
<td>Position</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Total cross section</td>
</tr>
<tr>
<td>$\sigma_s$</td>
<td>Scattering cross section</td>
</tr>
<tr>
<td>$\sigma_a$</td>
<td>Absorption cross section</td>
</tr>
<tr>
<td>$n$</td>
<td>Number density</td>
</tr>
<tr>
<td>$N$</td>
<td>Total column density</td>
</tr>
<tr>
<td>$k$</td>
<td>Extinction</td>
</tr>
<tr>
<td>$\tau$</td>
<td>Optical depth</td>
</tr>
<tr>
<td>$J$</td>
<td>Radiation source term</td>
</tr>
<tr>
<td>$B$</td>
<td>Planck function</td>
</tr>
<tr>
<td>$c$</td>
<td>Speed of light</td>
</tr>
<tr>
<td>$k_B$</td>
<td>Boltzmann constant</td>
</tr>
<tr>
<td>$T$</td>
<td>Temperature</td>
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## Fourier Transform Interferometry

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<tbody>
<tr>
<td>$\lambda$</td>
<td>Wavelength</td>
</tr>
<tr>
<td>$I$</td>
<td>Intensity of radiance seen by detector</td>
</tr>
<tr>
<td>$S$</td>
<td>Input radiance</td>
</tr>
<tr>
<td>$\nu$</td>
<td>Wavenumber</td>
</tr>
<tr>
<td>Symbol</td>
<td>Definition</td>
</tr>
<tr>
<td>---------</td>
<td>------------------------------------------------</td>
</tr>
<tr>
<td>$x$</td>
<td>Optical path difference</td>
</tr>
<tr>
<td>$t$</td>
<td>Time</td>
</tr>
<tr>
<td>$V$</td>
<td>Speed of moving mirror</td>
</tr>
<tr>
<td>$\theta$</td>
<td>Phase function</td>
</tr>
<tr>
<td>$\Delta z$</td>
<td>OPD sampling interval</td>
</tr>
<tr>
<td>$\sigma_n$</td>
<td>Nyquist frequency</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>Off-axis angle</td>
</tr>
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**Atmospheric Inverse Theory**

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<td>$y$</td>
<td>Measurement vector</td>
</tr>
<tr>
<td>$x$</td>
<td>State vector</td>
</tr>
<tr>
<td>$K$</td>
<td>Kernel or Jacobian or Weighting function</td>
</tr>
<tr>
<td>$F$</td>
<td>Forward model</td>
</tr>
<tr>
<td>$b$</td>
<td>Auxiliary information</td>
</tr>
<tr>
<td>$\epsilon$</td>
<td>Error on measurements</td>
</tr>
<tr>
<td>$\chi^2$</td>
<td>Cost function</td>
</tr>
<tr>
<td>$P(x)$</td>
<td>Prior atmospheric state</td>
</tr>
<tr>
<td>$P(y)$</td>
<td>Measurement probability</td>
</tr>
<tr>
<td>$P(x</td>
<td>y)$</td>
</tr>
<tr>
<td>$P(y</td>
<td>x)$</td>
</tr>
<tr>
<td>$S$</td>
<td>Covariance matrix</td>
</tr>
<tr>
<td>$\hat{x}$</td>
<td>Retrieved state</td>
</tr>
</tbody>
</table>

**Instrument Model**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x_c$</td>
<td>X coordinate of the centre of pixel</td>
</tr>
<tr>
<td>$y_c$</td>
<td>Y coordinate of the centre of pixel</td>
</tr>
<tr>
<td>$A$</td>
<td>Half-height of pixel</td>
</tr>
<tr>
<td>$B$</td>
<td>Half-width of pixel</td>
</tr>
<tr>
<td>$f$</td>
<td>Focal length</td>
</tr>
<tr>
<td>$r_{min}$</td>
<td>Distance from optical axis to nearest corner of pixel</td>
</tr>
<tr>
<td>$r_{c1}$</td>
<td>Distance from optical axis to one intermediate</td>
</tr>
</tbody>
</table>

xiv
corner of pixel

$r_{e2}$ Distance from optical axis to the other intermediate corner of pixel

$r_{\text{max}}$ Distance from optical axis to furthest corner of pixel

$w$ Apodization window

$SNR$ Signal-to-Noise Ratio

$TC$ Thermal Contrast

$BT$ Brightness Temperature

**Optical Design**

$z$ Satellite altitude

$w$ Pixel width

$M$ Magnification of the inverse telescope

$V$ Satellite ground speed

$y$ Along-track distance covered by the satellite in one scan

$\Theta$ Divergence

$t$ Dwell time for a single scan

$D$ Aperture diameter

$n$ Number of pixels in one row of the square array

$x_{\text{total}}$ Total optical path difference for single-sided interferogram

$m$ Number of samples in interferogram

$s$ Sampling rate

$\delta_i$ Sampling interval
CHAPTER 1

INTRODUCTION

1.1 Setting the Stage

Atmospheric ammonia (NH$_3$) is a highly reactive pollutant that has effects on the nitrogen cycle, air quality, and water quality. It is also a key contributor in reactions that form small aerosols which, if exposed to long-term, can have significant impact on cardiovascular and cardiopulmonary health (Crouse et al., 2012; Pope et al., 2009). Its short lifetime and high spatial variability makes obtaining global measurements a challenge. With new advances in radiometric instrument sensitivity and radiative transfer modelling, satellite observations of ammonia have been conducted using NASA’s Tropospheric Emission Spectrometer (TES, operational 2004-2018) (Shephard et al., 2011), NASA’s Cross-track Infrared Sounder (CrIS, operational 2011-present) (Shephard and Cady-Pereira, 2015), ESA’s Infrared Atmospheric Sounder Interferometer (IASI, operational 2006-present) (Clarisse et al., 2010), NASA’s Hyperspectral Thermal Emission Spectrometer (HyTES, first flights in 2012) (Kuai et al., 2019), and NASA’s Atmospheric Infrared Sounder (AIRS, operational 2002-present) (Warner et al., 2016). Though the previously mentioned instruments have been able to perform ammonia measurements, there is a lack of high-quality ammonia measurements with good coverage of Canada, leading to difficulties incorporating ammonia into atmospheric models and in creating policies to reduce ammonia emissions.

1.2 Instrument Goals and Motivation

The goal of this thesis work is to find an optimized satellite remote sensing approach designed specifically for ammonia measurement by combining forward modelling, sensor design, and
data retrieval algorithms. No current operational satellite instrument has been designed specifically to measure ammonia, leaving open the opportunity for an optimized instrument to provide coverage of Canada with good ground spatial resolution and a high signal-to-noise ratio. This project was developed in conjunction with Environment and Climate Change Canada (ECCC), and as such many of the specifications for the instrument were dictated by their requirements for spectral resolution, signal-to-noise ratio, and ground spatial resolution. The end result of this work will be a set of specifications for an instrument that can take ammonia measurements that meet the requirements as given by ECCC.

Figure 1.1 shows how the different sections of my research work together for the overall simulated retrieval of ammonia. My work can be broken up into three main sections, the first of which is the full instrument model (green). The input to the full instrument model is an NH$_3$ profile of choice (‘True NH3 profile’ in the chart). Making use of the SASKTRAN radiative transfer model, the full instrument model generates radiance as seen by the satellite observer, and calculates the interferogram as measured by an imaging Fourier Transform Spectrometer (IFTS). The Fourier transform of the interferogram is taken, resulting in an output ‘measured’ radiance spectrum (‘Output Radiance’). The second portion of my work is the convolution model (orange). Similar to the full instrument model, the convolution takes as an input a NH$_3$ profile (‘Input NH3 profile’). The convolution model also uses the SASKTRAN radiative transfer model to generate radiance, and then convolves this radiance with the instrument lineshape, giving a radiance spectrum as recovered by an IFTS (‘Calculated radiance’). Note that the convolution model is significantly faster than the full instrument model. The last piece of the research is the retrieval loop (blue), which makes use of the Rodgers retrieval theory (Rodgers, 2000). The retrieval loop begins with an initial guess for the NH$_3$ profile (‘Initial guess for NH3 profile’), and uses the convolution model to calculate the radiance that would be measured for the given NH$_3$ profile. This output from the convolution model is then compared to the ‘measured’ radiance from the full instrument model, and based on the differences between the two spectra, the guess for the NH$_3$ profile is adjusted. The new guess for NH$_3$ is then put back through the convolution model, for another iteration. The retrieval loop iterates in this way to find the statistically most likely NH$_3$ profile that would result in the radiance spectrum as generated by the full instrument.
model. These iterations continue until the measurement and the model agree to within some error. Once this agreement between measurement and model has been achieved, the process is said to have converged on a solution. After the retrieval loop has converged on a profile, the result is the ‘Retrieved NH3 profile’, and the process is finished.

**Figure 1.1:** Flowchart showing the overall process of work completed.

### 1.3 Outline

Chapter 2 gives an overview of the background knowledge required to sufficiently understand the work presented. It outlines ammonia’s role in the atmosphere, the environment, and its impacts on humans. Details on current ammonia measuring instruments are given, and the specific objectives for the proposed optimized ammonia measuring instrument are discussed. An outline of Fourier transform spectroscopy in the context of remote sensing is given, and the basics of Rodgers retrieval theory are detailed alongside a discussion of the current ammonia retrievals. In Chapter 3, my work with radiative transfer models and the absorption spectrum
of ammonia is outlined. This lays the groundwork for the use of SASKTRAN in both the full instrument model (shown in green in Figure 1.1) and the convolution model (shown in orange in Figure 1.1) for the project. Chapter 4 outlines the development of these instrument models: two separate models of an imaging Fourier transform spectrometer that serve two different purposes, and a comparison of the model outputs is presented. In Chapter 5, the simulated retrievals of NH$_3$ and surface temperature are described, with results shown, which forms the basis for the retrieval loop shown in blue in Figure 1.1. Chapter 6 outlines the proposed instrument design based on the requirements as set by ECCC, and gives an overview of how the final design decisions were made. This chapter uses all three sections of the research, working together as shown in Figure 1.1 to run multiple simulations and generate meaningful data to be analyzed. Chapter 7 summarizes the work and outlines further steps to be taken on this project.
CHAPTER 2

BACKGROUND

This chapter details the necessary background knowledge required to understand the work presented in later chapters. It begins with an overview of Earth’s atmosphere in general terms, and describes the propagation of radiance as it travels through the atmosphere using the radiative transfer equation. Ammonia’s role in the atmosphere as well as its effects on the environment and humans is discussed, and an overview of current ammonia measuring instruments is presented. The objectives for the proposed optimized ammonia measuring instrument are described, and an outline of Fourier transform spectroscopy in the context of remote sensing is given. The basics of Rodgers retrieval theory (Rodgers, 2000) are detailed and are accompanied by a discussion of current ammonia retrievals.

2.1 The atmosphere

The Earth’s atmosphere can be classified into several different regions, the boundaries of which are generally drawn where the temperature profiles changes from increasing to decreasing, or vice versa. The lowest layer of the atmosphere is the troposphere, which extends from the Earth’s surface to around 15-20 km, where the first inversion of the temperature profile occurs at what is called the tropopause. Above the tropopause is the stratosphere, which extends upwards to about 50 to 55 km, and is bounded by the stratopause. Continuing upwards, the mesosphere exists in the region between the stratopause and the mesopause, which occurs around 80 to 85 km. Past the mesopause is the thermosphere, extending all the way to 500 - 1000 km, where the thermopause is, and past the thermopause is the exosphere, which extends to about 100,000 km in altitude. Figure 2.1 shows a typical temperature profile in the Northern Hemisphere (shown up to 100 km), displaying the inversions in the
temperature profile occurring at the tropopause, stratospause and mesopause. For this work, the troposphere is of particular interest, as the majority of ammonia is found in the first few kilometers of the atmosphere closest to the surface.

Figure 2.1: A typical temperature profile in the Northern Hemisphere, using data from MSIS90 (Hedin, 1991).

Gaining knowledge of the composition of the atmosphere is of scientific interest, but is challenging to achieve. Remote sensing instruments can accomplish this by collecting measurements of the atmosphere from which information about the atmosphere can be retrieved, such as temperature profiles and species profiles (see Section 2.5). For my research, nadir measurements (in which the lines of sight of the instrument intersect the Earth’s surface) are of particular interest, as the majority of NH$_3$ is found in the first few kilometers of the atmosphere closest to the surface. Different species present in the atmosphere absorb or emit specific wavelengths of radiation, and create an absorption/emission spectrum that is indicative of the atmospheric composition at the time and location of a given measurement.

Remote sensing with instruments usually involves measuring a radiance spectrum. The
spectral radiance is the radiance of some surface per unit frequency or wavelength, where radiance is the flux of radiation emitted per unit solid angle per unit area of source. The SI unit of spectral radiance in wavelength is W/sr/m$^3$, but it can also be given in alternate units, such as photons/s/cm$^2$/nm/sr. In equations, radiance is commonly given the symbol $I$ or $S$. The radiative transfer equations describe how radiance changes as it passes through the atmosphere. Due to the main spectral features of ammonia occurring in the thermal-infrared (TIR) region, simplifications to the radiative transfer equations will be made due to the signal being dominated by thermal emission in the TIR region. The differential form of the radiative transfer equation is

$$dI(s) = -I(s)k(s)ds + J(s)k(s)ds,$$

(2.1)

where $dI(s)$ is the change in radiance across a layer, $I(s)$ is the spectral radiance (in photons/s/cm$^2$/nm/sr), $k(s)$ is the extinction, and $ds$ is the infinitesimal thickness of the layer. The first half of the equation describes how the incoming spectral radiance is attenuated, while the second half includes the source term $J(s)$, that describes the radiance that is emitted or scattered along element $ds$. The extinction is the probability per unit length that a photon travelling through the layer will be scattered or absorbed, and is thus the sum of the absorption and scattering.

In the TIR regime, scattered sunlight can be ignored, and so the source term is equal to the Planck function,

$$B_\lambda(\lambda, T) = \frac{2hc^2}{\lambda^5} \frac{1}{e^{hc/\lambda k_B T} - 1},$$

(2.2)

where $h$ is the Planck constant, $c$ is the speed of light, $k_B$ is the Boltzmann constant, $\lambda$ is the wavelength of the light, and $T$ is the temperature at that point on the path $s$. Units for the source term are the same as those for radiance. Being in the TIR regime, the extinction is equal to the absorption, $k_a(s)$. The absorption is calculated as a sum over the product of the absorption cross sections, $\sigma_{ai}(s)$, and the number densities, $n_{ai}(s)$, of a given species ($i$) for all absorbing species present in the layer,

$$k_a(s) = \sum_i \sigma_{ai}(s)n_{ai}(s).$$

(2.3)
The absorption is calculated in SI units of 1/m. The line of sight can be broken into a series of small segments, with one such homogeneous segment being shown in Figure 2.2. In this case, \( ds \) becomes \( \Delta s \), and Equation 2.1 can be used to determine the outgoing spectral radiance at point \( j + 1 \) along the line of sight, given the incoming radiance at point \( j \). This is assuming there is a change in radiance occurring within the segment due to thermal emissions and molecular absorption.

\[
\ln \left( \frac{I_{j+1} - B_j}{I_j - B_j} \right) = -k_j(s_{j+1} - s_j).
\] (2.4)

Rearranging to obtain

\[
I_{j+1} = I_j e^{-\tau_j} + (1 - e^{-\tau_j})B_j,
\] (2.5)

where the (unitless) optical depth \( \tau_j \) is defined as

\[
\tau_j = (s_{j+1} - s_j)k_j.
\] (2.6)

By dividing the line of sight of an observer into multiple segments assumed to be homogeneous, Equation 2.5 can be used to propagate radiance from the end of an observer’s line of sight through each of the segments to reach the observer. For nadir geometry, the line of sight intersects the ground, and the initial radiance can be modelled as the surface emission using a black body model.

The total column density (in molecules/cm\(^2\)) for a given species \( i \) is defined as
\[ N_i = \int n_i(s) ds. \]  \hspace{1cm} (2.7)

where \( n_i(s) \) is the number density of the species along the path \( s \). For remote sensing, generally two types of column densities are used: slant column density, and vertical column density. The slant column density integrates along the line of sight of the observer, giving a measurement of how much of the species is seen along the line of sight. Unless the line of sight has a viewing zenith angle of 0° (i.e. it is staring straight down), this will not describe the column density above some footprint on the surface. The vertical column density is the number of molecules per cm² as seen by an observer looking straight up from a point on the ground. The ratio between the slant column density and vertical column density is called the air mass factor. For this project, the vertical column density will be used, calculated by integrating the retrieved profile over altitude.

Figure 2.3 shows the outgoing radiance of Earth’s atmosphere, calculated using the SASKTRAN radiative transfer engine (Zawada, 2018). H₂O, CO₂, O₃, N₂O and CH₄ are the most prominent absorbing species in the calculated region, with the labels on Figure 2.3 showing in which spectral region each species provides the most absorption. The radiance in the range of 950–980 cm⁻¹ is highlighted in red in Figure 2.3. This is the area where the most ammonia absorption takes place, and thus is where the focus lies for this thesis. To calculate the radiance shown, SASKTRAN solves the radiative transfer equation (Equation 2.1), propagating the initial radiance through the layers of the atmosphere all the way up to the observer, with the aforementioned absorbing species attenuating the radiance along the way.

### 2.2 Ammonia in the atmosphere

Ammonia can be considered the principal form of reactive nitrogen going into the environment (Sutton et al., 2013). It has effects on the nitrogen cycle, as well as air and water quality. Augmented levels of atmospheric ammonia can cause eutrophication, and the decrease of plant diversity (Carfrae et al., 2004). Increasing ammonia concentrations in coastal waters can lead to a decrease in water quality, algal blooms, and disruptions in the fisheries habitats (Paerl et al., 2002). The lifetime of ammonia is generally assumed to be in the range of 12
Figure 2.3: Outgoing radiance of the atmosphere in the thermal infrared region, with major absorbing species labelled. Radiance in the range of 950–980 cm$^{-1}$ is highlighted in red, where the most absorption of NH$_3$ occurs.

to 36 hours (Paulot et al., 2017), which is extremely short compared to other atmospheric gasses that have lifetimes on the order of days or years, and is why the atmospheric impact of ammonia comes from its contributions to chemical reactions that generate pollutants (Xu and Penner, 2012). The majority of ammonia is found in the first few kilometers of the atmosphere; this is because it has a high affinity to water, and its incorporation into aqueous and acid particles is what effectively removes it from the atmosphere, as well as atmospheric scavenging (Ge et al., 2018).

The reactions of ammonia with acidic species leads to the production of secondary inorganic aerosols such as ammonium nitrate and ammonium sulfate (Doyle et al., 1979 (Stelson and Seinfeld, 1982)). These secondary inorganic aerosols can account for a large percentage of the mass of PM$_{2.5}$, in the range of 25-50% as found by Gautam et al., 2019 depending on
the location of measurement. Also known as fine particulate matter, PM$_{2.5}$ are aerosols that have a diameter less than 2.5 µm (Hertel et al., 2012). These particles are known to have impacts on human health, with a reduction in exposure to these fine particulates contributing to a longer life expectancy (Pope et al., 2009). Crouse et al., 2012 found links between long-term exposure to PM$_{2.5}$ and cardiovascular mortality, with the strongest association being with coronary heart disease. Exposure to PM$_{2.5}$ has also been linked to lung cancer (Pope III et al., 2002), and it is estimated that a difference in PM$_{2.5}$ concentration as small as 10 µg/m$^3$ is associated with a 1.5% increase in deaths overall (Schwartz et al., 2002).

Lamarque et al., 2010 shows that ammonia has increased by a factor of 5 from 1850 to 2000, and ammonia is one of the Intergovernmental Panel on Climate Change AR5 Representative Pathway Concentration (RPC) species that is projected to increase by the end of the 21st century, with some modelling scenarios predicting that the emissions of NH$_3$ will almost double by 2100 (Lamarque et al., 2011 Ciais et al., 2013). The majority of global NH$_3$ emissions come from agriculture - approximately 57% (Sutton et al., 2013). The remaining 43% comes from natural sources (21%), anthropogenic sources including the burning of fossil fuels (14%), and biomass burning (8%) (Sutton et al., 2013). For Canada specifically, 421 kt/yr (nearly 90%) of emissions comes from agriculture (Bittman et al., 2017). International conventions exist requiring mitigation of NH$_3$ emissions, but currently there are no Canadian guidelines for emissions targets or best agricultural practices (Bittman et al., 2017). Bittman et al., 2017 suggests several broad options for reduction of ammonia emissions (low-emission slurry application, reducing emissions from fertilizer application, reduced consumption of beef and pork), but also posits the strategy of mitigating emissions that pose the highest risk to humans and the environment, due to timing or location. The latter strategy would require both good modelling and high quality measurements to create regulations.

By estimating emissions for different atmospheric quantities, insights into the composition of the atmosphere can be gained, yearly trends can be analyzed, and hotspots for emissions can be identified. Emissions estimates are done using one of two strategies: bottom-up, which makes use of data currently known about emission activity in the area of interest, or top-down, which uses observations (e.g. from a satellite) to perform calculations. Emissions estimates for NH$_3$ vary, due to lack of knowledge about agricultural resources and differences
in the assumed lifetime of NH$_3$ (Luo et al., 2022). A study by Luo et al. (2022) estimated 78 (70–92) Tg a$^{-1}$, using a top-down method that used both IASI observations and GEOS-Chem model simulations, looking in the range of 2008 to 2018. A different study by Evangeliou et al. (2021) estimated annual emissions to be in the range of 190-210 Tg a$^{-1}$, much larger than the bottom-up estimate of 62 Tg a$^{-1}$ from the Community Emission Data System, CEDS (Luo et al., 2022). Although emissions estimates for NH$_3$ have been done, these estimates vary quite a bit depending on the exact strategy of estimation.

Designing a dedicated instrument optimized for ammonia detection, the goal of this work, is done with the intention of eventually building the instrument and generating a data set of ammonia measurements that have high spatial and temporal resolution. Having such a data set is important for the accuracy of model performance for academic interests, but it can also affect policies developed using the model to assess the impact of policy actions (Reis et al., 2009). A study done by Gilliland et al. (2003) suggested strong seasonal variations in NH$_3$ emissions (~70% higher in June compared to fall and winter months), and that the inclusion of these variations may be significant for model performance. Erisman et al., 2009 discusses what they refer to as the ‘ammonia gap’ - the difference between emissions based ammonia concentrations (from models) and measured air concentrations. This ammonia gap combined with the effect that NH$_3$ emissions have on model performance shows that more information from air measurements is needed to increase model performance.

Despite the many impacts it can have on human health as well as the environment, the actual concentration of ammonia in the atmosphere is generally very low. Measurements of NH$_3$ are typically given in units of parts per billion volume (ppbv, or simply ppb). This describes the volume occupied by the gas, in this case NH$_3$ per volume of air. Shephard et al. (2011) considered profiles with a surface Volume Mixing Ratio (VMR) greater than 5 ppbv to be polluted. Such small concentrations result in a weak spectral signal, requiring a high signal-to-noise ratio from the instrument to ensure that moderately polluted profiles can still be detected. This signal-to-noise requirement, combined with the desired coverage, spectral resolution, and ground spatial resolution, creates tight criteria for an optimized instrument to detect ammonia.
2.3 Current ammonia-measuring instruments

High-quality ammonia measurements are difficult to acquire, and require a combination of a good signal-to-noise ratio (SNR) and high spectral resolution to be successful. Instruments such as the Tropospheric Emission Spectrometer (TES, Shephard et al., 2011), the Infrared Atmospheric Sounding Interferometer (IASI, Walker et al., 2011), the Cross-track Infrared Sounder (CrIS, Shephard and Cady-Pereira, 2015), the Hyperspectral Thermal Emission Spectrometer (HyTES, Kuai et al., 2019), and the Atmospheric Infrared Sounder (AIRS, Warner et al., 2016) have all successfully performed ammonia retrievals. While these instruments were not designed specifically for the detection of NH\textsubscript{3}, the spectral region covered allowed for the retrievals to be performed. A short overview of each of these instruments and how they have been used to retrieve ammonia is provided in the following subsections.

2.3.1 TES

TES is an imaging infrared Fourier-transform spectrometer onboard the National Aeronautics and Space Administration’s (NASA) Aura platform, launched on July 15, 2004 (Shephard et al., 2011). It has a high spectral resolution (0.1 cm\textsuperscript{-1}, 0.06 cm\textsuperscript{-1} unpodized), a ground footprint of 5km×8km, and a low brightness temperature noise of 0.1-0.2 K (Shephard et al., 2011). The Aura platform is in a Sun-synchronous polar orbit, with a 16-day exact repeat cycle, and a near-repeat every 2 days (Beer et al., 2001). Figure 2.4 shows the coverage provided by TES during a single day. Measuring in the range of 650–3050 cm\textsuperscript{-1}, TES’s combination of high spectral resolution and high SNR makes it a prime candidate for ammonia detection (Beer et al., 2001). In Shephard et al. (2011), ammonia retrievals were performed using the TES data, using microwindows to reduce the impact of interfering species. Due to the low degrees of freedom (i.e. low amount of information available), a transformation matrix was developed to take the retrieved ammonia profile and reduce the influence of the a priori data, resulting in data point(s) that more accurately reflect the information gained from the retrieval (Shephard et al., 2011). These points are referred to as the Representative Volume Mixing Ratio (RVMR) (Shephard et al., 2011), and the averaged TES RVMR values are plotted on a map in Figure 2.5. See Section 2.6 for details.
on the calculation of the RVMR. The SNR sensitivity study done in the Shephard et al., 2011 paper estimated the TES minimum level of ammonia detectability to be a profile with a peak ammonia concentration value of 1 ppbv.

![Figure 2.4: Map of the coverage achieved during a typical day of TES global surveying. Reprinted with permission from Beer et al., 2001 © The Optical Society.](image)

### 2.3.2 CrIS

CrIS is an across-track scanning Fourier-transform instrument that has a 2200 km swath, a spectral resolution of 0.625 cm\(^{-1}\), and a spectral noise level near 0.04 K (Shephard and Cady-Pereira, 2015). CrIS measures over the spectral range of 650–2550 cm\(^{-1}\) (Strow et al., 2013). Operated by the USA Joint Polar Satellite System (JPSS) program (a collaboration between the National Oceanic and Atmospheric Administration (NOAA), the Department of Defense (DoD) and NASA), it resides on the Suomi National Polar-orbiting Partnership (NPP) satellite, which was launched on 28 October 2011 (Shephard and Cady-Pereira, 2015). CrIS has a 3×3 array of circular pixels, with each pixel having a 14 km ground footprint diameter (Shephard and Cady-Pereira, 2015). From the retrievals done in Shephard and Cady-Pereira (2015), CrIS has a minimum peak detection limit of 1 ppbv. The retrievals have limited information, typically less than one degree of freedom, giving effectively an average mixing ratio value instead of a true profile with independent pieces of information.
2.3.3 IASI

IASI is a Michelson-type Fourier transform spectrometer onboard the EUMETSAT MetOp platform, which measures in the range of 645–2760 cm\(^{-1}\) at an unapodized spectral resolution of 0.25 cm\(^{-1}\) (Walker et al., 2011). Launched on October 19, 2006 (Razavi et al., 2009), it is a scanning instrument, with a 2400 km swath containing 2×2 arrays of pixels with a 12.3 km ground footprint diameter (Walker et al., 2011) and a brightness temperature noise in the range of 0.15-0.2 K (Shephard and Cady-Pereira, 2015). Measurements from IASI were used in Walker et al. (2011) to retrieve total column amounts, with estimates of up to 6.8
mg m$^{-2}$. These retrievals showed correspondence between levels of high ammonia detection and intensively farmed regions.

2.3.4 AIRS

The AIRS instrument is a grating spectrometer, measuring 2378 separate spectral channels in the range of 650 to 2670 cm$^{-1}$ with a ground spatial resolution of 13.5 km (Warner et al., 2016). Launched on board the Earth Observing System (EOS) Aqua Spacecraft on May 4, 2002 (Pagano et al., 2010), the data retrieved from the AIRS measurements has been compiled into a daily global map of ammonia (with a resulting 45 km$^2$ spatial resolution), which is able to show areas with persistent elevated levels of NH$_3$, and correlate these areas with cropland usage (Warner et al., 2016). Noise levels in our area of interest are $\sim$0.35 K (Pagano et al., 2003).

2.3.5 HyTES

HyTES is a 512 pixel push-broom grating imaging spectrometer, built and managed by the NASA Jet Propulsion Laboratory (Kuai et al., 2019). With its first flights in July 2012, HyTES has been flown several times on the low-altitude Twin Otter aircraft, and has had a flight on the high-altitude NASA ER-2 research aircraft (Kuai et al., 2019). It makes use of 256 spectral channels measuring in the range of 7.5 to 12 $\mu$m, giving a spectral resolution around 2 cm$^{-1}$ (Kuai et al., 2019). At a flight altitude of 1 km, HyTES has a pixel size of 2 x 2 m, which would roughly translate to a pixel size of 1.2 km at an orbital altitude of 600 km (Kuai et al., 2019). The noise level of HyTES is around 0.2 K (Hulley et al., 2016). A paper by Kuai et al. (2019) shows the use of HyTES data to study three NH$_3$ plumes from a feedlot (with low thermal contrast), a power plant (with high thermal contrast), and a wildfire (with high thermal contrast), all in the USA. The smoldering wildfire had a retrieved NH$_3$ concentration of 5 ppb, the powerplant 10-15 ppb, and the feedlot 50 ppb.
2.3.6 Instrument Objectives

The previously mentioned instruments were not specifically designed with ammonia measurement as the primary objective, while the instrument developed in this thesis is solely focused on the measurement of ammonia, with all design choices being made with this goal in mind. Other ammonia-measuring instruments such as TES and IASI performed methane retrievals in addition to the ammonia retrievals. The nearest windows in which methane is typically retrieved, 1290-1310 cm\(^{-1}\) for TES (Worden et al., 2012) and 1210-1290 cm\(^{-1}\) for IASI (De Wachter et al., 2017), were deemed to be too far from the NH\(_3\) windows, and would add unnecessary complexity into the design. As measuring methane was not the original intention of this project, it was decided that this project would focus solely on the measurement of ammonia. There are other instruments which are able to detect ammonia to a certain extent, but the need for measurements with a higher spatial resolution, better coverage of Canada, and higher precision and accuracy remains.

Designing an instrument specifically for NH\(_3\) measurement allows for the optimization of parameters to ideally provide daily mapping of NH\(_3\) in Canada. The main objective is to increase the spatial resolution of measurements while keeping reasonable spatial coverage and sufficient SNR for precise retrievals. Table 2.1 shows the goal and threshold requirements of the instrument, developed in collaboration with ECCC scientists. The goal values are the ideal values of the given parameters for recovered measurements, while the threshold values are the maximum acceptable values for the parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Goal value</th>
<th>Threshold value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spectral Resolution (cm(^{-1}))</td>
<td>0.05</td>
<td>0.1</td>
</tr>
<tr>
<td>Spatial resolution per pixel (km)</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>Brightness noise level (K) at 270 K</td>
<td>0.05</td>
<td>0.1</td>
</tr>
</tbody>
</table>

**Table 2.1:** List of goal and threshold requirements for NH\(_3\) detecting satellite.

Ideally, the ground spatial resolution would be on the scale of 1 km, which would provide good resolution while still allowing for reasonable coverage per image. The lowest acceptable spectral resolution for the instrument is 0.1 cm\(^{-1}\), to ensure the narrow signal from NH\(_3\) is
captured by the measurement. A brightness noise level of 0.1 K or less at 270 K is required, to be able to distinguish the weak NH$_3$ signal from background noise. The previously described instruments fall short of the criteria laid out in Table 2.1, hence the need for a dedicated instrument.

Due to the high spectral resolution required for the instrument, a grating spectrometer is not the ideal choice, as most have a maximum practical resolution around $\sim 0.2 \text{ cm}^{-1}$, which does not meet the threshold requirement for resolution (Kaufmann et al., 2022). In general, the Fourier transform spectrometer (FTS) is more complex than a grating spectrometer, but the FTS has the Fellgett advantage, also known as the multiplex advantage. Perkins, 1987 explains that a Fourier Transform Infrared spectrometer can achieve a much higher SNR in comparison to an equivalent scanning monochromator. An interferometer sees all wavelengths at once, compared to a dispersive instrument that sees one wavelength at a time (Perkins, 1987). The advantage is quantified by the equation

$$
\text{Fellgett’s advantage} = \sqrt{\frac{\nu_1 - \nu_2}{\Delta \nu}},
$$

(2.8)

where $\nu_1$ and $\nu_2$ are the limits of the spectrum in question, and $\Delta \nu$ is the resolution. In words, the Fellgett advantage is equal to the square root of the number of sample points in the spectrum. For this instrument’s purposes, using the threshold resolution of 0.1 cm$^{-1}$ and a range of 920-1010 cm$^{-1}$, the Fellgett advantage is calculated to be a factor of 30. Higher resolutions and/or wider spectral ranges increase the Fellgett advantage. Factors such as the beam-splitter efficiency and detector frequency response stop an FTS from fully realizing the theoretical calculated Fellgett advantage potential, but for detector-noise-limited systems the advantage is enough to make the FTS the principal choice for the infrared region (Perkins, 1987).

Due to the weak signal from NH$_3$, a high SNR is required to collect meaningful data. A filtered band spectrometer could be another option for this project, but the finite number of wavelengths it can measure is limiting, compared to the larger spectrum generated by the FTS. Overall, the FTS is the obvious choice for this project. Thus, we move forward with the idea that the Fourier transform spectrometer is the best instrument type for this project.
2.4 Remote Sensing with Fourier transform spectrometry

Interferometers merge two (or more) sources of light to create an interference pattern, which can be analyzed to extract information about the incoming light. A Fourier Transform Spectrometer is an instrument that uses an interferometer and induces a path difference between the two sources of light, recording the intensity of the interference pattern as a function of path difference. This recording is known as an interferogram. The spectrum of the incoming light will determine the shape of the interferogram, as different wavelengths of light will interfere differently for a given optical path difference. Thus, using the constructive and destructive interference of electromagnetic radiation, information about the spectrum of the incoming light is recorded by the FTS in the interferogram. The Fourier transform operation is able to take a function of distance \( f(x) \) and transform it into a function of wavenumber \( g(\nu) \), where the wavenumber is just the inverse of the wavelength. By taking the Fourier transform of the interferogram, a function of optical path difference, a function is obtained that describes the strength of the incoming light as a function of wavenumber. In other words, the Fourier transform of the interferogram generates a radiance spectrum.

Compared to a grating-based spectrometer, the FTS is capable of a much higher spectral resolution (Jahromi et al., 2021), which allows for better retrievals of atmospheric species. The following sections describe the operation of the basic Michelson interferometer as well as the details unique to an imaging FTS.

2.4.1 Michelson interferometer

Michelson interferometers are a common choice to use in an FTS setup. Specific variations in the configuration are possible, but the overall operation remains the same. Figure 2.6 shows the setup of a Michelson interferometer.

As seen in Figure 2.6, the input beam of collimated light is split into two beams at the beamsplitter, each of which travels down one arm of the interferometer. The beams each reflect off of the mirror at the end of the respective arm, and are once again split at the
The focusing optics recombine a portion of each of the beams, and the light reaches the detector. By moving one of the mirrors at the end of the interferometer arm, an optical path difference (OPD), denoted by \( x \), between the two beams is created. With zero path difference, constructive interference of the recombined beams occurs and the measured intensity is at a maximum. Maxima also occur when the OPD is an integral multiple of \( \lambda \). For monochromatic light of wavelength \( \lambda \), displacing the moving mirror by a distance of \( \lambda/4 \) gives a total path difference of \( \lambda/2 \), creating destructive interference, resulting in no signal being detected. This also occurs for OPDs of the form \( (n + \frac{1}{2})\lambda \), where \( n = 0, 1, 2, \ldots \). The variation in intensity seen by the detector due to the interference of the two beams is recorded for different OPDs, and generates an interferogram. Note that the following analysis switches to using wavenumber instead of wavelength, as the Fourier transforms are done in wavenumber-distance pairs. The wavenumber is defined as

\[
\nu = \frac{1}{\lambda},
\]  

(2.9)
where $\lambda$ is the given wavelength. The signal intensity of a monochromatic source is

$$I_0(x) = S(\nu_0)(1 + \cos(2\pi\nu_0x)), \quad (2.10)$$

where $S(\nu_0)$ is the input radiance at a given wavenumber $\nu_0$. The signal intensity seen by the detector from a polychromatic input beam at a given OPD $x$ is simply a superposition of multiple monochromatic sources,

$$I_p(x) = \int_{0}^{\infty} S(\nu)(1 + \cos(2\pi\nu x))d\nu. \quad (2.11)$$

The spectrum that created the interferogram can be recovered using a Fourier transform,

$$S(\nu) = \int_{0}^{\infty} I(x)e^{-j2\pi\nu x}dx, \quad (2.12)$$

where $I(x)$ is the modulated interferogram data, generated by subtracting the mean from the interferogram data.

The largest difference in OPD is referred to as the Maximum Optical Path Difference (MOPD). The choice of MOPD is what determines the resolution to which the spectrum can be recovered with the Fourier Transform. If an IFTS with some given MOPD observes a monochromatic source of wavenumber $\nu_1$, the recorded interferogram will have the shape of a cosine wave, centred at the OPD of zero, and truncated at $\pm x_{MOPD}$. This interferogram can be thought of as an infinite cosine wave multiplied by a boxcar function that is equal to 1 in the range $[-x_{MOPD}, x_{MOPD}]$, and 0 elsewhere. Recall that the Convolution Theorem states that the multiplication of two functions in one Fourier domain is equal to the convolution of the Fourier transform pairs of the functions in the other Fourier domain. The Fourier transform pair of the infinite cosine is a delta function at $\nu_1$, and the Fourier transform pair of the boxcar signal is the sinc function. The convolution of these two functions results in the recovered spectrum taking the form of a sinc function centred on the wavenumber $\nu_1$,

$$\text{sinc}(2\pi x_{MOPD}(\nu - \nu_1)). \quad (2.13)$$

Now recall the Rayleigh criterion for resolution: two lines can be resolved if the distance between their peaks is bigger than the distance between the line’s peak and its first minimum. The first minimum of the sinc function occurs when
which is the same as saying it occurs when

\[ \nu - \nu_1 = \frac{1}{2x_{MOPD}}. \]  

(2.15)

So per the Rayleigh criterion, the minimum distance between two lines that is resolvable is $1/2x_{MOPD}$.

There are two main scanning methods for interferometers. The step-scan method involves the moving mirror stopping at discrete intervals, gathering signal, and then moving to the next OPD; all of the intensity recorded for a single data point is gathered at the same OPD. This mode allows for an increase in instrument sensitivity and the removal of the atmospheric transmission variations. The time required for the step-scan method is variable depending on the specific implementation. For example, a ground-based astronomical instrument developed by ABB requires 2 seconds to step between each scan, but can undersample (see Section 2.4.2) by a factor of 10 (F. J. Grandmont, personal communication, October 24, 2022). Rapid step-scanning methods have been studied by ABB Ltd., but the technology remains at a technology readiness level of 2 (F. J. Grandmont, personal communication, October 24, 2022).

The continuous scan method involves the moving mirror moving at a constant speed, so the intensity collected for a single data point occurs within a small range of OPDs. The interferogram of the source is recorded quickly, and then, in some cases, a scan of a nearby background position is taken (Naylor et al., 2005). Figure 2.7 shows an intensity fringe near the zero path difference (ZPD), and also marks the point on the fringe that the step and scan method would detect.

Choosing to use the step-scan method would increase the cost and complexity of the design, and potentially require more time for each scan, depending on whether we choose to model based on the newer rapid-scan methods. The precision required in the instrumentation to implement this method is high. For the purposes of an instrument to detect ammonia, the continuous scan method is more favourable. Equation 2.11 is modified to incorporate the changing OPD over time interval $(0, t_f)$:
Figure 2.7: Intensity fringe near ZPD, with the intensity at exactly ZPD marked in orange.

\[ I_p(x_{avg}) = \int_0^t \int_0^\infty S(\nu)(1 + \cos(2\pi\nu(x_0 + Vt)))d\nu dt, \]  \hspace{1cm} (2.16)

where \( V \) is the speed of the moving mirror, \( x_0 \) is the starting OPD of the measurement, \( t \) is the time that has passed since the beginning of the measurement (\( t=0 \) at \( x_0 \)), and \( x_{avg} \) is the average OPD for the point. Figure 2.8 shows two interferograms (single-sided, see Section 2.4.2) under identical conditions, one having been generated using the step-scan method, and the other with continuous scanning.

2.4.2 Options for FTS

For some instruments, the time needed to acquire an interferogram that meets the resolution requirements of the projects is larger than the amount of time allotted per scan to meet the coverage requirements. To reduce the amount of time required for a single scan at a given scanning rate, the number of samples must decrease. There are two methods that can be used to reduce the number of samples in the interferogram: using single-sided interferograms, and undersampling.
Single-Sided Interferograms

For an instrument with a given maximum OPD, a typical (double-sided) interferogram is recorded with samples being taken while the OPD varies from \(-x_{\text{max}}\) to \(x_{\text{max}}\), where \(x_{\text{max}}\) is the MOPD. For a single-sided interferogram, the samples taken do not go all the way to the negative of the MOPD, and will either begin at the ZPD or at some smaller negative OPD value \((-x_{\text{min}})\). For this project, a small number of samples (20, per the recommendation of ABB) will be taken on the negative side of the interferogram, to aid in the phase correction. The phase correction is done following the method described in Mertz, 1967.

A short, double-sided interferogram, using equal amounts of samples on either side of the peak, is used in phase correction. Figure 2.9 shows the full (single-sided) interferogram, as well as the points that make up the short double-sided interferogram. Figure 2.10 shows the spectrum and phase calculated using the short double-sided interferogram. The real and
imaginary parts of the recovered spectrum from the double-sided interferogram do not show visible absorption lines - there is hardly any detail in the spectrum due to the shortened MOPD resulting in a low spectral resolution (recall Equation 2.15). The spectrum and phase plotted in Figure 2.10 have been interpolated to the higher resolution wavenumber array used in the calculation of the single-sided interferogram recovered spectrum (necessary for the phase correction). It is the phase calculated from the short double-sided interferogram that will be used to phase correct the spectrum from the single-sided interferogram.

![Figure 2.9: Single-sided interferogram and its accompanying short double-sided interferogram.](image)

Care is taken at this point to distinguish between the weighting function and the apodization function for the single sided interferogram. The weighting function used for the single sided interferogram must be such that the central fringe and its neighbouring points are not counted twice, compared to the more distant fringes (Mertz, 1967). Ben-David and Ifarraguerrí, 2002 gives the criteria that the weighting function $w(x)$ must satisfy the re-
Figure 2.10: Magnitude and phase of calculated spectrum using the short double-sided interferogram.

\[ w(x_0 - x) + w(x_0 + x) = 1 \text{ in the range } -x_{\text{min}} \leq x \leq x_{\text{min}}. \]

If this criteria is not met, the contrast of absorption lines is reduced (Mertz, 1967). For simplicity, a piecewise weighting function is used, comprising of a ramp function going from \(-x_{\text{min}}\) to \(x_{\text{min}}\), and all points greater than \(x_{\text{min}}\) having a weighting of 1. The weighting function must always be used, but an apodization function can be added onto the interferogram as well to obtain a smoother end spectrum. Figure 2.11 shows the chosen weighting function used for single sided interferograms.

Taking the Fourier transform of the weighted and apodized single-sided interferogram gives the magnitude and phase spectra seen in Figure 2.12.

Note that the spectrum recovered from the single-sided interferogram has more detail than that from the short double-sided interferogram - the absorption lines in the spectrum can now be seen due to the higher MOPD. This higher-resolution radiance must first be
Figure 2.11: Weighting function used for single-sided interferograms.

Phase corrected before it can be of use. From Chase, [1982] the phase corrected spectrum $S(\nu_i)$ is

$$S(\nu_i) = R(\nu_i) \cos \theta(\nu_i) + I(\nu_i) \sin \theta(\nu_i),$$  \hspace{1cm} (2.17)

where $R(\nu_i)$ is the real component of the spectrum after the Fourier transform, $I(\nu_i)$ is the imaginary component of the spectrum after the Fourier transform, and $\theta(\nu_i)$ is the phase function. The proper phase function is found from the short double-sided interferogram, while the real and imaginary components of the spectrum come from the single-sided interferogram. Figure 2.13 shows the phase corrected spectrum.

Undersampling

Another option to reduce the time needed to acquire an interferogram is to undersample the interferogram. Information theory dictates that the highest frequency component able to be recovered is determined by the sampling spacing, per the Nyquist sampling theorem:

$$\Delta z \leq \frac{1}{2\sigma_n},$$  \hspace{1cm} (2.18)

where $\Delta z$ is the OPD sampling interval in cm, and $\sigma_n$ is the Nyquist frequency in cm$^{-1}$. This is true for any signal that has components spanning the interval from 0 to $\sigma_n$cm$^{-1}$. For a band-limited signal with non-zero components in between the frequency limits $\sigma_{min}$
and $\sigma_{\text{max}}$, the minimum required OPD sampling interval is instead given by the Shannon sampling theorem:

\[ \Delta z \leq \frac{1}{2(\sigma_{\text{max}} - \sigma_{\text{min}})}. \]

(2.19)

Note that the narrower the band, the more savings can be found from the Shannon sampling theorem. Taking fewer samples of the interferogram than is dictated by the Nyquist theorem (i.e. undersampling) results in the aliasing of the signal to lower wavenumbers when transformed back into radiance-space. Sampling that is coarser than dictated by the Shannon sampling theorem will not allow the spectrum to be fully recovered.

Figure 2.14 shows a fully sampled interferogram, as well as two undersampled interferograms, undersampled by factors of 2 and 4, respectively. Note that for the lower sampling rates, the same underlying interferogram is being sampled.
Figure 2.13: Spectra calculated using single-sided interferogram, and the phase-corrected spectrum

2.4.3 Imaging FTS

An IFTS uses an array of detector pixels as opposed to one singular pixel, allowing the instrument to have multiple lines of sight. Figure 2.15 shows a ray diagram for an on-axis and off-axis pixel on the focal plane. Note that the off-axis angle $\alpha$ is the same angle of the light entering and exiting the Michelson interferometer.

The OPD of the off-axis pixel is modified by the incident angle $\alpha$,

$$x_{i,j} = x_0 \cos(\alpha_{i,j}),$$  \hspace{1cm} (2.20)

where $x_0$ is the OPD for the on-axis pixel, and $\alpha_{i,j}$ is the off-axis angle for the pixel located at position $(i,j)$. As the IFTS steps through different OPD values, each pixel views the intensity corresponding to its line of sight, allowing data collection for multiple lines of sight to occur simultaneously.
Figure 2.14: Interferograms generated from instrument model, showing a fully sampled interferogram, and undersampled interferograms (with undersampling factors of 2 and 4).

2.5 Rodgers retrieval methods

Spectral measurements contain information about the atmospheric content at the time and location of the measurement. This information can be extracted from the measurement through what is known as the retrieval process, which is formulated as an inverse problem. Rodgers, 2000 presents an overview of the inverse problem and methods for solving, which will be used in this work. Equations 2.21 through 2.38 present the Rodgers, 2000 approach used for retrievals. The forward model models the physics of the light propagating through
Figure 2.15: Ray diagram showing an on-axis pixel with position (h, v) and off-axis pixel with position (i, j), where r represents the distance between the two pixels, $\alpha$ is the off-axis angle, and b is the image distance (recreated following Kumar Sha, 2013).

the atmosphere and through the instrument, and is defined by Rodgers, 2000 as

$$F(x, b) = y + \epsilon, \quad (2.21)$$

where $x$ is the vector of length $n$ that is of interest, $b$ is auxiliary information, $y$ is the vector of $m$ measurements, and $\epsilon$ is the vector of error associated with the measurements. For example, in this work $x$ is the log of the Volume Mixing Ratio of NH$_3$, and $y$ is the spectra measured by the instrument. The model parameter $x$ to the forward model is unknown, but the measurements $y$ are known. To obtain the vector $x$, the forward model must be inverted. Atmospheric inverse problems are non-linear and fundamentally ill-posed (i.e. the measurements do not contain enough information to fully recover $x$). Finding a solution to this problem begins with the solution to the linear inverse problem,

$$y = Kx, \quad (2.22)$$

where $K$ is an $m \times n$ matrix, assumed to be full rank. For the case where $n=m$, $K$ is square and invertible, and the exact solution is $x=K^{-1}y$. If $n > m$ (underdetermined case, also known as ill-posed), there are infinitely many solutions as there is not enough information from the measurements to fully retrieve $x$. Additional information from implementing constraints, more measurements, or lowering the resolution of the retrieval grid is required for a solution. If $n < m$ (overdetermined case), there are no solutions that perfectly match all the data, proving the need for error within the model to allow for any discrepancies in the measurement.
values. The determination of the ideal solution \( \mathbf{x} \) that fits within error criteria is done by minimizing the least square difference between the measurements and the model,

\[
\chi^2 = (\mathbf{y} - \mathbf{Kx})^T (\mathbf{y} - \mathbf{Kx}).
\] (2.23)

Taking the derivative of \( \chi^2 \), setting the derivative equal to zero, and solving for \( \mathbf{x} \) gives

\[
\mathbf{x} = (\mathbf{K}^T \mathbf{K})^{-1} \mathbf{K}^T \mathbf{y}.
\] (2.24)

Retrievals model measurements as probability density functions to allow for experimental error and noise in the measurements. Considering the Gaussian probability density function,

\[
P(\mathbf{y}) \sim \exp \left[ -\frac{1}{2} (\mathbf{y} - \mathbf{\bar{y}})^T \mathbf{S}_y^{-1} (\mathbf{y} - \mathbf{\bar{y}}) \right],
\] (2.25)

where \( \mathbf{S}_y \) is a covariance matrix representing correlation of error between channels. For channels \( i \) and \( j \),

\[
\mathbf{S}_{ij} = \epsilon \{(y_i - \bar{y}_i)(y_j - \bar{y}_j)\}. \quad (2.26)
\]

Using \( \mathbf{Kx} \) as the best estimate for \( \mathbf{\bar{y}} \), the probability of measurement \( \mathbf{y} \) occurring for a given \( \mathbf{x} \) is

\[
P(\mathbf{y}|\mathbf{x}) \sim \exp \left[ -\frac{1}{2} (\mathbf{y} - \mathbf{Kx})^T \mathbf{S}_y^{-1} (\mathbf{y} - \mathbf{Kx}) \right],
\] (2.27)

where the maximum likelihood solution occurs as the maximum of this function. The least squares difference is now

\[
\chi^2 = (\mathbf{y} - \mathbf{Kx})^T \mathbf{S}_y^{-1} (\mathbf{y} - \mathbf{Kx}).
\] (2.28)

Setting the derivative of \( \chi^2 \) to zero gives a most probable solution of

\[
\mathbf{x} = \left( \mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K} \right)^{-1} \mathbf{S}_y^{-1} \mathbf{K}^T \mathbf{y}.
\] (2.29)

If \( \mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K} \) is non-invertible, a proper solution cannot be found without additional information. A simple way of adding knowledge is a priori information, which is information about the atmosphere that is known prior to taking measurements. Representing this information as a Gaussian probability density function,

\[
P(\mathbf{x}) \sim \exp \left[ -\frac{1}{2} (\mathbf{x} - \mathbf{x}_a)^T \mathbf{S}_a^{-1} (\mathbf{x} - \mathbf{x}_a) \right],
\] (2.30)
where \( x_a \) is the prior knowledge of vector \( x \), the least squares equation becomes

\[
\chi^2 = (y - Kx)^T S_y^{-1} (y - Kx) + (x - x_a)^T S_a^{-1} (x - x_a), \tag{2.31}
\]

and the solution for \( x \) becomes

\[
\hat{x} = x_a + (K^T S_y^{-1} K + S_a^{-1})^{-1} K^T S_y^{-1} (y - Kx_a). \tag{2.32}
\]

This is the maximum a posteriori solution: the vector \( x \) for which the probability of \( x \) is maximized for a given measurement vector \( y \).

The retrieval of atmospheric trace gasses is a moderately non-linear problem, and as such it cannot be perfectly inverted, but can be solved by linearizing the system and iteratively solving using the Gauss-Newton method. The term \( Kx \) in Equation 2.31 is replaced by the non-linear model of the particular problem, \( F(x) \),

\[
\chi^2 = (y - F(x))^T S_y^{-1} (y - F(x)) + (x - x_a)^T S_a^{-1} (x - x_a). \tag{2.33}
\]

Taking the derivative of \( \chi^2 \) and setting it to 0 gives

\[
-\left[ \nabla_x F(x) \right]^T S_y^{-1} [y - F(x)] + S_a^{-1} (x - x_a) = 0. \tag{2.34}
\]

Now, \( K \) is the Jacobian matrix, and is defined as the first derivative of the forward model,

\[
\nabla_x F(x) = \frac{\partial F(x)}{\partial x} = K. \tag{2.35}
\]

This allows us to define the function upon which the Gauss-Newton method will act

\[
g(x) = -K^T S_y^{-1} [y - F(x)] + S_a^{-1} (x - x_a), \tag{2.36}
\]

as well as its derivative

\[
\nabla_x g(x) = K^T S_y^{-1} K + S_a^{-1} - \left[ \nabla_x K^T \right] S_y^{-1} (y - F(x)). \tag{2.37}
\]

The Gauss-Newton method can now be applied to find the root of the gradient of the cost function (2.36), which minimizes the cost function (2.33) itself. All \( \nabla_x K^T \) terms are set to 0 (as Gauss-Newton ignores second derivatives). Subbing in Equations 2.36 and 2.37 to the Gauss-Newton equation gives

\[
x_{i+1} = x_i - \left[ \nabla_x g(x_i) \right]^{-1} g(x_i). \tag{2.38}
\]

Equation 2.38 is repeatedly applied to the problem until convergence is achieved.
2.6 Existing Retrievals

As discussed in Section 2.3, there are multiple instruments that currently take measurements from which ammonia can be retrieved. The TES paper by Shephard et al., [2011] gives lots of detail and insight into their retrieval process. A Rodgers-style retrieval is performed on the natural logarithm of the VMR, after the retrievals of temperature, water vapor, ozone, methane, carbon dioxide, clouds, surface temperature, and surface emissivity (Shephard et al., 2011). Shephard et al., 2011 used a priori profiles for the retrievals derived from the GEOS-Chem chemical transport model simulations of 2005 global distributions of ammonia. Three different NH\textsubscript{3} a priori profiles were generated: ‘polluted’, which averaged all profiles with surface VMR greater than 5 ppbv, ‘moderately polluted’, which averaged all profiles with between 1 ppbv and 5 ppbv at the surface or had greater than 1 ppbv between the surface and 500 hPA, and ‘unpolluted’, which averaged all profiles with less than 1 ppbv between the surface at 800 hPa (Shephard et al., 2011). Once the retrieval has been performed, the RVMR value is calculated in an attempt to reduce the influence of the prior profile. Given the relatively weak signal of NH\textsubscript{3}, in general the retrieval provides at most one Degree of Freedom for Signal (DOFS), which is why the RVMR value is calculated.

For the RVMR calculation, the transformation matrix makes use of the sum of the rows of the averaging kernel (SRAK). The procedure goes from the greatest to least amount of information content using the SRAK. The total DOFS is obtained from the trace of the averaging kernel. Next, the vertical resolution of each retrieval level is calculated, using the full width at half maximum of the row of the averaging kernel for that level. The level that corresponds to the peak in the SRAK is selected, and the calculated vertical resolution for that level dictates which other levels will be combined into the RVMR value. This means that all of the rows of the averaging kernel that fall within this selection criteria are then combined to create a single row of the transformation matrix. Note that after this combination, these levels used can no longer be used in the determination of further RVMR points. This procedure is repeated to create further rows of the transformation matrix, until the information content remaining is below some threshold value. Once the transformation matrix has been obtained, it is convolved with the retrieved profile to calculate the RVMR.
value(s). More information on RVMR can be found in Shephard et al., 2011.

Similar the TES retrievals, I also used a Rodgers-style retrieval on the natural logarithm of the VMR. Unlike the TES retrievals though, I did not perform retrievals of any other parameters prior to the retrieval of NH$_3$, and the TES retrievals retrieved NH$_3$ in isolation, while I retrieved surface temperature alongside NH$_3$. The resolution of the TES radiance was 0.06 cm$^{-1}$, while my radiance profiles were of a 0.1 cm$^{-1}$ resolution, requiring some slight adjustments to the equations presented in Shephard et al., 2011 when calculating SNR values. My retrievals used the same prior profiles as Shephard et al., 2011, as well as the same selection criteria used to assign priors to measurements. More detail on the retrievals used for this project are provided in Chapter 5.

A case similar to that presented in Shephard et al., 2011 was modelled by my code, to compare my work to the TES retrieval. The Shephard paper shows two retrievals performed on the measurement, identical other than the choice of prior. Based on the figures presented in Shephard et al., 2011, I chose the true profile value to be 0.9$\times$ the value of the polluted prior profile, in an attempt to have a similarly polluted ‘true’ profile. Retrievals were performed using both the moderately polluted prior (Figure 2.17) and the polluted prior (Figure 2.16). These figures resemble those in Shephard et al., 2011, and show the dependence of the shape of the retrieved profile on the prior. Both figures show the RVMR value as a red asterisk, with the highest sensitivity occurring around 1-2 km, and a retrieved RVMR value in the range of 2.5-3.5 ppbv.

2.7 Problem to be solved

As described in Section 2.3, ammonia retrievals are possible with data already acquired from several different instruments, but these data sets do not have both high spatial resolution and full daily coverage of Canada. The goal of this thesis work is to design an instrument to fill this gap, that can provide a data set with 1 km spatial resolution and 0.1 cm$^{-1}$ spectral resolution, and that provides daily measurements of Canada in its entirety. Note that these requirements were developed in collaboration with ECCC scientists.

Given the limitations imposed by the requirements of noise and coverage, two paths
are considered for this project. The first is to plan for a single instrument to fulfill all requirements given - said instrument would require highly specialized customized parts, and would likely have a very high cost. The other option would be to have multiple cheaper instruments working together in tandem to provide the necessary coverage. By allowing the requirements to be fulfilled in this way, there is a reduction in cost from the potential to use more commercially available components as opposed to custom made ones. The reduction in cost and ability to use commercial parts is appealing, and there is no strong argument in favour of having one sole instrument. Thus the decision is made to design a smaller and more cost-effective instrument that provides less spatial coverage but fulfills all other requirements, keeping in mind that the end product would have several of these instruments fly at the same time to provide the total spatial coverage required for this project.

**Figure 2.16:** Retrieval performed on measurement with true profile equal to 0.9× the value of the polluted prior profile.
Figure 2.17: The same retrieval as in Figure 2.16 using a moderately polluted prior profile instead of a polluted prior profile.

Providing that the instrument does not require a highly specialized orbit and is within certain volume restraints, there are options available to fly the payload on a commercial rocket by renting space. SpaceX has a smallsat rideshare program that allows for payloads to be put onto their rocket and launched into space. In terms of cost, a payload of 50 kg launched into low Earth orbit would cost around $0.3M (SmallsatRideshare program n.d.). The SpaceX rideshare program has been successfully used by the GHGsat project, which focuses on measuring Methane emissions. The GHGsat constellation currently comprises six satellites, the most recent three having been launched in May of 2022 about a SpaceX Falcon 9 rocket (Greenhouse Gas Monitoring from Space: GHGSat Launches Three New Satellites with SpaceX 2022).

Working with the knowledge that the instrument will make use of a Fourier Transform...
Spectrometer and will use the Rodgers retrieval framework to perform retrievals on the data, a model has been built to simulate the measurement and retrieval process. This model takes in numerous inputs that dictate the instrument specifications, the observer geometry, and the atmospheric conditions, and generates an output radiance spectrum. This is the spectrum that is then used for the retrieval that results in a retrieved ammonia profile. Chapter 6 investigates the effects of different combinations of parameters on the resulting retrieval, and presents the resulting specifications that represent the optimized configuration of the instrument, allowing to fulfill all requirements set for this project.

2.8 The Approach

This chapter has given an overview of the background knowledge necessary for an understanding of the work presented in the chapters that follow. My research can be divided into three distinct sections that interact with one another to allow for an analysis of different instrument configurations. The next three chapters of this thesis will cover one of the three sections. Chapter 3 gives an overview of how atmospheric signals are modelled using the radiative transfer engine SASKTRAN, discusses the interfering species of ammonia, and explains what brightness temperature is and how it is used in this work. Chapter 4 delves into the instrument models themselves, and how we are able to model a Fourier Transform Spectrometer in two different ways. This chapter discusses finer details such as detector noise, filters, transmission, and the detector array. Chapter 5 uses the instrument models from Chapter 4 to produce a radiance spectrum, and applies the theory discussed in Section 2.5 to retrieve NH₃ as well as surface temperature. By using these three different pieces together, a full view of the instrument is available, and different test cases can be run to determine an optimized configuration, as is discussed in Chapter 6. Chapter 7 summarizes the work presented and discusses the future work remaining for this project.
Chapter 3
Radiative Transfer

This chapter gives an overview of how the radiance entering the optimized remote sensing system is modelled. It begins with a discussion about signal modelling and how the SASKTRAN radiative engine is used to model signals. The brightness temperature, a metric used in this thesis to estimate the detectability of a given NH$_3$ profile, is defined, and is used to discuss interfering species and a strategy (microwindowing) to mitigate their impact on ammonia retrievals. The absorption spectrum of ammonia is examined, as is the distribution of ammonia over Canada taken from an ECCC forecast model.

3.1 Signal Modelling

Two of the most common viewing geometries for remote sensing are limb and nadir, shown in Figure 3.1. In a nadir configuration, the instrument’s line of sight intersects the Earth, as opposed to the limb configuration, where the line of sight starts outside the atmosphere, passes through different layers of the atmosphere, and exits the atmosphere. Limb geometry allows for a much higher vertical resolution of measurements, while nadir geometry is able to give measurements with higher ground spatial resolution. Due to the high ground spatial resolution requirements for the instrument, a nadir viewing configuration is more suited to the project.

The radiative transfer equation, as discussed in Section 2.1, can be used to model the radiance as seen by an observer, given information about the atmospheric composition and observer geometry. My fully independent calculations (using the radiative transfer equation) were used to verify SASKTRAN TIR to within 0.1% (shown in Figure 3.2).

SASKTRAN TIR is a radiative transfer engine designed specifically for the thermal in-
Figure 3.1: Viewing geometry for nadir configuration (left), showing the line of sight intersecting the Earth. Viewing geometry for limb configuration (right), showing the line of sight passing through the layers of the atmosphere, as well as the tangent altitude.

Infrared regime created by Warnock, 2020, which was built upon the existing SASKTRAN radiative transfer engine developed by Zawada, 2018. The SASKTRAN framework is a more elegant tool that can calculate radiance for multiple lines of sight, and can calculate weighting functions. It has a number of built in climatologies and optical properties, as well as options for the Bidirectional Reflectance Distribution Function. Figure 3.3 shows spectra generated by SASKTRAN TIR at a high resolution, as well as a typical instrument resolution.

3.2 Brightness Temperature

The brightness temperature, a metric used to estimate the level of detectability of a NH$_3$ profile, is defined as the temperature (calculated here in Kelvin) a black body would have to be to emit a certain spectral radiance and can be obtained by inverting the Planck function:

$$T_b = \frac{hc}{k_B \lambda} \ln^{-1} \left( 1 + \frac{2hc^2}{I_\lambda \lambda^5} \right), \quad (3.1)$$

where $h$ is the Planck constant, $c$ is the speed of light, $k_B$ is the Boltzmann constant, $\lambda$ is the wavelength of the light, and $I_\lambda$ is the spectral radiance for wavelength $\lambda$. Given a measured radiance, brightness temperatures can be calculated for each point in the spectrum. Looking at the difference in brightness temperatures between an unpolluted and a polluted NH$_3$ profile gives an idea of how detectable the polluted profile would be. Figure 3.4 shows the brightness temperature differences for NH$_3$ and the relevant interfering species. The strong absorption lines from the presence of CO$_2$ and H$_2$O can be seen in the top panel of Figure 3.4. The NH$_3$ absorption does not create such strong lines in the brightness temperature profile itself, but
looking at the difference between unpolluted and polluted profiles, the presence of NH$_3$ can clearly be seen. The interfering species make the retrieval of NH$_3$ more difficult.

A preliminary study was done to look at the impact of the choice of temperature profile and water vapour profile. Typically, both of these parameters would be retrieved prior to doing an NH$_3$ retrieval. The level to which these parameters are known will impact the retrieval of NH$_3$. Since the surface temperature value had a large impact on the retrieval of NH$_3$, it was decided that this parameter would be retrieved alongside NH$_3$ (see Section 5.2).

A shift in temperature profile (not including the surface temperature) of $\pm 1$ K resulted in (on average) a difference in about 0.2 ppbv in the retrieved NH$_3$ profile. A change in the water vapour profile of $\pm 5\%$ resulted in (on average) a difference in 0.25 ppbv in the retrieved NH$_3$ profile. More work is needed to determine how well the instrument would be
Figure 3.3: Radiance generated by SASKTRAN TIR radiative transfer engine, showing both high-resolution radiance as well as radiance generated at a typical instrument resolution of 0.5 cm$^{-1}$.

To mitigate the effect of the interfering species on the NH$_3$ retrieval, a strategy known as ‘microwindowing’ can be implemented, which involves only performing retrievals using points on the radiance spectrum that do not have a strong signal from the interfering species. Figure 3.5 shows microwindows near the area with the most NH$_3$ signal, based on those shown in Shephard et al., 2011.

The brightness temperature noise levels of TES, IASI and CrIS are 0.1–0.2 K, 0.15–0.2 K, and 0.04 K respectively (Shephard and Cady-Pereira, 2015). The fairly polluted profile (peaking at 12.6 ppbv) used in Figure 3.5 results in a signal higher than these noise levels, but shows the need for low noise levels if accurate measurement of moderately polluted profiles is to be achieved.
### 3.3 Ammonia Spectroscopy and Distribution

Using data from the HITRAN database (https://hitran.org/) allowed for a closer look at the absorption spectrum of NH$_3$. A significant amount of absorption occurs around 967 cm$^{-1}$, which corresponds to the $\nu_2$ vibrational mode of the NH$_3$ molecule (symmetric bending) (David, 1996).

The relatively weak signal from NH$_3$ makes it difficult to measure NH$_3$ profiles with small number densities. The amount of thermal contrast (defined as the difference between the surface temperature and the air temperature at the bottom of the profile, from Shephard...
Figure 3.5: Same brightness temperature differences as shown in Figure 3.4 with microwave-windowed data shown. All data not used is shaded in grey. The peaks in absorption of species other than NH$_3$ are blocked, and as such their effects on the NH$_3$ retrieval are minimized.

et al., 2011) in a scene can contribute to the detectability. Shephard et al., 2011 found that a high thermal contrast increases the detectability of profiles.

ECCC provided Global Environmental Multi-scale – Modelling Air-quality and CHemistry (GEM-MACH) files. GEM-MACH is ECCC’s comprehensive air-quality forecast model, and is run twice a day over North America (Canada, 2022). It contains a full description of atmospheric chemistry and meteorological processes, and the meteorology is integrated in-step with the chemistry (Canada, 2022). The GEM-MACH files provided by ECCC contain data for one hour a day on the 10th of each month for the year of 2020, and gives a good idea of what realistic thermal contrast and maximum NH$_3$ values would be across Canada. The maximum NH$_3$ values from the GEM-MACH model for July 10, 2020 are plotted in Figures 3.6. Previously, I had been working with averaged profiles from Shephard et al., 2011 to gen-
erate radiance measurements, but with the provided dataset, I was able to incorporate many different NH₃ profiles into SASKTRAN using code developed by Nicholas Lloyd, a Senior Research Scientist at the University of Saskatchewan. His code was developed in such a way that a chosen date, latitude and longitude were taken as an input, and then the appropriate NH₃ profile and surface temperature were output. To ensure the thermal contrast described by the GEM-MACH files was preserved, the temperature profile from the dataset was also used. As the temperature profile was only defined up to an altitude of about 16 km, this temperature profile was merged with the default temperature profile from SASKTRAN-TIR: below 10 km, the GEM-MACH profile was used, in between 10 km and 15 km, the GEM-MACH and SASKTRAN-TIR default temperature profile were merged (using a simple linear weighting that gradually decreased/increased the weight of the respective profile as altitude increased), and above 15 km, the default profile was used.

**Figure 3.6:** Maximum NH₃ at a given coordinate from the GEM-MACH dataset provided by ECCC for July 10, 2020.
Using the established SASKTRAN TIR radiative transfer engine to model the incoming radiance, the challenges of interfering species and weak signal due to low concentrations of ammonia are apparent. Care must be taken in the instrument design to ensure that the small NH$_3$ signals can be measured.
CHAPTER 4
INSTRUMENT MODELS

To model the measurement of radiance from an IFTS instrument, two separate models were developed to fulfill differing needs in the simulation and retrieval process. Both models were developed in Python, and were developed with help from Jeff Langille and his IFTS model (https://arggit.usask.ca/jeff/ifts-model/-/tree/main/ifts_model). Both models take as input SASKTRAN generated radiance that has been put through a basic sensor model. The sensor model implements a simple Gaussian spatial point spread function that accounts for how each pixel collects radiance around the central line of sight. As stated in Section 2.3.6, the chosen instrument type is a Fourier transform spectrometer, which will be implemented in the form of a Michelson interferometer.

4.1 Specifications

The goal of the designed observing system is to achieve daily mapping of ammonia in Canada at a 1 km ground spatial resolution. The instrument itself and its orbit couple to give the overall observing specifications. Assuming a satellite altitude of 600 km and a polar orbital period of 96 minutes, the rotation of the Earth between successive orbital passes has a maximum shift of 1900 km (at 44° latitude, which we are taking to be Canada’s lowest point in latitude). As a nadir infrared instrument, meaningful data can be collected both during daytime and nighttime, so instead of each orbital pass needing to cover a swath of 1900 km, each pass must only cover 950 km in swath. During the day, 950 km strips separated by 1900 km are covered, with the in-between gaps being later covered during the night time passes. A spectral resolution of 0.1 cm\(^{-1}\) is required, to be able to detect the weak \(\text{NH}_3\) signal. Trying to have a singular instrument fulfill all the requirements of this project would
be complex and would likely have a high cost. A smaller and less complicated instrument would be less costly to build, fly and test. Once a proof of concept has been developed, it would be reasonable to simply manufacture multiple instruments that fly together to provide the necessary coverage.

Assuming the use of a $256 \times 256$ pixel array, there are different options for the configurations that fulfill these parameters. The investigation of the difference specifications was greatly aided by Frédéric Grandmont and Stéphane Lantagne from ABB Ltd. One option put forth by ABB was to use the ABB patented inverse image slicer to essentially ‘re-arrange’ the incoming radiance. With a $128 \text{km} \times 512 \text{km}$ field of view (FOV), the FOV can be sliced in half to make two $128 \text{km} \times 256 \text{km}$ slices, and then using specialized optics to essentially ‘stack’ the two slices on top of each other to result in a square image to be projected onto the detector. Using the image slicer results in a wider but shorter FOV, allowing less time for collecting signal, but increases the swath covered in one measurement.

Another option to increase the coverage provided by the instrument would be to implement across-track scanning. The instrument would have an additional scanning mirror (not to be confused with the moving mirror in the Michelson interferometer setup), which would operate in a square wave pattern. This would allow the instrument to take a $256 \text{km} \times 256 \text{km}$ image whose edge is on the path of the satellite, and then move the scanning mirror to then take an image on the opposite side of the satellites path. This would continue, with the scanning mirror allowing the FOV to switch between the two ‘tracks’. Note that this configuration would halve the stare time allocated to each image, assuming a 100% duty cycle. See the stare pattern in Figure 4.1.

As previously mentioned, using multiple instruments on the same platform is another strategy that can be used to meet the daily coverage requirements. Assuming 1 pixel covers $1 \text{ km}^2$, using four instruments each with a $256 \times 256$ detector array would provide the required coverage per scan of 950 km without requiring cross-track scanning. Two instruments modified to have a $128 \text{km} \times 512 \text{km}$ FOV by the inverse image slicer would also provide the required coverage.

The use of the inverse image slicer or the across-track scanning increases the coverage per scan, but reduces the time available to obtain the interferograms. Using the inverse image
Figure 4.1: Proposed stare pattern for satellite to increase swath.

slicer to have a 128km×512km FOV as opposed to a 256km×256km FOV results in the dwell
time being halved, and the across-track scanning with two tracks as shown in Figure 4.1
would also halve the time available to obtain the interferograms.

Discussions with ABB introduced more guidelines for the proposed instrument. A maxi-
mum sampling rate of 363 Hz is proposed based on the ABB team’s experience with 256×256
detector arrays. Similarly, an F# near 1.4 or 1.5 is suggested to be the limit for an instru-
ment such as this one. The large FOV is expected to pose problems with fringe visibility
when reaching the maximum OPD at the corner pixels - to remedy this, ABB suggested the
inclusion of an inverse telescope in front to reduce the FOV by some factor, which would also
require expanding the input aperture by the inverse of this factor.

There is no required orbit for this project, though the two most promising options would
be an inclined orbit or a polar orbit. An inclined orbit with an inclination near 65° or so could be done in an attempt to maximize the time the instrument spends over Canada. This would mean that the measurements at a given position are not necessarily always taken at the same time of day, but this would give smaller gaps in between adjacent swaths. The polar orbit has an inclination near 90°, with the instrument passing over the North and South poles during its orbits. The calculations done for the swath required for coverage were done using a polar orbit, and we move forward on the assumption that this is the orbit used for this project, as it is a common orbit that could allow the instrument to be a part of a rideshare program, as opposed to requiring its own launch (as mentioned in Section 2.7).

4.2 Full instrument model

The full instrument model was developed to allow for a realistic measurement to be generated, by simulating all of the steps to generate interferograms, add in noise, and take the Fourier transform to recover the spectrum. This model allows for fine-tuning of many parameters, but the downside is that it has a long runtime. Using the theory shown in Section 2.4, a step-by-step implementation of the interferogram generation process is utilized, as opposed to the convolution model, which makes use of the Instrument Lineshape (ILS) to simulate the use of the IFTS (see Section 4.3).

4.2.1 Filters

A filter is a critical element to include in the front-end optical design of the instrument. Filters are used to avoid stray light entering from other wavelengths - if undersampling is to be used, additional radiance coming from wavelengths outside of the range of interest can have a strong impact on the recovered radiance. To get a sharp cutoff, a bandpass filter is used in conjunction with a lowpass and a highpass filter. To model these filters, the transmission values from similar filters made by Alluxa, a manufacturer of high-performance optical filters, were used, and were shifted in wavelength to accommodate the needs of the project. Transmission values are available on their website (www.alluxa.com) for free. The 6000-500 OD3 Bandpass Filter was used as a basis for the bandpass filter, and the 224 OD5
Ultra Steep Longpass Filter was used as the basis for both the lowpass and highpass filters.

The resulting transmission in the bandpass area is around 65%, as can be seen in Figure 4.2. Figure 4.3 presents the same data as Figure 4.2 but uses a log scale for transmission to better show the rejection region. The overall transmission outside of the desired range is on the scale of 1e-5.

![Figure 4.2: Bandpass, lowpass and highpass filters used to create the overall filter for the model.](image)

### 4.2.2 Optics

The optical analysis considered for this project was kept to a basic level. A file containing the instrument’s optical specifications and detector specifications is used to pass along information to the model that is required for simulation, such as the integration time of a single scan, the entrance aperture, the field of view, the inverse telescope magnification, and the pixel size. The choice of these parameters is discussed later in Chapter 6.
4.2.3 Noise

Using the theory laid out in Section 2.4, an interferogram is generated using the filtered radiance and the instrument specifications. Noise is then added to this interferogram. To aid in the simulation of noise, a detector with reasonable specifications was found that could give an idea of what noise levels could be expected for this instrument. The chosen detector is the MARS VLW Infrared Detector. The datasheet for this detector gives information about the expected noise behaviour. The Noise Equivalent Differential Temperature (NEdT) value is the temperature difference that would generate a signal that is equal to the detector’s noise. The NEdT value measured for the MARS VLW detector is less than 25 mK (at 300K and 11 µm). The readout noise is the noise generated in the process that converts the stored
charge of each pixel into the voltage to be measured, and is given as 1000 electrons. For this project, readout noise, shot noise, and detector noise were all added to the interferogram. The following assumption was made about the relationships between different types of noise:

\[ \text{Noise}^2_{\text{NEdT}} = \text{Noise}^2_{\text{Readout}} + \text{Noise}^2_{\text{Shot}} + \text{Noise}^2_{\text{Detector}}. \]  

(4.1)

The detector noise in the above equation is the combination of all other noise sources into a single term. The shot noise follows a Poisson distribution, and as such we use the standard deviation to show the noise level, which is the square root of the average number of events (the average number of events is taken to be \(18 \times 10^6\) electrons per the detector datasheet), resulting in a shot noise value of 4301 electrons. To calculate the detector noise value in electrons, the NEdT must first be converted to electrons.

The Planck equation (Equation 3.1) is used to calculate the difference in spectral radiance caused by an increase in 25 mK of temperature. This difference in radiance value is then converted to a photon count (scaled by some factor in \(1/\text{s/sr/cm}^2/\text{nm}\)) by using the photon energy:

\[ E = \frac{hc}{\lambda}, \]  

(4.2)

where \(h\) is the Planck constant, \(c\) is the speed of light, and \(\lambda\) is the wavelength of the light (using 11\(\mu\)m as given by the data sheet).

This value is then converted to a (scaled) electron count using the detector’s quantum efficiency, 60%. It is assumed that the experimental setup held constant certain values, so that a constant in units of \(1/\text{s/sr/cm}^2/\text{nm}\) could be calculated from the other parameters given in the datasheet (noise calculated at 50% well fill, with a total charge handling capacity of 37e6 electrons). Dividing out this constant from the scaled electron count resulted in an NEdT value of 6809 electrons. This NEdT value in electrons was then used to calculate the detector noise using Equation 4.1, resulting in a detector noise level of 5183 electrons.

To add the noise values to the model, the shot noise is first added to the incoming photon count when generating the interferogram, using Poisson statistics. The interferogram is then converted to units of electrons, and both the readout noise and detector noise are added at
this level, with the assumption that both follow a normal distribution. Figure 4.4 shows two interferograms, one with noise and one without.

Figure 4.4: Interferograms generated using the full instrument model, one without the addition of noise (blue) and one with noise added (orange).

Recall that the noise calculations were done using the information that the NEdT value is less than 25 mK, at half well fill. Due to the fairly small input aperture and short dwell time of the instrument (details on how these parameters were calculated shown in Chapter 6), the amount of electrons captured is significantly less than the half well fill benchmark, and thus the noise level relative to the signal level increases beyond the given level of 25 mK - closer to 100-150 mK. Due to the weakness of the NH$_3$ signal, this significantly impacts the ability to retrieve useful information from the measurement. To remedy this, a group of 4 adjacent pixels forming a square are grouped together to create a ‘super-pixel’. Interferograms with noise are generated for each pixel, and then the four interferograms are averaged together.
The Fourier transform of this averaged interferogram is taken, and the resulting spectrum used to retrieval the NH$_3$ profile.

The noise for each data point is required when performing retrievals on the radiance extracted from an interferogram (see Chapter 5). To calculate the noise for each point, first the standard deviation of the (unscaled) out-of-band radiance is calculated using the unapodized interferogram. This value is then scaled by the same radiometric scaling factor as is used to scale the radiance (see Section 4.2.5), with the final result being an array of error values, each one corresponding to a radiance value.

### 4.2.4 Transmission

To simulate the averaging of the incoming light over a single pixel, the pixel is divided into an 3×3 grid, and interferograms are generated for each sub-pixel. Those interferograms are then averaged together to generate the interferogram for the overall pixel. Apodization is not a hard requirement, but is used in this case to prevent ringing, which gives a smoother end spectrum. The chosen apodization for this project is a Hanning window, a commonly used apodization function. The Hanning window is defined as:

$$w(n) = 0.5 - 0.5 \cos \left( \frac{2\pi n}{M-1} \right), \quad 0 \leq n \leq M - 1,$$

where $M$ is the number of points in the window. Figure 4.5 shows a sample Hanning window, peaking in magnitude at one in the centre, and tapering off to zero near the edges. Note that the window shown in Figure 4.5 is one that would be used for a double-sided interferogram. For the single-sided interferograms used in this project, the peak of the interferogram coincides with the peak of the Hanning window, with the window tapering to 0 at the MOPD of the long side, and the points on the short side are multiplied by the same apodization coefficient as their counterparts on the long side i.e. $w(-x) = w(x)$.

Section 2.4.2 discusses how single sided interferograms are used to obtain an end spectrum, which involves taking the complex Fourier transform of both a short symmetric double-sided interferogram, and the full single-sided interferogram. The double sided interferogram is then used to phase correct the single sided interferogram. Both interferograms are apodized before
the Fourier transform is taken.

4.2.5 Radiometric scaling

Once the spectrum has been extracted from the interferogram by using a Fourier transform, a process known as radiometric scaling is applied, which scales the output to adjust the units and give meaningful data. The radiometric scaling in this model is done by putting a spectrum of constant value through the model (filters included), generating an interferogram. The same procedure described in Section 2.4.2 is used to phase correct using a short double-sided interferogram, and an output spectrum is obtained. A scaling factor is calculated by taking the ratio of the input constant radiance to the output spectrum generated by the constant input. By multiplying the measurement output unscaled radiance by this scaling factor...
factor, the original units of radiance are recovered, and the effects of the filters are essentially undone.

### 4.3 Convolution model

During a retrieval, the forward model is run several times over as the program iterates towards the optimal solution. Thus, the speed of the retrieval is directly tied to the speed of the forward model. The full instrument model previously developed, though detailed, is slow running, and so a convolution model was developed. As the name suggests, the convolution model takes radiance and convolves it with an instrument line shape to model the measured radiance. The convolution of two functions, \( f \) and \( g \), is defined as

\[
(f * g)(\nu) = \int_{-\infty}^{\infty} f(\nu')g(\nu - \nu')d\nu',
\]

where \( \nu \) is the independent variable on which \( f \) and \( g \) depend, and \( \nu' \) is a variable for integration purposes. For the convolution model presented here, \( \nu \) and \( \nu' \) are wavenumber.

The convolution of two functions describes how the shape of one function is modified by the other. For our purposes, the convolution of the high-resolution radiance with the instrument lineshape describes how passing the radiance through the instrument will change the output that is given. Equation [4.4] describes the general convolution for continuous functions. We make use of the equation for discrete functions:

\[
(f * g)[n] = \sum_{m=-\infty}^{\infty} f[m]g[n - m].
\]

To implement this in Python, a matrix was created, with each row containing the line-shape for the corresponding wavelength. This matrix is then multiplied by the high-resolution radiance, to give the output radiance. A similar strategy is used to transform the weighting functions, used in the retrievals (see Chapter 5). If the instrument lineshape used is representative of the instrument model, the simulated radiance can be calculated without having to go through and generate an interferogram. As this model is used in the iterations for retrievals, there is no need to add in noise.
To create the instrument lineshape to be used, two theoretical lineshapes were combined to accurately model the most important effects of the instrument on the radiance. The instrument uses a imaging detector, and as such off-axis effects must be taken into consideration. Equations 4.6 through 4.9 as well as Table 4.1 describe the lineshape of an off-axis rectangular pixel per Genest and Tremblay, 1999. The full piecewise equation is shown in Table 4.1, where $v_0$ is the wavenumber of the line, and $f$ is the focal length of the collimating lens. $x_c$ and $y_c$ are the coordinates of the centre of the pixel, and $A$ and $B$ are the half-height and half-width of the pixel, respectively. $r_{\text{min}}$, $r_{c1}$, $r_{c2}$, and $r_{\text{max}}$ are calculated as follows:

$$r_{\text{min}} = \left[ (x_c - A)^2 + (y_c - B)^2 \right]^{1/2},$$

$$r_{c1} = \left[ (x_c - A)^2 + (y_c + B)^2 \right]^{1/2},$$

$$r_{c2} = \left[ (x_c + A)^2 + (y_c - B)^2 \right]^{1/2},$$

$$r_{\text{max}} = \left[ (x_c + A)^2 + (y_c + B)^2 \right]^{1/2}.$$  

Note that Table 4.1 assumes that $r_{c1} \leq r_{c2}$. If this is not the case, the X and Y coordinates can be exchanged (Genest and Tremblay, 1999).

<table>
<thead>
<tr>
<th>Wave Number Range</th>
<th>ILS Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>$v &lt; \frac{v_0}{(1+r_{\text{min}}^2/f^2)^{1/2}}$</td>
<td>0</td>
</tr>
<tr>
<td>$\frac{v_0}{(1+r_{\text{min}}^2/f^2)^{1/2}} &lt; v &lt; \frac{v_0}{(1+r_{c1}^2/f^2)^{1/2}}$</td>
<td>$1 - \frac{1}{2\pi} \arcsin \frac{y_c - B}{f(v_0/v^2 - 1)^{1/2}} - \frac{1}{2\pi} \arcsin \frac{x_c - A}{f(v_0/v^2 - 1)^{1/2}}$</td>
</tr>
<tr>
<td>$\frac{v_0}{(1+r_{c1}^2/f^2)^{1/2}} &lt; v &lt; \frac{v_0}{(1+r_{c2}^2/f^2)^{1/2}}$</td>
<td>$1 - \frac{1}{2\pi} \arcsin \frac{y_c - B}{f(v_0/v^2 - 1)^{1/2}} - \frac{1}{2\pi} \arccos \frac{y_c + B}{f(v_0/v^2 - 1)^{1/2}}$</td>
</tr>
<tr>
<td>$\frac{v_0}{(1+r_{c2}^2/f^2)^{1/2}} &lt; v &lt; \frac{v_0}{(1+r_{\text{max}}^2/f^2)^{1/2}}$</td>
<td>$1 - \frac{1}{2\pi} \arccos \frac{x_c + A}{f(v_0/v^2 - 1)^{1/2}} - \frac{1}{2\pi} \arccos \frac{y_c + B}{f(v_0/v^2 - 1)^{1/2}}$</td>
</tr>
<tr>
<td>$v &gt; \frac{v_0}{(1+r_{\text{max}}^2/f^2)^{1/2}}$</td>
<td>0</td>
</tr>
</tbody>
</table>

**Table 4.1:** Instrument lineshape for an off-axis rectangular pixel, as given by Genest and Tremblay, 1999.

By convolving this equation with the Fourier transform of the Hanning window (used to apodize the interferogram, accounts for the finite OPD), the finalized instrument lineshape is acquired. This is the lineshape that is convolved with the high-resolution radiance. Note that this lineshape changes depending on the position of the pixel of interest.
4.4 Comparison of Measurements

Figure 4.6 shows the radiances generated using both models, using both a reference and a polluted NH$_3$ profile. The inset figure shows the area of interest around 967.5 cm$^{-1}$ where the most NH$_3$ absorption takes place.

![Radiance Spectra](image)

**Figure 4.6:** A portion of the radiance spectra generated using SASKTRAN high-resolution radiance and each of the full instrument model and convolution model, for reference and polluted NH$_3$ profiles.

Both models are able to capture the effect of an off-axis pixel, and show the appropriate wavenumber shift (not pictured). As can be seen in Figure 4.6, there is more variability in the full instrument model spectra due to the addition of noise in the interferogram, while the convolution model does not include any noise. The absorption features around 965 cm$^{-1}$ and 967.5 cm$^{-1}$ are displayed clearly in both the convolution modelled radiance and the full instrument modelled radiance, but be aware that this is for a fairly polluted NH$_3$ profile, and the detectable signal is quite small. For more moderately polluted profiles and unpolluted profiles, the impact that NH$_3$ makes in the spectrum becomes smaller, especially when taking into consideration the noise level. The full instrument model and the convolution model both describe the behaviour of an IFTS instrument, with the slower, more detailed full instrument...
model serving its purpose to simulate a measurement, and the quicker convolution model being better suited to its use in the iterative retrieval process.
Chapter 5

Rodgers Retrieval

This chapter uses the Rodgers retrieval framework, first introduced in Chapter 2, to develop a retrieval process that makes use of both the full instrument model and the convolution model (outlined in Chapter 4). The retrieval process retrieves an ammonia profile alongside a surface temperature value, as an incorrect surface temperature value was found to have strong impacts on the ammonia retrieval if done by itself. Results from preliminary retrievals are shown and discussed.

5.1 NH$_3$ retrieval

There is a dedicated Python library built by my research group that implements the Rodgers framework efficiently (https://arg.usask.ca/docs/skretrieval/). It has a framework that allows for Rodgers-style retrievals to be performed using parameters passed into the retrieval. The retrieval results obtained from the skretrieval framework were verified with my own independent calculations. Once both the full instrument model and convolution model had been developed, the full model was used to generate the true simulated radiance for the retrieval ($y$ as described in Section 2.5), and the convolution model was used to generate radiance in the iterative retrieval process ($F(x)$ as described in Section 2.5). The methodology for the retrieval of NH$_3$ used for this project is very similar to that used by Shephard et al., 2011, described in Section 2.6.

Recall from Section 2.5 the idea of a priori information, also simply called a ‘prior’. The prior in a retrieval is information about the atmosphere that is known before measurements have been taken, which is added into a retrieval if there is not already enough information to find a proper solution. The choice of priors for the retrievals in this thesis are based on
those presented in Shephard et al., 2011: one unpolluted, one moderately polluted, and one polluted prior option. In the early stages of development, priors were selected manually based on the pollution level of the input NH$_3$ profile, but selection was then automated to better reflect the process to be used for instrument retrievals. Similar to Shephard et al., 2011, the SNR and the thermal contrast were used to determine which prior profile to used. The SNR is calculated, using the equation from Shephard et al., 2011:

$$SNR = \frac{(BT_{Bkgd} - BT_{NH3})}{NEDT},$$  \hspace{1cm} (5.1)

where the NEdT is the noise equivalent differential temperature, the minimum temperature difference that can be detected by a thermal sensor. An NEdT value of 25 mK is used, given by detector specifications (see Section 4.2.3). $BT_{Bkgd}$ and $BT_{NH3}$ are the brightness temperature values for a background spectral area and the spectral area with the most NH$_3$ absorption, respectively. To avoid having to perform another model run to get $BT_{Bkgd}$ at the same wavenumber as $BT_{NH3}$, $BT_{Bkgd}$ is estimated using a nearby window:

$$BT_{Bkgd} = \frac{BT_{968.3} + BT_{968.4}}{2} - (0.073 + 0.013TC)$$ \hspace{1cm} (5.2)

where $TC$ is the thermal contrast. The correction on the end is from a method developed by Shephard et al., 2011 to account for small differences in the estimated background brightness temperature and the true background in the NH$_3$ spectral region. $BT_{NH3}$ is the average of the 2 values near the peak of the signal:

$$BT_{NH3} = \frac{BT_{967.3} + BT_{967.4}}{2}$$ \hspace{1cm} (5.3)

The previous equations averaged two values, as opposed to Shephard et al., 2011’s three values, due to the coarser resolution of this instrument (0.1 cm$^{-1}$, as opposed to TES’s 0.06 cm$^{-1}$ resolution). Note that the wavenumbers given in Equations 5.2 and 5.3 are for the theoretical on-axis pixel. Due to the wavenumber shift experienced in off-axis pixels, the wavenumbers are adjusted accordingly for the pixel in question to ensure that the proper signal and background brightness temperatures are captured.

The shape of the retrieved profile is heavily influenced by the shape of the prior. Similar
to Shephard et al., 2011, 3 sets of priors are used: a polluted prior (with a maximum NH$_3$ value around 12 ppbv), a moderately polluted prior (with a maximum NH$_3$ value around 1.3 ppbv), and an unpolluted prior (maximum NH$_3$ value of 0.04 ppbv). The initial guess for the retrieval is also selected from one of the three previously described profiles. The initial guess is simply the first profile put into the iterative process of the retrieval; it is $x_0$ in Equation 2.38. For polluted and moderately polluted cases, the initial guess is the same as the prior. For the unpolluted case, the unpolluted profile is used as the prior, and the moderately polluted profile is used as the initial guess. The unpolluted profile is not used as the initial guess to avoid falling into null space during the retrieval (Shephard et al., 2011).

To determine which set of initial guess and prior profiles are to be used in the retrieval, the method as described in Shephard et al., 2011 was followed. In Shephard et al., 2011 a simulated sensitivity analysis was performed, with the end result showing a roughly linear relationship between SNR and thermal contrast for each profile type. The linear relationship for polluted profiles had a larger slope than that for moderately polluted profiles, and the unpolluted profile linear fit had a slope near 0. These linear fits were used to estimate the NH$_3$ profile type.

From each measurement, the SNR is calculated as shown in Equation 5.1 and the thermal contrast is calculated (after pre-processing, to ensure a reasonable value for the surface temperature). If the absolute value of the SNR is less than 0.5, the unpolluted prior and moderately polluted initial guess are used. If the absolute value of the SNR is greater than 0.5, then the distances from each point to the straight-line fit of each of the unpolluted, moderately polluted, and polluted best-fit lines are calculated:

\[ d = \sqrt{(x-TC)^2 + (y-SNR)^2}, \]

where

\[ x = (SNR + TC/\alpha - \beta) / (\alpha + 1/\alpha), \]

\[ y = \alpha x + \beta, \]

and $\alpha$=[0.001, 0.225, 0.762], and $\beta$ = [0.116, -0.126, 0.270]. The shortest distance from the
SNR/TC point to the best fit line determines which of the cases outlined previously is used for the prior and initial profiles.

As mentioned in Section 4.2.3, the noise corresponding to each radiance point is calculated using the noisy interferogram. To create the covariance matrix for the measurements, first a variance matrix is created by taking the outer product of the error values array with itself. A correlation matrix is then created: since Hanning apodization is being used on the interferogram prior to calculating the radiance, the correlation matrix is created by using the Fourier Transform of the Hanning function. The variance matrix and the correlation matrix are then multiplied together to give the covariance matrix for the measurements.

Figure 5.1 shows the results of a sample retrieval done. The true NH$_3$ profile is shown in black, and is used in the full instrument model to generate a noisy spectrum. This spectrum is the data upon which the retrieval is performed. For this retrieval, the prior and the initial guess (labelled ‘Prior’ and ‘Calc 0’ in the legend, respectively) were both chosen to be the moderately polluted profile. The iterations of the retrieval process calculated using Equation 2.38 are shown as the various coloured lines, with the final retrieved profile (‘Final Calc’) shown in pink. The RVMR is also noted as a pink asterisk (calculated per Shephard et al., 2011). Note that it is the log of the VMR that is retrieved, as was done in Shephard et al., 2011. The shape of the retrieved profile will depend heavily on the prior used in the retrieval, due to the limited pieces of information available. The retrieval shown in Figure 5.1 resembles a similar retrieval done by Shephard et al., 2011 and gives confidence that the procedure is being done correctly.

5.2 Surface Temperature retrieval

While investigating the influence of other factors on the retrieval (Section 3.2), it was discovered that the assumed surface temperature strongly impacts the retrieval. Since a nadir instrument is being modelled, the line of sight of the instrument intersects the Earth’s surface, and as such the surface temperature essentially dictates the baseline magnitude of the radiance. An estimate for surface temperature that is far from the true value will strongly impact the retrieval, giving unreasonable profiles of retrieved NH$_3$, or in the worst case scenario will
‘break’ the retrieval (no convergence). To avoid this, the retrieval of the surface temperature is incorporated into the NH$_3$ retrieval so they are done simultaneously. In addition to this, pre-processing is done prior to the retrieval. Recalling that the surface temperature has an approximately linear relationship with the average radiance, we are able to make a first step in the pre-processing by using the difference between the average modelled radiance value and the average measured radiance value. This difference is then multiplied by the weighting function (averaged over wavenumber) for the surface temperature, and then is added to the initial guess of surface temperature to give a closer starting point for the retrieval. Then the retrieval of NH$_3$ and surface temperature proceed simultaneously. The retrievals are able to recover the surface temperature with errors in the range of ± 0.002 K, or ± 0.04 K if microwindows are used.

Figure 5.2 shows the values of the surface temperature over the iterations of another sample retrieval. The true surface temperature, 295 K, is marked by a grey line. Iteration #0 is the retrieval’s initial guess of the surface temperature, i.e. the value after pre-processing is completed, and the successive iterations are shown in blue. For this particular retrieval, 4 iterations were required, so the value for Iteration #4 is the final retrieved surface temperature value. The value for surface temperature before pre-processing was 300 K, and as can be seen in Figure 5.2, the pre-processing adjusts the surface temperature value by nearly 5 K, to already get a reasonable estimate of the surface temperature, with only small adjustments to the value being made in the retrieval process.

The coupled ammonia and surface temperature retrieval is now used to investigate the impact of different instrument specifications on the quality of the retrievals.
Figure 5.1: Retrieval done on a sample profile, with the default moderately polluted profile being used as both the prior and the initial guess.
Figure 5.2: Iterations of a surface temperature retrieval.
Combining the signal modelling laid out in Chapter 3 and the instrument models developed in Chapter 4, a retrieval process is designed in Chapter 5 that outputs a retrieved ammonia profile and surface temperature value. The quality of the retrieved parameters will depend on the instrument specifications, and so a study of the combinations of different parameters is done, with the goal of obtaining the reasonable retrievals, while adhering to pre-determined requirements and the physical limitations of the instrument.

6.1 Selecting Instrument Specifications

Figure 6.1 contains a block diagram of the optical system for the instrument model. The incoming light first passes through an inverse telescope. The inverse telescope is used since the large FOV for the desired coverage cannot be supported by the interferometer, and would likely cause issues with fringe visibility at high OPDs for corner pixels. The inverse telescope reduces the FOV and requires an expansion of the aperture inside the interferometer compared to the aperture stop on the outside, as the product of the area of the aperture and the solid angle of the FOV must remain constant. After passing through the inverse telescope, the light then travels into the interferometer itself, the specifics of which are described in Section 2.4 in detail. The interferometer generates an interference pattern, which passes through the camera system. The camera has some F# that is defined by the focal length of the focusing lens and the diameter of its entrance pupil. The camera then focuses the interference pattern onto a detector - a 256×256 pixel detector array is chosen for our purposes.

To be able to achieve the spatial resolution, spectral resolution, and noise levels to meet
Figure 6.1: Block diagram for the layout of the optical system.

the project requirements, the available options for optics are limited. ABB provided me
with a spreadsheet that linked together different design parameters such as F#, FOV, pixel
size, telescope magnification, etc., which allowed me to posit different scenarios to see what
would be feasible. A few hard limits were set from the beginning: per the advisement of
ABB, the maximum sampling rate is set to be 363 Hz. The maximum sampling rate of
the MARS VLW infrared detector (used in Section 4.2.3 for noise calculations) is 320 Hz,
and so a goal sampling rate of 320 Hz or less is set, with a threshold level of 363 Hz. The
maximum array divergence (after passing through the inverse telescope) was set to be $12^\circ$, a
limit of the interferometer itself. A minimum F# of 1.5 was set. Some key equations from
the spreadsheet are as follows:

$$\text{FOV}_{\text{pixel}} = z \sin (\Theta_{\text{pixel}}), \quad (6.1)$$

where $z$ is the altitude of the satellite, and $\Theta_{\text{pixel}}$ is the pixel divergence before passing through
the inverse telescope. $\Theta_{\text{pixel}}$ is calculated as

$$\Theta_{\text{pixel}} = \frac{w}{fM}, \quad (6.2)$$

where $f$ is the focal length, $M$ is the magnification of the inverse telescope and is less than
1, and $w$ is the width of the square pixel. The divergence of the full array (after passing
through the inverse telescope) is

$$\Theta_{\text{array}} = M\Theta_{\text{pixel}}n, \quad (6.3)$$

where $n$ is the number of pixels in one row of the (square) pixel array. The divergence of the
full array is limited to $12^\circ$. The sampling rate is calculated as
\[ s = \frac{m}{t}, \quad (6.4) \]

where \( m \) is the number of samples, and the dwell time \( t \) is found to be

\[ t = \frac{y}{V}, \quad (6.5) \]

where \( y \) is the along-track distance covered by the satellite in a single scan, and \( V \) is the satellite ground speed. The number of samples required in the interferogram is found to be

\[ m = \frac{x_{\text{total}}}{\delta_i}, \quad (6.6) \]

where \( x_{\text{total}} \), the total OPD for a single-sided interferogram, is \( x_{\text{min}} + x_{\text{max}} \), and the sampling interval is

\[ \delta_i = \frac{0.95}{2\sigma_{\text{max}}}, \quad (6.7) \]

as defined by ABB. Note that the spreadsheet can also take into account undersampling, which reduces the sampling rate by some integer factor, due to fewer samples being required. The aperture stop diameter is

\[ D_{\text{stop}} = MD_{\text{inside}}, \quad (6.8) \]

where the aperture inside the instrument is calculated as

\[ D_{\text{inside}} = \frac{f}{F\#}. \quad (6.9) \]

Recall that the chosen detector, first introduced in Section 4.2, is the MARS VLW Infrared Detector, which has a pixel size of 30 \( \mu \)m, and a square detector of 256\( \times \)256 pixels. By fixing the pixel size and adhering to the aforementioned limitations, there are only a few parameters left to be selected: focal length, the telescope magnification factor, and the undersampling factor (see Section 2.4.2 for more detail on undersampling an interferogram).

An MOPD of 5 cm was selected. To allow for a balance of aperture diameter and pixel coverage, a focal length of 100 mm and a magnification of 0.3x for the inverse telescope was
selected. This results in each pixel covering a 0.6 km × 0.6 km square on the ground (also known as its ‘ground footprint’), and the instrument having an aperture stop size of 20 mm. Recall the requirement of a pixel footprint of at least 1 km × 1 km. Having nearly halved the footprint of the pixel, now it will be more difficult to obtain the global coverage desired, but to obtain a 1 km × 1 km pixel footprint would reduce the size of the input aperture stop and reduce the amount of signal able to be captured in a single scan. Because of the higher than expected noise (discussed in Section 4.2.3), the interferograms from four neighbouring pixels were averaged together to reduce the noise level. Thus, the effective spatial resolution is 1.2 km × 1.2 km. This could be reduced to 1 km × 1 km, but the reduced coverage is undesirable, and so the pixel coverage will remain 1.2 km × 1.2 km. By averaging four interferograms together to reduce noise, the noise level reduces and is under the threshold level of 0.1 K.

For the selection of the undersampling factor, the more the interferogram is undersampled, the less time is required to capture an interferogram, but the noise level increases and there is loss of the modulation efficiency. Both a factor of 2 and a factor of 3 for undersampling were investigated, as an undersampling factor of 3 would allow the instrument to make use of the ABB patented inverse image slicer (see Section 4.1), giving a swath of 307 km (compared to the swath of 153 km without the slicer). Alternatively, this could allow for the square wave scanning mirror to be used, which also doubles the swath. Table 6.1 shows the differences between the two undersampling configurations.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Non-Slicing Case</th>
<th>Slicing Case</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dwell time (s)</td>
<td>22.12</td>
<td>11.06</td>
</tr>
<tr>
<td>Across track width (km)</td>
<td>153.6</td>
<td>307.2</td>
</tr>
<tr>
<td>Along track length (km)</td>
<td>153.6</td>
<td>76.8</td>
</tr>
</tbody>
</table>

Table 6.1: Specifications for two cases investigated.

Recall the discussion in Section 4.1 regarding the coverage required for daily mapping of Canada, and the options available to increase the swath of a given instrument. With the assumption of a Low Earth Orbit (LEO) at around 600 km, and the knowledge that a TIR instrument can measure in both daytime and nighttime, it was calculated that for daily coverage, each orbital pass must cover 950 km in swath. To use the configuration with
no slicing, seven instruments would be required to achieve this coverage, while the slicing option reduces this number to four. Obviously, reducing the number of instruments required to provide full Canadian coverage is desirable, but if there is a substantial difference in the quality of data recovered from the configurations, using the slicing with an undersampling factor of 3 might not be viable.

6.2 Preliminary Case Comparison

To compare how the two configurations stack up against each other, a suite of tests were ran. Three different factors were varied:

- **Surface Temperature**: Surface temperatures of 288 K, 295 K, and 300 K were used to provide different levels of thermal contrast.

- **Ammonia Pollution Level**: Polluted (maximum value of 20 ppbv), moderately polluted (maximum value of 4 ppbv) and unpolluted (maximum value of 0.8 ppbv) profiles were used in the generation of interferograms.

- **Microwindows**: Cases were ran using the full spectrum to perform the retrieval, or using a select set of microwindows only (see Section 3.2 for more information on microwindowing)

For each combination of these factors, a measurement was generated for both the slicing and non-slicing configuration using the full instrument model (see Section 4.2), and a retrieval was performed using the framework described in Chapter 5. Note that due to time constraints, the tests run were run on one super-pixel only, which was centred on the optical axis.

Due to the low amount of information available from the nadir measurements, the shape of the retrieved profile depends heavily on the prior, making it difficult to compare exactly how well the retrievals are performing. Instead, the performance is evaluated by calculating the total column density (Eq. 2.7) of the retrieved profile, and comparing it to the total column density of the true profile.
The following figures show a sample of results from the panel of tests, for a surface temperature value of 295 K. Figures 6.2, 6.4, and 6.6 display the brightness temperature calculated from the data from the two different configurations. Figures 6.3, 6.5, and 6.7 show retrievals performed on simulated radiance as seen by the non-slicing configuration and the slicing configuration. Figures 6.8 and 6.9 show the brightness temperature and retrievals with the same parameters as Figure 6.5 but uses select microwindows (shown in Figure 3.5) to perform the retrieval, as opposed to the full spectrum.

The top panel of the brightness temperature figures show the brightness temperature calculated for both the non-slicing case (‘Case 0’) and the slicing case (‘Case 1’), as well as for a reference spectrum with no ammonia present (‘No NH\textsubscript{3}’). The bottom panel displays the difference between the brightness temperature without any ammonia, and that of one of the measured cases. This panel better shows the ammonia signal, which can be difficult to see in the top panel. For moderately polluted and polluted profiles, the distinct ammonia signal can be identified. This signal increases in intensity as the thermal contrast increases, increasing the detectability of the profile. Figure 6.8 shows the microwindowed data, with grey panels put over unused data.

Each retrieval figure contains four panels. The first two panels show the retrieval process for the non-slicing case (Case 0, first panel) and the slicing case (Case 1, second panel). The true state of NH\textsubscript{3} that was input into the full instrument model is shown in black. The prior used for the retrieval is shown as a grey dashed line - for some cases it may overlap with the initial guess (‘Calc 0’). The first two panels show the progression of the retrieval, as well as the final retrieved profile (‘Final Calc’). The asterisk shown is the calculated RVMR, per the definition of Shephard et al., 2011, discussed in Section 2.3. The text above the first two panels describes the retrieved Surface Temperature (ST\textsubscript{ret}) as well as the calculated SNR.

The third panel shows the retrieved VMR profile with error shading, and gives details on the calculated column density values in molecules/cm\textsuperscript{2} for both cases, as well as for the true state. The fourth panel is the same as the third, but shows the log(VMR), which is the actual retrieved quantity.

Both configurations initially perform well when looking at the final retrieved product. In general, retrievals performed on both moderately polluted and polluted profiles give rea-
Figure 6.2: Brightness temperature calculated for the non-slicing case (Case 0) and the slicing case (Case 1) for an unpolluted profile.

Reasonable results for both sets of cases, but when dealing with unpolluted profiles, the lack of signal is a barrier and the retrievals perform much worse. As expected from Shephard et al., 2011, an increased thermal contrast increases the detectability of the profile. The use of microwindows (described in Section 3.2) on the radiance data attempts to remove the effects of interfering species, but at the cost of losing other information that can better the retrieval. Using microwindows still gives reasonable results (not as good as those when using the full spectrum), but for unpolluted cases, the reduction in information is most noticeable and results in a worse retrieval. Between the two cases, the error on the column density is generally higher for the slicing case.
Figure 6.3: Figure showing the retrieval performed on the non-slicing case (Case 0) and the slicing case (Case 1) for an unpolluted profile.

6.3 Full Image Generation

As both configurations initially look viable, further investigation is required to detail the differences between the non-slicing and slicing specifications. Thus, a large-scale run was complete. A full image as seen by the IFTS was run, i.e. each pixel in the 256×256 grid generated its own interferogram, the interferograms within each super-pixel were averaged together, the retrieval was performed on this interferogram, and an output profile and total column density value were generated. The GEM-MACH datasets were used to provide surface temperature as well as the NH$_3$ profile. To maintain the thermal contrast from the GEM-MACH dataset, the dataset’s temperature profile was also used below 10 km, and was merged.
with the default SASKTRAN-TIR temperature profile above 10 km, to account for the lack of GEM-MACH temperature data above 16 km. The output is a grid of retrieved column density values and their errors.

Due to the large amount of interferograms required to be generated, using a regular desktop computer would require an extraordinary amount of time to generate interferograms for 65,536 pixels and perform retrievals on the 16,384 super-pixels. The University of Saskatchewan’s high performance computing cluster, Plato, was used to be able to run the required code in parallel, greatly reducing the time required to obtain results. To save on time and memory, the run on Plato performed microwindowed retrievals only.

The measurement grid is centred over the city of Missisauga, ON, located at 43.6° N, 79.6° W, and the GEM-MACH dataset from May 10th, 2020 was used to provide the temperature,
Figure 6.5: Figure showing the retrieval performed on the non-slicing case (Case 0) and the slicing case (Case 1) for a moderately polluted profile.

surface temperature, and NH\textsubscript{3} values. Figure 6.10 shows the coverage of the simulations done, shown in white, with the optical axis (over-top of the city of Missisauga) shown in red. This time and location was selected as the grid contained a mixture of polluted, moderately polluted, and unpolluted profiles. Figure 6.11 shows the true column density values plotted over a map showing Missisauga and the surrounding area, as given by GEM-MACH. Figures 6.12 and 6.13 are similar to Figure 6.11 showing the retrieved column density values for the non-slicing (2\times undersampled) and slicing (3\times undersampled) cases, respectively.

In Figure 6.11, an area of elevated column density is seen on the left hand side of the grid. Both the non-slicing case (Figure 6.12) and the slicing case (Figure 6.13) are able to detect this polluted area, although both cases do overestimate it significantly. Note also the ring pattern, seen prominently in Figure 6.13 and only slightly in Figure 6.12. This pattern
Figure 6.6: Brightness temperature calculated for the non-slicing case (Case 0) and the slicing case (Case 1) for a polluted profile.

is likely due to the interference fringe pattern from the interferometer. Recall that for any given optical path difference, the image generated by the interferometer is a fringe interference pattern.

6.4 Surface Temperature Impact on Retrievals

For the full grid run, microwindowed retrievals were used for the sake of time. Discussed in Section 3.2 the surface temperature value used in the retrievals has a large impact on the NH$_3$ retrievals, hence the decision to incorporate the surface temperature retrieval into the NH$_3$ retrieval. Looking at the differences between the true surface temperature and the retrieved surface temperature for the gridded microwindow retrievals, there are differences as
Figure 6.7: Figure showing the retrieval performed on the non-slicing case (Case 0) and the slicing case (Case 1) for a polluted profile.

large as 0.05 K, with the mean absolute difference being near 0.005 K. Figure 6.14 shows the microwindowed retrieval for one super-pixel, where the retrieved value is much larger than the true profile. For this case, a surface temperature of 267.99 K was retrieved, which is around 0.05 K lower than the true surface temperature, 268.04 K. This offset surface temperature gives a different baseline radiance for the convolution model compared to the measurement from the full instrument model, and the retrieval increases the NH$_3$ profile in order to try to minimize the difference between the two. Now a retrieval on the same measurement is done using the full spectrum, to see how it would impact the quality of retrieval. The full spectrum retrieval results are shown in Figure 6.15. The retrieved surface temperature is different than the true surface temperature value by less than 0.001 K, and the calculated
Figure 6.8: Brightness temperature calculated for the non-slicing case (Case 0) and the slicing case (Case 1) for a moderately polluted profile, showing microwindows used in retrieval.
column density is much closer to the true value and has lower error. This pixel was one of the more extreme cases of a poor surface temperature retrieval, and shows the impact that the surface temperature has on the retrieved NH$_3$ profile. A few other pixels were investigated, and the use of the full spectrum retrieval again resulted in a better surface temperature and NH$_3$ profile retrieval.

From the full grid microwindowed retrievals, only about 15% of the surface temperature retrievals are within 0.001 K of the true value, with nearly 50% of the retrievals having an absolute difference of 0.005 K or higher. Due to the impact of a proper surface temperature retrieval on the column density retrieved, if microwindowed retrievals are to be used to avoid the effects of interfering species, it would be my suggestion that the surface temperature is
Figure 6.10: Coverage of the instrument, centred over the city of Missisauga (shown in red).

retrieved using the full spectrum before the NH$_3$ retrieval is performed.

### 6.5 Prior Selection

As previously stated, the prior selection is an important part of the retrieval. The selection scheme for all previous figures is described in Section 5.1 and is now referred to as the ‘automatic’ selection scheme. This prior selection strategy was developed by Shephard et al., 2011, by performing a sensitivity study to determine the relationship between thermal contrast and SNR for each of the three pollution level categories. Due to time constraints, I used the same prior selection scheme as Shephard et al., 2011, but wanted to see how it would compare to what I refer to as a ‘manual’ selection scheme. For the ‘manual’ prior selection,
the maximum NH$_3$ VMR value for the GEM-MACH profile (i.e. the true profile put into the full instrument model to generate the measurement) was used to determine which prior to select. If the maximum VMR value was greater than 5 ppbv, the polluted profile was selected as the initial and prior profiles. If the maximum VMR value was greater than 1 ppbv but less than 5 ppbv, the moderately polluted profile was selected as the initial and prior profiles. If the maximum VMR value was less than 1 ppbv, the unpolluted profile was selected as the prior profile, and the moderately polluted profile was selected as the initial profile. Using the same grid measurements as before, a second round of retrievals was ran, with the manual prior selection scheme. Figures 6.16 and 6.17 show the calculated column density values from this secondary run.

Figure 6.11: Column density values as given by GEM-MACH dataset.

The different areas of prior selection can be seen clearly in the figures previous - there are two main areas of pollution, a large area near the edge of the left hand side of the grid,
and then a small oval area centred horizontally on the grid in the lower half. These polluted areas line up with the true polluted areas as can be seen in 6.11. They are very similar in shape to where the polluted areas of the true grid can be found, and is more localized than the polluted region detected using the automatic prior selection scheme. This indicates that more work should be done with the automatic prior selection scheme, to optimize it for the given instrument specifications.

6.6 Error analysis

The error on the column density of the retrieved profiles was calculated, and the column density with its error range was compared to the true column density values. Figure 6.18 through 6.21 show how many retrieved column density values were within error range of the
true value, shown for both non-slicing and slicing cases, as well as manual and automatic prior selection. For all cases, in the area of strong pollution, a good portion of the retrieved column density values are within error. Looking at Figure 6.21 compared to Figure 6.17, it can be seen that the areas where the unpolluted prior was selected (most prominently in the upper right hand corner) are rarely within error range.

6.7 Overall Performance

Recalling Table 6.1 to evaluate the overall performance of the instrument. This instrument design achieves the threshold spectral resolution of 0.1 cm$^{-1}$ by having an MOPD of 5 cm. The spatial resolution of each individual pixel is 0.6 km $\times$ 0.6 km, but with the super-pixel strategy an overall ground spatial resolution of 1.2 km $\times$ 1.2 km is achieved, which is still
Figure 6.14: Ammonia retrieval with poor surface temperature retrieval - using microwindows.

below the threshold values. The brightness noise levels for the non-slicing case and the slicing case are 0.04 K and 0.08 K, respectively, both of which meet the threshold level of 0.1 K, and the first of which meets the goal level of 0.05 K.

Overall, both the slicing and non-slicing configurations are viable options for an ammonia detecting instrument. Though the slicing configuration does come with an increase in noise, it still meets the required noise level of 0.1 K or less in brightness temperature noise. A poorly retrieved surface temperature value can have strong effects on the retrieved ammonia profile. If microwindows are to be used to reduce the impact of interfering species on the NH₃ retrievals, it is suggested that the surface temperature retrieval be carried out beforehand using the full spectrum, as the microwindowed temperature retrievals have a higher error for retrieved surface temperature and thus give a worse NH₃ retrieval.
Figure 6.15: Retrieval for the same measurement as Figure 6.14, using the full spectrum instead of microwindows only.
Figure 6.16: Retrieved column density values for non-slicing case, with the manual prior selection scheme.
Figure 6.17: Retrieved column density values for slicing case, with the manual prior selection scheme.
Figure 6.18: Number of retrieved column density values that are within error of the true value for the non-slicing case with automatic prior selection.
**Figure 6.19:** Number of retrieved column density values that are within error of the true value for the non-slicing case with manual prior selection.
**Figure 6.20:** Number of retrieved column density values that are within error of the true value for the slicing case with automatic prior selection.
Figure 6.21: Number of retrieved column density values that are within error of the true value for the slicing case with manual prior selection.
Chapter 7

Summary and Future Work

7.1 Summary

Atmospheric ammonia (NH$_3$) is a difficult to measure atmospheric pollutant, due to its short lifetime (on the order of hours) (Paulot et al., 2017) and its high spatial variability. The largest sources of global NH$_3$ emissions are from agriculture and natural sources - making up 78% of all emissions (Sutton et al., 2013). Ammonia is highly reactive, with the majority of its environmental impact coming from its involvement in chemical reactions that generate pollutants like nitrate and ammonium (Xu and Penner, 2012). Ammonia has effects on the nitrogen cycle, air quality, and water quality, and is a contributor in the formation of small aerosols that can impact cardiovascular and cardiopulmonary health if exposed to long-term (Crouse et al., 2012, Pope et al., 2009).

In recent years, the advancements in radiative transfer modelling and radiometric instrument sensitivity have allowed satellite measurements of ammonia to be made. Measurements taken by instruments such as NASA’s Tropospheric Emission Spectrometer (TES, Shephard et al., 2011), NASA’s Cross-track Infrared Sounder (CrIS, Shephard and Cady-Pereira, 2015), ESA’s Infrared Atmospheric Sounder Interferometer (IASI, Clarisse et al., 2010), NASA’s Hyperspectral Thermal Emission Spectrometer (HyTES, Kuai et al., 2019), and NASA’s Atmospheric Infrared Sounder (AIRS, Warner et al., 2016) have been used to perform ammonia retrievals. Though reasonable results are obtained, these instruments fall short of the desired daily high-resolution mapping of NH$_3$ in Canada. Designing a dedicated instrument for ammonia allows for the optimization of instrument parameters to attain certain requirements that allow NH$_3$ to be successfully retrieved, which is difficult due to its weak signal and high spatial variability. The requirements for this dedicated ammonia instrument are a spectral...
resolution of 0.1 cm$^{-1}$ or less, and a brightness noise level of 0.1 K or less at 270 K. A spatial resolution of 1 km is desired.

For this instrument, a Fourier Transform Spectrometer is selected, due to the Fellgett advantage in the thermal infrared regime allowing for a higher signal-to-noise ratio, which is desirable due to the weak NH$_3$ signature (Perkins, 1987). Specifically, an imaging FTS is used, allowing the instrument to have multiple lines of sight. Two different models are developed to model the behaviour of the IFTS: the full instrument model, and the convolution model. Both models use high-resolution radiance generated by SASKTRAN TIR (Warnock, 2020), a well-developed radiative transfer model. The input NH$_3$ profiles and surface temperature values were taken from a GEM-MACH dataset provided by ECCC. To preserve the thermal contrast from the GEM-MACH dataset, the GEM-MACH temperature profile was used in the model, merged with the default SASKTRAN-TIR temperature profile above 10 km to account for the GEM-MACH’s lack of data above 16 km. The full instrument model generates the interferograms as would be measured by the IFTS, and takes into account radiance filtering, phase correction, radiometric scaling, and the addition of noise at the interferogram level. This model allows options for single sided interferograms as well as undersampling, which are both used for this instrument. By taking the Fourier transform of the interferogram, an output spectrum is recovered. The convolution model takes the high-resolution radiance and directly convolves it with the instrument lineshape. Note that the lineshape is such that it models the effects of an off-axis square pixel, as is required for this detector. The convolution model was developed as a faster method to model the IFTS effects, and is used in the retrieval which requires modelling radiance several times over.

After the two models were developed, they were incorporated into a retrieval process, based on the Rodgers retrieval methods. Taking the output from the full instrument model, the retrieval chooses which prior and initial NH$_3$ profiles are to be used in the retrieval. The iterative retrieval process uses the convolution model to determine the statistically most likely NH$_3$ profile to have resulted in the radiance as generated by the full instrument model. The retrieval of surface temperature was incorporated into the NH$_3$ retrieval, to be done simultaneously, as the surface temperature sets the ‘baseline’ radiance, and having the incorrect surface temperature in the retrieval results in NH$_3$ retrieval values that are unreasonable.
Pre-processing is done for the surface temperature, making a single step on its own, and further small adjustments are carried out alongside the retrieval of NH$_3$. Due to the low degrees of freedom in the NH$_3$ retrieval, total column density values are calculated post-retrieval to better evaluate the performance of the retrieval.

Looking at the specifications for the instrument, limitations were imposed to ensure the instrument was realistic: the maximum sampling rate must be 363 Hz or less, the maximum array divergence is 12°, and the minimum F# is 1.5. Balancing the aperture diameter to ensure there is enough input light with the pixel FOV was the largest challenge, and constrained the choices for other parameters. Due to the low number of photons incident upon the instrument per measurement, the noise level from a single pixel measurement was higher than desired, and so ‘super-pixels’ were used: the interferograms from four adjacent pixels (in a square) were averaged together before taking the Fourier Transform, resulting in a lower noise level. Two leading scenarios emerged: one in which the undersample factor was 2, and one in which the undersample factor was 3. The second scenario would allow for the instrument to either implement across-track scanning or use the ABB patented inverse image slicer, both of which would double the across-track coverage in a single pass (going from 153 km to 307 km).

A suite of tests were run to do a preliminary evaluation of these two scenarios. Retrievals were run on scenarios which varied three factors: thermal contrast, pollution level, and microwindowing. Microwindowing is a technique used that takes certain spectral points that don’t have a strong signal from an interfering species, and uses only those points in the retrieval. At this point, results for both cases were deemed reasonable, and so further testing proceeded.

A large-scale run was then completed, using the full grid of 256×256 pixels. For each super-pixel in the grid, a microwindowed retrieval was performed, generating a full image of total column density values. The grid is centred over the city of Mississauga, and the input NH$_3$ and surface temperature values were once again taken from the GEM-MACH dataset. These images were generated for each undersampling scenario. Both cases were able to measure elevated ammonia levels, though the retrieved column density values were, in general, larger than the true column density values. The surface temperature retrievals
were retrieved with differences as large as 0.05 K, with the mean absolute difference being 0.005 K. Using a full spectrum retrievals resulted in better performance for both the surface temperature (differences closer to 0.001 K) and the retrieved NH$_3$ profile (lower errors and column density values closer to the true values). Overall, both scenarios meet the performance standards set for the project, but the non-slicing case has a lower brightness noise level (0.04 K) than the slicing case (0.08 K).

7.2 Future Work

There is still room for improvement within the full instrument model. Currently, there is no Analog-to-Digital Converter (ADC) included, which would convert the signal from the detector to one that can be recorded by the onboard computer. This would be introduced after the generation of the interferogram, before the Fourier transform to recover the radiance.

Two prior selection schemes were used in this thesis when running full grid retrievals—an automatic selection scheme, using the strategy outlined by Shephard et al., [2011], and a manual scheme, which used knowledge of the true ammonia profile to select which prior to use in the retrieval. More work needs to be done to adjust the automatic prior selection scheme to be optimized for the specifications of this instrument, as the selected prior profile has a large impact on the retrieval due to the low information content.

The retrieval process retrieves only two parameters: NH$_3$ and surface temperature. All other atmospheric parameters (temperature profile, other species such as O$_3$, H$_2$O, CO$_2$) have the same profiles used in measurement generation as in the retrievals. The effects of water vapour interference were studied briefly, but a more thorough study and simulation of the retrievals of these parameters is required. As well, all scenes were assumed to be cloud-free. Shephard et al., [2011] performed a cloud sensitivity study on the impact for their NH$_3$ retrievals, and discovered that increased cloud optical depth decreases the information content in the NH$_3$ retrieval. Due to the weak signal of NH$_3$, the level to which we can retrieve interfering species is important, and ties into the use of microwindows, which were briefly investigated in this paper. More work needs to be done to determine the level to which the interfering species can be retrieved with the instrument in its current state, and
how this changes the impact of microwindowing the data prior to performing retrievals.

The next large step would be to prototype the instrument. When searching for filters and detectors that are similar in configuration to what is required for the project, there were few viable options that came up. Ideally, commercially produced components would be used to reduce costs, as opposed to custom made components, but the highly specialized specifications of the instrument might mean that off-the-shelf components are not suitable. Specialized components like the inverse image slicer and/or the components required for across-track scanning would need to be sourced. As well, using multiple instruments means that multiples of the components would need to be purchased eventually. For the prototyping phase, a single instrument can be developed, with the intention of building multiple identical instruments in the future to attain coverage requirements.
References


Journal of Geophysical Research, 115(D13), D13302–n/a.


Gautam, S., Patra, A. K., & Kumar, P. (2019). Status and chemical characteristics of ambient 
PM2.5 pollutions in China: A review. Environment, development and sustainability, 
21(4), 1649–1674.

for global modeling of upper atmospheric NH from freezing clouds. Proceedings of the 
National Academy of Sciences - PNAS, 115(24), 6147–6152.

Genest, J., & Tremblay, P. (1999). Instrument line shape of Fourier transform spectrometers: 
5438–5446. https://doi.org/10.1364/AO.38.005438

estimates for the eastern United States based on ammonium wet concentrations 
and an inverse modeling method (Gilliland, A. B., R. L. Dennis, S. J. Roselle, and 
T. E. Pierce (2003), Seasonal NH3 emission estimates for the eastern United States 
based on ammonium wet concentrations and an inverse modeling method, J. Geophys. 
- Atmospheres, 108(D15), 4477–n/a.

Greenhouse gas monitoring from space: Ghgsat launches three new satellites with SpaceX. 
space-ghgsat-launches-three-new-satellites-with-spacex/

Laboratory, Massachusetts Institute of Technology.

atmosphere (Hedin, A. E. (1991), Extension of the MSIS Thermosphere Model into the 

Hertel, O., Skjoth, C., Reis, S., Bleeker, A., Harrison, R., Cape, J., Fowler, D., Skiba, U., 
Simpson, D., Jickells, T., Kulmala, M., Gyldenkærne, S., Sorensen, L., Erisman, J., 
& Sutton, M. (2012). Governing processes for reactive nitrogen compounds in the 


