Modeling the Zeeman Effect in Planetary Atmospheric Radiative Transfer and Applications

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Atmospheric science
PhD Thesis

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Abstract

Remote sensing is about retrieving distant physical properties from locally observed radiation. The first step to remote sensing is to describe, or model, the radiative transfer. Without locating the origin of the observed radiation, and without proper interpretation of what it represents, understanding and utilizing instrumental results are nearly impossible. The focus of my thesis is on how radiation interacts with a weakly magnetized medium by means of the Zeeman effect. One molecule of particular interest affected by the Zeeman effect is the oxygen molecule. The thesis work started by an implementation of a module for the Zeeman effect in an existing radiative transfer model. Later works has applied this module to Earth and Mars radiative transfer.

The high relative concentration of the oxygen molecule in Earth’s atmosphere, and the fact that the molecule interacts with sub-millimeter radiation, has made it a prime target for temperature retrievals using both ground- and satellite-based radiometers. The Zeeman effect is important for molecular oxygen at mesospheric altitudes on Earth, where the geometry of the magnetic field and of the observation influence the polarized absorption of radiation. Simulations of ground-based measurements by a radiometer in Bern, Switzerland, have the Zeeman module reproduce the dependency on observational geometry for the local magnetic field, partly validating the module. Simulations of satellite measurements comparing the Zeeman module to a fast, parameterized, implementation of the Zeeman effect for numerical weather predictions also indicates that the module works. There are small discrepancies between the two models but both are close to the satellite measurements given the noise of these measurements. Work to move beyond simulation space and analyze these satellite measurements to find the atmospheric temperatures at high altitudes also show promising results.

Besides Earth applications, the module has been used for Mars conditions, where only trace amounts of molecular oxygen is available. Mars does not have a global magnetic field but instead have several magnetic sources scattered throughout its crust. This gives a magnetic field that is significantly weaker than on Earth and with much more structures. It is possible to utilize the Zeeman effect on molecular oxygen to measure the magnetic field of Mars. The last part of this thesis work suggests a measurement scheme for a satellite capable of retrieving the horizontal components of the Martian crustal magnetic field. It shows the expected errors associated with such a measurement scheme.
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My work was supervised by Associate Professor Mathias Milz at the Department of Computer Science, Electrical and Space Engineering, Luleå University of Technology, Kiruna, Sweden. Co-supervision was provided by Professor Stefan A. Buehler at the Meteorological Institute, University of Hamburg, Germany, and by Jana Mendrok at the Department of Earth and Space Sciences, Chalmers University of Technology, Gothenburg, Sweden. All three of you have helped me immensely in all aspects of the work leading to this thesis. Associate Professor Patrick Eriksson at the Department of Earth and Space Sciences, Chalmers University of Technology, Gothenburg, Sweden, has been equally helpful for my research. Paraphrasing and perhaps butchering the saying, these four are the giants on whose shoulders my work has relied upon most directly, and for this I am ever grateful to you. Another important person for my work is Oliver Lemke at the Meteorological Institute, University of Hamburg, Germany. His help with programming issues have been great, and if the other four are scientific giants, then Oliver cheerfully provided me with the metaphorical ladder I used for the climb. Thank you Oliver.

I have been extremely lucky during my time as a PhD student. I have traveled and seen the world. In order I visited Russia, the Netherlands, Japan, the United States, France, the United Kingdoms, Germany, and Austria. Each place has its own importance. In Russia, the Netherlands, the United States, Japan, and Austria I presented my work at conferences and meetings. The inspiration found by listening to and trying to understand the problems and solutions that others are presenting at these conferences have focused my efforts, and the feedback received on my own presentations from the audience have greatly improved my work. I spent months in each of Japan, France, the United Kingdoms, and Germany working on different projects or taking courses. In Japan we explored new possibilities, in France we experienced a great course on atmospheres, in the United Kingdoms we emphasized detailed model comparisons, and in Germany we expanded our capabilities for simulations. These “we” are different groups of people — before the visits, most were strangers to me but they are now friends and colleagues. Meeting these people made my years as a PhD student much more interesting and precious to me.

Kiruna has been my home for the majority of my adult life. I moved here as a master student. I will leave with a PhD. To my former fellow master students and to my fellow PhD students and colleagues at Space Campus in Kiruna and at campus in Luleå, you have made my time in the North fun.

I do not like writing acknowledgments. There are simply too many of you out
there that contributed, either directly or indirectly, either by a lot or by a little, to my work that I cannot name you all. To these unnamed co-authors, colleagues, funders, teachers, fellow students, friends, and family members, if you read this and feel that I should thank you, then you are correct. Thank you all.
By Swedish tradition a PhD thesis can be preceded by a Licentiate thesis. I followed this tradition, and my Licentiate thesis (Larsson, 2014) is available from the website of Luleå University of Technology. This PhD thesis is an extension of the Licentiate thesis. As such, both of the papers appended to the Licentiate thesis are also appended to this work, and a large part of the introduction to the papers, the “kappa”, is repeated from the original work with minor changes.
CHAPTER 1

Introduction

Remote sensing is widely used for determining atmospheric parameters. A satellite orbiting a planet can use remote measurements to observe large volumes of a planet’s atmosphere to study many different phenomena. For instance, both the chemistry and the temperature structures of the atmosphere can be studied on a global scale. Remote sensing also allows for the vast data mining necessary in weather forecasting for Earth. It is often the only reasonable option available to gather these meteorological data, as \textit{in situ} measurements above Earth’s surface is difficult to perform on sufficient scales to significantly impact forecasting.

At the heart of remote sensing is radiative transfer. Without locating the origin of the observed radiation, and without proper interpretation of what it represents, understanding and utilizing instrumental results are nearly impossible. A key part to understand how radiation propagates through an atmosphere is to be able to compute the molecular absorption of atmospheric gases.

The work for this thesis has focused on one aspect of the problem of molecular absorption, namely on modeling an effect that magnetism has on the absorption of molecular oxygen in the microwave region, and the applications of this in remote sensing. Known as the Zeeman effect, the radiation is polarized and the spectral lines are split when the molecule is placed in an external magnetic field. This is because molecular oxygen has two ‘free’ electrons that can interact with the magnetic field, causing the molecular energy levels to slightly change.

A good model of the Zeeman effect propagation has important applications in a wide range of research areas from meteorology to planetary physics. Commonly used meteorological instruments, for instance the Special Sensor Microwave Imager/Sounder (SSMIS; Kunkee et al., 2008; Swadley et al., 2008), measure the molecular oxygen electromagnetic spectrum to attain temperature profiles, e.g., by sounding at different frequency bins. Molecular oxygen is useful for these types of measurements on Earth because of its high and constant abundance up to high altitudes, which results in strong and stable spectral features. In the lower atmosphere the Zeeman effect can be ignored since spectral lines are strongly pressure-broadened, which hides the Zee-
man effect. For molecular oxygen at high pressures, a special effect on propagation called line mixing is important. Line mixing introduce the problem that lines cannot be treated as fully separate and additive features of the gas, but the lines will mix together. In the stratosphere and above, however, the Zeeman effect is important for measurements. The atmosphere is a connected system, so measurements from both high and low altitudes are useful for numerical weather prediction applications. The ability to consistently model both the Zeeman effect and line mixing is therefore important for measurements

Another application for a Zeeman effect model is in the quantification of magnetic fields. Although in a completely different frequency region and for other molecules and atoms, the Zeeman effect has been used to determine the magnetic field at the sun and other stars (see, e.g., Berdyugina and Solanki, 2002, and works cited therein). The methods applied in solar physics are not likely to be useful on planets. This is because the magnitude of the magnetic field is very different at most planets compared to the magnetic field strength of most stars. The smaller magnetic field strength of planets causes Zeeman split lines to overlap to a larger extent, and thereby better hide the magnetic signal. In short, more detailed analysis is necessary for weak magnetic fields than for strong magnetic fields.

To put the Zeeman effect in the context of radiative transfer, computer model simulations are necessary. The Atmospheric Radiative Transfer Simulator (ARTS; Buehler et al., 2005; Eriksson et al., 2011a) has therefore been central to this thesis. This is the software that my work, in order, first extended with a Zeeman effect module, and then utilized in practical applications. ARTS models the propagation of polarized radiation through a three-dimensional planetary atmosphere of the user’s choice.

This thesis begins with a chapter covering the basic theory of radiative transfer and how this can be modeled. Basic radiative transfer is explained in Section 2.1, and basic atmospheric absorption is explained in Section 2.2. The connection to retrievals of physical parameters is briefly touched on in Section 2.3. This chapter is by necessity neither exhaustive nor very detailed. Examples of the consequences of my work on simulations in ARTS are presented in Chapter 3, which also has some discussion on observational geometries. Chapter 4 expands on some applications of the theoretical work. The presented applications include ongoing efforts to retrieve temperatures up to the mesopause of Earth, and an expansion on the idea of using the Zeeman effect to retrieve magnetic fields on Mars. The last chapter summarizes the appended publications and concludes the thesis.
Chapter 2

Theory

This chapter describes the theoretical basis required by the reader to understand the implementation and operation of the Zeeman effect in electromagnetic radiative transfer modeling. The descriptions below focus on molecular oxygen spectroscopy. Most of the theory can be directly applied to other molecules or atoms, but in no way is this chapter general and I will not always attempt to point out when and where it is general.

2.1 Basic Radiative Transfer

2.1.1 Scalar Radiative Transfer

2.1.1.1 Beer’s Law

When radiation passes through the atmosphere, some of the radiation will be absorbed. This is known as Beer’s law. One way to visualize Beer’s law in a simplified
Theory

way is by holding a piece of paper in front of a strong lamp. A significant part of the light from the lamp will not reach you, the observer, anymore, but some will. The equation that governs how much of the incoming light that reaches the observer in this case is

\[ \frac{dI}{d\vec{r}} = -\alpha I, \] (2.1)

where \( \alpha \) is the absorption coefficient of the medium, \( I \) is the total intensity, and \( d\vec{r} \) is the infinitesimal distance the radiation is transferred, i.e., the thickness of the paper in the example. The above equation may be solved for a distinct homogeneous layer as

\[ I_{\text{out}} = I_{\text{in}} e^{-\alpha |\vec{r}|}, \] (2.2)

where \( I_{\text{in}} \) is the incoming radiation to the layer and \( I_{\text{out}} \) is the outgoing radiation from the layer. Imagining the outgoing radiation encountering another layer of some other properties that it also has to pass through before it can be observed, then the incoming radiation to this second layer is already reduced by the first layer but the radiation will also be reduced by the second layer — Equation 2.2 is applied for both layers, with the incoming radiation to the second layer being the outgoing radiation of the first layer. Imagining several such layers stacked after one-another before the radiation can be observed, it should be clear that the radiation that is observed is

\[ I_{k+1} = I_k e^{-\alpha_k |\vec{r}_k|}, \text{ or} \]
\[ I_n = I_0 \prod_{k=0}^{n-1} e^{-\alpha_k |\vec{r}_k|}, \] (2.3)

where the \( k \) index now represents a layer such that \( I_k \) is the incoming radiation from the source and \( I_{k+1} \) is the outgoing radiation, with \( I_0 \) as the original source of radiation and \( I_n \) as the observed radiation. The other two variables give the layer absorption coefficient and layer thickness. Note that the upper equation leads to the lower equation.

2.1.1.2 Planck’s Law

The warmth of an atmosphere will cause it to radiate, acting like a source of radiation. This thermal source of radiation can be described by Planck’s law. Planck’s law gives the maximum emission from a thermal source that randomly emits photons. Sources emitting at these levels are called blackbody radiators. The emission from a blackbody is

\[ B = \frac{2hf^3}{c^2} \frac{1}{e^{hf/k_BT} - 1}, \] (2.4)

where \( h \) is Planck’s constant, \( f \) is the frequency, \( c \) is the speed of light in vacuum, \( k_B \) is Boltzmann’s constant, and \( T \) is the temperature.

If the frequency is low, the Rayleigh-Jeans approximation

\[ B \approx B_{RJ} = \frac{2f^2k_BT}{c^2} \] (2.5)
2.1. Basic Radiative Transfer

is close to Planck’s law, and is derived by inserting the first order Taylor expansion
\[ e^{hf/k_B T} \approx 1 + \frac{hf}{k_B T} \tag{2.6} \]
into Planck’s law when \( hf/k_B T \ll 1 \). It is not very common to use Rayleigh-Jeans approximation in full calculations instead of Planck’s law. There is not much computational time to be saved by switching away from Planck’s law. It is, however, a common practice to convert total intensity at low frequencies to a construct known as brightness temperature by
\[ T_{RJ} = \frac{I_c^2}{2f^2 k_B}. \tag{2.7} \]
The idea of the above equation is that if the intensity measured, \( I \), is from a blackbody radiator, then, in the Rayleigh-Jeans approximation, \( T_{RJ} \) is the temperature of this blackbody radiator. This conversion turns out, in atmospheric scenarios, to be quite good for intuitively understanding total intensity data in low frequency ranges. As is described below, the brightness temperature is connected to the real temperature of the atmosphere. The practice to convert to brightness temperatures directly from Planck’s law also exist (and is in fact more common).

2.1.1.3 Combining Emission and Absorption

By combining absorption and emission to solve the scalar radiative transfer problem for a non-scattering medium in local thermodynamic equilibrium, we get
\[ \frac{dI}{dr} = -\alpha (I - B). \tag{2.8} \]
This means that the radiation after a single optically thin layer is
\[ I_{\text{out}} = I_{\text{in}} e^{-\alpha |\vec{r}|} + B (1 - e^{-\alpha |\vec{r}|}). \tag{2.9} \]
The above is similar to Equation 2.2, assuming that an atmospheric layer acts as an additional homogeneous source for the total radiation. Also similar to Equation 2.2 is that we can imagine a situation with several subsequent layers absorbing and emitting radiation so that
\[ I_{k+1} = I_k e^{-\alpha_k |\vec{r}|} + B_k (1 - e^{-\alpha_k |\vec{r}|}), \text{ or} \]
\[ I_n = I_0 \left[ \prod_{k=n-1}^{k=1} e^{-\alpha_k |\vec{r}|} \right] + \sum_{i=1}^{i=n-1} B_i \left( \prod_{k=i+1}^{k=n} e^{-\alpha_k |\vec{r}|} - \prod_{k=i}^{k=n-1} e^{-\alpha_k |\vec{r}|} \right), \tag{2.10} \]
where a pseudo-layer at index \( n \) has been introduced with zero absorption to simplify the expression. Note again that the first equation leads to the latter equation.

There are two very simple cases of Equations 2.8 and 2.9 that can be imagined to understand why brightness temperature is such an intuitive quantity. The first case
is when $\alpha = 0$ throughout the transfer. In this scenario, the only outgoing radiation is the incoming radiation. Imagine observing the surface from a downward-looking satellite with no atmospheric absorption. The only thing limiting your field of view in this case is the planetary surface itself. The atmosphere will appear perfectly clear, which is why frequency ranges with $\alpha \approx 0$ are often called window channels. The brightness temperature of the surface is understood as the surface emissivity times the Planck function of the surface temperature. If the surface emissivity is known, then the brightness temperature retrieved from a window channel is therefore only a function of the physical temperature of the surface itself.

The second case is when $\alpha$ is so large that the thermal emission of a thin layer approximates a blackbody radiator. In such an atmosphere, the outgoing intensity of the layer depends solely on the temperature of the layer. At very high altitudes, the absorption coefficient will once again approach zero. Even though the absorption coefficient is high close to the surface, it will drop with increasing altitude either because the number density of the absorbing molecule drops with increasing altitude, because pressure broadening decreases with increasing altitude, or because of a combination of both of these effects. (Pressure broadening and molecular absorption are discussed in the next section.)

Again, imagine observing this optically thick atmosphere from the perspective of a downward-looking satellite. The physical surface of the planet below is hidden. What is instead observed is a blurry atmospheric layer. We know that at the top of this layer $\alpha \approx 0$, because from some point the total intensity remains unchanged throughout the rest of the propagation path. The bottom of the blurry layer must be the last part of the atmosphere that act as a blackbody radiator, i.e., where $\exp(-\alpha|\vec{r}|) \approx 0$. The total intensity registered at the satellite is thus a weight of the thermal emissions over the blurry atmospheric layer. Consequently, the brightness temperature is the mean weighted temperature of the blurry layer.

### 2.1.1.4 For Non-Local Thermodynamic Equilibrium

Equation 2.8 is not the basic form of the radiative transfer equation. It is only applicable when absorption and emission coefficients are equal, which is the case for a medium in local thermodynamic equilibrium. In a more general case, the scalar radiative transfer problem for a non-scattering medium is

$$\frac{dI}{dr} = -\alpha_a I + \alpha_e B,$$

(2.11)

where $\alpha_a$ is the absorption coefficient as before (though often of a different numerical value) and $\alpha_e$ is the emission coefficient. For a brief description of these two variables see Subsection 2.2.1.3. In short, if they are not equal, then there will be a flow of energy into or out from the local layer of the medium: the medium absorbs a different amount of radiation to what it emits such that there is a local flow of energy. Thus,
there is no local thermodynamic equilibrium. Even in this case, it is possible to define

\[
\frac{dI}{d\vec{r}} = -\alpha_a \left( I - \frac{\alpha_e}{\alpha_a} B \right).
\] (2.12)

This is because the form above is intuitive since it clearly shows that non-local thermodynamic equilibrium radiative transfer changes the ratio between emission and absorption to something other than unity. In essence, with \( B \to (\alpha_e/\alpha_a)B \), the same approach as Equation 2.10 can be taken for the layered solution (the ratio between \( \alpha_a \) and \( \alpha_e \) is independent of \( \vec{r} \) in a homogeneous layers). So \( I_n \) can often be found from

\[
I_{k+1} = I_k e^{-\alpha_{a,k}|\vec{r}_k|} + \frac{\alpha_{e,k}}{\alpha_{a,k}} B_k (1 - e^{-\alpha_{a,k}|\vec{r}_k|}), \text{ or}
\]

\[
I_n = I_0 \prod_{k=n-1}^{k=1} e^{-\alpha_{a,k}|\vec{r}_k|} + \sum_{i=1}^{i=n-1} \frac{\alpha_{e,i}}{\alpha_{a,i}} B_i \left( \prod_{k=n}^{k=i+1} e^{-\alpha_{a,k}|\vec{r}_k|} - \prod_{k=n-1}^{k=i} e^{-\alpha_{a,k}|\vec{r}_k|} \right). \] (2.13)

The form above is only applicable when \( \alpha_a/\alpha_e \) can be accounted for externally (see, e.g., López-Puértaz and Taylor, 2001; Goussev, 2002, for more details), so some care has to be taken to determine \( \alpha_a \) and \( \alpha_e \) before applying Equation 2.13.

### 2.1.2 Polarized Radiative Transfer

Polarization is neglected in scalar radiative transfer but can intuitively be understood from imagining radiation as a stream of oscillating photons. If there is an average directionality of oscillation, then the radiation is said to be polarized.

There are polarizing effects on radiation in the atmosphere. These include, e.g., reflection, scattering and the Zeeman effect. The scalar equations previously discussed cannot handle this polarization properly. One problem is that rotation due to reflection may turn one kind of polarization into another. This means that we are required to solve the radiative transfer simultaneously for different directionality of polarization.

In a three-dimensional Cartesian coordinate system with the radiation propagating in the \( \hat{z} \)-direction, radiation can oscillate with any directionality in the \( x-y \) plane. If the average oscillation is along, e.g., the \( \hat{x} \)-axis, then the polarization is linear and \( \hat{x} \)-directional. If the oscillation change directionality over time (i.e., there is a phase difference between the propagation of \( \hat{x} \)-directional and \( \hat{y} \)-directional radiation), then the radiation is circularly polarized. If there is no average directionality, the radiation is said to be unpolarized. Different levels of ellipticity occur, and these can be described by, e.g., the Stokes vector.

#### 2.1.2.1 The Stokes Vector

The challenge tackled by the Stokes formalism is to describe the polarized intensity of radiation in the fewest possible terms in what is called the Stokes vector. There
are six independent polarization bases in Stokes formalism. Of these, four are linearly oriented and two are circularly oriented. These are described in the list below by six commonly used names, unit vectors describing their main directionality in the x-y plane, and small artistic arrows showing the same directionality graphically:

Vertical: $\hat{e}_v = \begin{bmatrix} 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} \uparrow \end{bmatrix}$,

Horizontal: $\hat{e}_h = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} \rightarrow \end{bmatrix}$,

Plus 45°: $\hat{e}_{+45°} = \begin{bmatrix} \cos\left(\frac{\pi}{4}\right) & \sin\left(\frac{\pi}{4}\right) & 0 \end{bmatrix} \begin{bmatrix} \nearrow \end{bmatrix}$,

Minus 45°: $\hat{e}_{-45°} = \begin{bmatrix} \cos\left(\frac{7\pi}{4}\right) & \sin\left(\frac{7\pi}{4}\right) & 0 \end{bmatrix} \begin{bmatrix} \searrow \end{bmatrix}$,

Left Circular: $\hat{e}_{lc} = \begin{bmatrix} 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} \circ \end{bmatrix}$,

Right Circular: $\hat{e}_{rc} = \begin{bmatrix} 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \circ \end{bmatrix}$.

From a naïve perspective, one might think that only two linear polarization bases are required to describe the ellipticity of the polarization. However, if we consider that the intensity along $\hat{e}_v$ and along $\hat{e}_h$ is equal if all of the intensity is along $\hat{e}_{+45°}$, it is clear to see that more than two linear polarization bases are required because it is otherwise unknown that the intensity along $\hat{e}_{-45°}$ is nil. For the circular polarizations this 'off-axis' geometry is not valid and we are left with only two possible circular polarization states.

It is possible to simplify the problem further than to use a six-numbered vector. This is because the total intensity of vertical and horizontal polarization must be the same as the total intensity of circular polarization, and the total intensity of off-axis polarization. The Stokes vector, $\vec{I} = [I, Q, U, V]^\top$, is now possible to define. The notations I use for the Stokes vector follow Eriksson et al. (2011a), with

$$I \equiv I_v + I_h = I_{+45°} + I_{-45°} = I_{lc} + I_{rc}, \quad (2.14)$$

$$Q \equiv I_v - I_h, \quad (2.15)$$

$$U \equiv I_{+45°} - I_{-45°}, \quad (2.16)$$

$$V \equiv I_{lc} - I_{rc}, \quad (2.17)$$

where $I$ is the total intensity, $Q$ is the difference between horizontal and vertical polarization intensities ($\hat{e}_v, \hat{e}_h$), $U$ is the difference between plus and minus 45° polarization intensities ($\hat{e}_{+45°}, \hat{e}_{-45°}$), $V$ is the difference between left and right circular polarization intensities ($\hat{e}_{lc}, \hat{e}_{rc}$), $I_v$ is the total intensity along $\hat{e}_v$, $I_h$ is the total intensity along $\hat{e}_h$, $I_{+45°}$ is the total intensity along $\hat{e}_{+45°}$, $I_{-45°}$ is the total intensity along $\hat{e}_{-45°}$, $I_{lc}$ is the total intensity along $\hat{e}_{lc}$, and $I_{rc}$ is the total intensity along $\hat{e}_{rc}$. The possibility to confuse $I$ above with $I$ in, e.g., Equation 2.8 is intentional. If $Q = U = V = 0$ throughout a transfer, then there is no need to use the Stokes vector and the two $I$s are identical.
2.1.2.2 Beer’s Law

In order to rewrite Beer’s law from its scalar form of Equation 2.1 to work with the Stokes vector, it is necessary to convert the absorption coefficient of Equation 2.35 to a matrix (see, e.g., Emde et al., 2004). The vector form of Beer’s law becomes

\[
\frac{d\vec{I}}{d\vec{r}} = -K \vec{I},
\]  
(2.18)

to which a layered solution, in analog of Equation 2.3, is

\[
\vec{I}_{k+1} = e^{-K_{k|\vec{r}_k}} \vec{I}_k, \quad \text{or} \quad \vec{I}_n = \left[ \prod_{k=n-1}^{k=1} e^{-K_{k|\vec{r}_k}} \right] \vec{I}_0.
\]  
(2.19)

In the above, \( K \) is the propagation matrix, which by necessity to work with the Stokes vector is a \( 4 \times 4 \) matrix. Note that the main difference between Equations 2.3 and 2.19 is that the order of execution is important so that each layer ‘remembers’ the previous layers’ state of polarization. Also note that if \( K \) is diagonal for all layers, and there is no polarization in the initial radiation, then Equations 2.3 and 2.19 give the same results.

As a mathematical reminder, the natural exponential of a square matrix \( A \) is defined as

\[
e^A \equiv \sum_{n=0}^{\infty} \frac{1}{n!} A^n.
\]  
(2.20)

There are ways to numerically approximate a solution to the infinite sum above, but I will not detail any here (see instead, e.g., Moler and Van Loan, 2003).

For unpolarized absorption, the propagation matrix will be

\[
K_I = \begin{bmatrix}
\alpha_I & 0 & 0 & 0 \\
0 & \alpha_I & 0 & 0 \\
0 & 0 & \alpha_I & 0 \\
0 & 0 & 0 & \alpha_I \\
\end{bmatrix},
\]  
(2.21)

since reduction of each polarization state is equal, and if the incoming radiation is fully polarized, then its Stokes components are reduced in the same way as its total intensity. In the unpolarized case, the scalar Beer’s law (Equation 2.1) and vector Beer’s law (Equation 2.18) are interchangeable, i.e., \( \alpha = \alpha_I \). Most absorption lines behave unpolarized and will therefore simply reduce the total amount of radiation following Beer’s law with the above propagation matrix.

If there is a polarizing influence on the attenuation, the propagation matrix will be

\[
K_A = \begin{bmatrix}
\alpha_I & \alpha_Q & \alpha_U & \alpha_V \\
\alpha_Q & \alpha_I & 0 & 0 \\
\alpha_U & 0 & \alpha_I & 0 \\
\alpha_V & 0 & 0 & \alpha_I \\
\end{bmatrix},
\]  
(2.22)
where the individual indexes show the influence on different polarization components. If the absorption is polarizing, scalar and vector Beer’s law are not interchangeable. The absorption coefficient $\alpha_I$ is still the total absorption, but $\alpha_Q$, $\alpha_U$ and $\alpha_V$ are the differences between the absorption coefficients of their respective Stokes components.

One example of an application of polarizing attenuation is reflection from the ground, where some energy is lost and there is a difference in how polarization components interact with the surface as a function of, e.g., incoming angle.

If there is a polarizing influence on the refraction, which causes a rotation of polarization, the matrix will be

$$K_B = \begin{bmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & \beta_V & \beta_U \\
0 & -\beta_V & 0 & -\beta_Q \\
0 & -\beta_U & \beta_Q & 0
\end{bmatrix}, \quad (2.23)$$

where the main delaying polarization component is marked by the indexes. Each $\beta$ is thus representative of the polarization rotation caused by phase delays between the perpendicular polarizations indicated by the index. For example, if there is a difference in propagation speed between vertical and horizontal polarizations (non-zero $\beta_Q$), then some linear polarization will turn into circular (and vice versa) while the radiation propagates. One example of phase delay in the atmosphere is Faraday rotation, which is caused by the rotation of electrons in a magnetic field and influences the propagation of circular polarization.

Note that if there are several different influences on the polarization state of the radiation, then the sum of all these types of propagation will give the effective $K$. For instance, the Zeeman effect is influenced by both attenuation and phase delay, and must therefore be described by

$$K = \begin{bmatrix}
\alpha_I & \alpha_Q & \alpha_U & \alpha_V \\
\alpha_Q & \alpha_I & \beta_V & \beta_U \\
\alpha_U & -\beta_V & \alpha_I & -\beta_Q \\
\alpha_V & -\beta_U & \beta_Q & \alpha_I
\end{bmatrix}, \quad (2.24)$$

### 2.1.2.3 Planck’s Law

Planck’s law in Stokes vector form reads

$$\vec{B} = \begin{bmatrix}
B \\
0 \\
0 \\
0
\end{bmatrix}, \quad (2.25)$$

where $B$ is the scalar Planck’s law of Equation 2.4. Blackbody radiation is random, and will as such only affect the $I$ component of the radiation. The thermal emission from the atmosphere can still carry polarization because the emission itself depends on the propagation matrix.
2.1. Basic Radiative Transfer

The conversion to brightness temperature is also slightly different in vector form than in scalar form. I again use the notation by Eriksson et al. (2011a), who define

$$\vec{T}_{BRJ} = \left( \frac{c^2}{4 f^2 k_B} \right) \begin{bmatrix} I \\ Q \\ U \\ V \end{bmatrix} = \begin{bmatrix} T_{BRJI} \\ T_{BRJQ} \\ T_{BRJU} \\ T_{BRJV} \end{bmatrix}.$$  \hspace{1cm} (2.26)

In this notation, $T_{BRJI} + T_{BRJQ}$ is the brightness temperature for the vertical polarization component. $\vec{T}_{BRJ}$ can be either from a Rayleigh-Jeans approximation or directly from Planck’s law, but the above is for Rayleigh-Jeans.

2.1.2.4 Combining Planck’s Law and Beer’s Law

In analogy to Equation 2.8, the vector radiative transfer equation is

$$\frac{d\vec{I}}{dr} = -K_a \left( \vec{I} - \vec{B} \right).$$ \hspace{1cm} (2.27)

In similar analogy to Equation 2.10, this has a solution for homogeneous layers as

$$\vec{I}_{k+1} = e^{-K_a |\vec{r}_k|} \vec{I}_k + \left( 1 - e^{-K_a |\vec{r}_k|} \right) \vec{B}_k,$$

$$\vec{I}_n = \left[ \prod_{k=n-1}^{k=1} e^{-K_a |\vec{r}_k|} \right] \vec{I}_0 + \sum_{i=n-1}^{i=1} \left( \prod_{k=n}^{k=i+1} e^{-K_a |\vec{r}_k|} - \prod_{k=n-1}^{k=i} e^{-K_a |\vec{r}_k|} \right) \vec{B}_i,$$ \hspace{1cm} (2.28)

where pseudo-layer $n$ has $K_n = 0$. Again, the upper equation leads to the lower equation for the full solution. The main differences between Equations 2.10 and 2.28 is again that the order of multiplication is important (as explained for Beer’s law above, the polarization state of the radiation going into and out of each layer is important).

2.1.2.5 For Non-Local Thermodynamic Equilibrium

The analogy from the scalar radiative transfer Equation 2.11 also works in non-local thermodynamic equilibrium. The formalism reads

$$\frac{d\vec{I}}{dr} = -K_a \vec{I} + K_a \vec{B},$$ \hspace{1cm} (2.29)

which still can be written for convenience as

$$\frac{d\vec{I}}{dr} = -K_a \left( \vec{I} - K_a^{-1} \vec{B} \right).$$ \hspace{1cm} (2.30)

Similar as for the scalar layered equation, the vector layered solution also must carry the emission-to-absorption ratio for each layer. The layered solution follows from
Equation 2.28 and just need the change: $\vec{B}_i \rightarrow \mathbf{K}^{-1}_{a,i}\vec{B}_i$. The solution for $\vec{I}_a$ is thus

$$\vec{I}_{k+1} = e^{-\mathbf{K}_{a,k} |\vec{r}_k|} \vec{I}_k + (1 - e^{-\mathbf{K}_{a,k} |\vec{r}_k|}) \mathbf{K}^{-1}_{a,k}\mathbf{K}_{e,k}\vec{B}_k,$$

$$(2.31)$$

with the same limitations as for Equation 2.13.

2.1.2.6 Sensor Orientation

One important property of polarization to keep in mind is the sensor orientation. If the medium is polarizing and radiative transfer is considered in layers, then calculations in each layer are most easily performed by considering the orientation of the sensor as the reference coordinate system. This is because the effects that cause polarization are usually oriented according to some local field that may or may not change between the layers. For example, the propagation associated with the Zeeman effect is oriented along the magnetic field and the propagation associated with reflection from the surface is oriented with respect to the normal of the surface.

Reorienting the local effects on the linear polarization to the sensor coordinate system may be done by considering Equation 2.27 in a sensor coordinate system as

$$\mathbf{L}^{-1} \frac{d\vec{I}}{d\vec{r}} = -\mathbf{K'} \left( \mathbf{L}^{-1} \vec{I} + \vec{B} \right),$$

$$(2.32)$$

where the prime on $\mathbf{K'}$ is there to denote the propagation in a rotated coordinate system, and $\mathbf{L}$ is the rotation matrix to change the Stokes vector from the sensor coordinate system to the rotated coordinate system (see, e.g., Mishchenko et al., 2002)

$$\mathbf{L} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos 2\eta & -\sin 2\eta & 0 \\ 0 & \sin 2\eta & \cos 2\eta & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix},$$

$$(2.33)$$

where $\eta$ is the counterclockwise angle of rotation of the sensor’s linear polarization directionality to the locally polarizing effect’s linear polarization directionality. It follows from Equation 2.32 that

$$\mathbf{K} = \mathbf{L} \mathbf{K'} \mathbf{L}^{-1},$$

$$(2.34)$$

and that by this operation the polarization is oriented according to the sensor for each layer.
2.2 Atmospheric Line Absorption

To model atmospheric radiative transfer properly requires knowledge of how molecules and matter in an atmospheric volume interact with the radiation. The main way by which molecules interact with radiation is through absorption/emission lines. The effective atmospheric absorption may be approximated from the line-by-line scalar absorption profile as

$$\alpha(f) = \sum_s n_s \sum_{l_s} S_{l_s} F_{VVH}(f) F_{l_s}(f), \quad (2.35)$$

where $n_s$ is the number density of molecule $s$, $S_{l_s}$ is the line strength of line $l_s$, $F_{VVH}$ is a far wing correction factor, and $F_{l_s}$ is the line’s shape as a function of the frequency $f$. I will ignore polarization throughout this section as it is mostly not important for line absorption. To take polarization into account, simply apply

$$K(f) = \alpha(f) \Phi, \quad (2.36)$$

where $\Phi$ represents the polarization effects. The only effect that I am aware of where line absorption is noticeably polarized so that Equation 2.36 is important in planetary atmospheres is the Zeeman effect, and while parts of this is covered in this section, the reader is referred to Paper I and sources therein for details on this polarization.

For other lines, the absorption is identical for all polarization states so $\Phi = 1$.

The factor $F_{VVH} = f \tanh(h f / 2 k_B T) / f_{0, l_s} \tanh(h f_{0, l_s} / 2 k_B T)$, where $f_{0, l_s}$ is the central frequency of line $l_s$, is a necessary correction to standard line shapes. It is mostly important for low frequencies near the line center, as it approaches unity near the line center at different rate if $f < f_{0, l_s}$ or $f > f_{0, l_s}$. The line shape itself approaches zero when $f$ is far from $f_{0, l_s}$, so the factor does not matter as much then. For some more details on this correction factor, please see Huber and van Vleck (1966).

Absorption is considered additive for all absorption lines and all gases in the atmosphere. Lines are considered to have one frequency, but due to physical effects (mainly caused by pressure and temperature), the lines will be broadened to cover a wide frequency range, and sometimes even shift the central frequency of the line. This section discuss absorption/emission lines and their shapes, as well as their physical causes. The aim is to provide an intuitive and mathematical understanding of the underlying physics of lines.

2.2.1 Line Strength

Line strength is the absorption rate of a line per path length of propagation path and per molecule. This subsection will discuss the definition and derivation of the line strength. More detailed definitions and derivations can be found, e.g., in the works by Hilborn (1982) and by Šimečková et al. (2006). In simple terms, the strength of a transition depends on the total rate of change of the molecule’s state levels — the higher the rate of change, the stronger the line.
2.2.1.1 Generating a Photon

Perhaps the most basic problem involved in radiative transfer is the generation of photons. An electron-atom or an electron-molecule system that generates photons is composed of several discrete energy levels. A transition between two of these energy levels changes the total energy of the system. Considering two energy levels \(E_j\) and \(E_i\), for levels \(j\) and \(i\), between which the electron can change, the energy of the transition is simply the difference between these energy levels

\[
\Delta E = E_j - E_i. \tag{2.37}
\]

These energy levels are difficult to observe directly, but the photons generated by this transition can readily be observed by a radiometer or spectrometer. The energy states themselves are sums of different different contributions

\[
E_j = E_{e,j} + E_{v,j} + E_{r,j} + E_{s,j} + \cdots, \tag{2.38}
\]

where \(E_{e,j}\) is the electronic energy state, \(E_{v,j}\) is the vibrational energy state, \(E_{r,j}\) is the rotational energy state, and \(E_{s,j}\) is the spin energy state. The triple dots are there for all other energy states (e.g., nuclear interactions). Many of these energy states can remain the same through a transition and it is often intuitive to make this distinctions between transitions.

The photons generated with energy \(\Delta E\) will have the frequency

\[
f_{ji} = \frac{|\Delta E|}{h}. \tag{2.39}
\]

Here and below the dual subindex \(ji\) means a transition from \(E_j\) to \(E_i\), and oppositely \(ij\) is a transition from \(E_i\) to \(E_j\). As a rule of thumb, transitions between electronic energy states are seen in the ultraviolet or visible electromagnetic spectra, transitions between vibrational energy states are seen in the infrared electromagnetic spectra, and transitions between rotational energy states are seen in the microwave electromagnetic spectra. Throughout this work, a transition is interchangeably called a line. The frequency associated with a line is called the central frequency of the line. Absorbing a photon of the right frequency increases the energy of the electron-atom or electron-molecule system. Conversely, emitting a photon decreases the energy of the system. I will for simplicity refer to absorbing and emitting species as molecules below.

2.2.1.2 Rate of Transitions

Transitions can happen through spontaneous decay, induced decay, and induced absorption. The spontaneous decay rate of level \(E_i\) is described by the Einstein \(A\)-coefficient, \(A_{ji}\), with units of decays per second from state \(j\) to state \(i\). The induced decay and induced absorption are described by the Einstein \(B\)-coefficients. If for all entities of a molecule there are initially \(n_j\) molecules in state \(E_j\), the Einstein \(A\)-coefficient can be used to calculate the number of these molecules in this state after some time \(t\) by

\[
n_j(t) = n_j(0)e^{-\tau \sum A_{ji}}, \tag{2.40}
\]
2.2. Atmospheric Line Absorption

where the initial number in the state is \( n_j(0) \). This can intuitively be understood from the idea that the number of molecules in state \( E_j \) is a function of the natural decay rate of state \( E_j \) to state \( E_i \). The sum of all Einstein \( A \)-coefficients will then naturally give the spontaneous decay time of \( E_j \),

\[
t_{s,j} = \left( \sum_i A_{ji} \right)^{-1},
\]

(2.41)

so that the rate of decay of the number of molecules of state \( E_j \) can be rewritten as

\[
n_j(t) = n_j(0) e^{-t/t_{s,j}}.
\]

(2.42)

Induced decay and induced absorption are both aptly named since they occur as a function of the external electromagnetic fields. Considering the simple case with only the transition between states \( E_1 \) and \( E_2 \) and the states are balanced then there is a relationship between the radiation-induced \( B \)-coefficients and the natural decay rate of the \( A \)-coefficient

\[
n_2A_{21} = n_1B_{12}u(f_{21}) - n_2B_{21}u(f_{21}),
\]

(2.43)

where \( u(f_{21}) \) is the energy density of the field per frequency at frequency \( f_{21} \), \( B_{21} \) is the induced emission, \( n_j \) is the number of molecules in state \( E_j \) in the volume, and \( B_{12} \) is the induced absorption. Both of Einstein’s \( B \)-coefficients are in units of decays per second per energy density per frequency. The external field at the natural frequency of the level \([u(f_{21})]\) is inducing both additional absorption and additional emission. In this work, the field inducing emission and absorption is assumed to be the Planck field. In, e.g., lasers, the external field is artificially inducing emissions and will not be the Planck field.

The line strength is by Šimečková et al. (2006) the right-hand of Equation 2.43 per entity of the molecule. This means

\[
S_{21}(T) = \frac{1}{n} \left[ n_1B_{12} - n_2B_{21} \right] \frac{\hbar f_{21}}{c^2}
\]

(2.44)

where \( 1/n \) means it is per entity of the (isotopic) molecule. The distribution of molecular states in local thermodynamic equilibrium follows the Maxwell-Boltzmann distribution

\[
n_j = n g_j e^{-E_j/k_bT}/Q(T),
\]

(2.45)

where \( g_j \) is a constant of the energy level \( i \), and \( Q(T) \) is the sum of all possible states. Known as the partition function,

\[
Q(T) = \sum_j g_j e^{-E_j/k_bT},
\]

(2.46)
it is calculated and described in detail, e.g., the work by Fischer et al. (2003) for several atmospheric molecules. Inserting Equation 2.43 with Equation 2.45 into Equation 2.44, the line strength can be written

\[ S_{21}(T) = \frac{g_2 A_{21}}{Q(T)} \frac{c}{8 \pi f_{21}} \left[ e^{-E_1/k_B T} - e^{-E_2/k_B T} \right]. \]  

(2.47)

To translate the strength at a reference temperature to the line strength at another temperature, it is necessary to know one of the energy levels, the energy associated with the inherent frequency of the transition, and the ratio of the total integrated partition sum at two temperatures. Adapting the reference line strength to the line strength at any temperature for Equation 2.35 is done by

\[ S_{ls}(T) = S_{ls}(T_0) \frac{S_{21}(T)}{S_{21}(T_0)} = S_{ls}(T_0) \frac{Q(T)}{Q(T_0)} \frac{e^{-E_1/k_B T} - e^{-E_2/k_B T}}{e^{-E_1/k_B T_0} - e^{-E_2/k_B T_0}}, \]  

(2.48)

where \( S_{ls}(T_0) \equiv S_{21}(T_0) \) if the same source for the total integrated partition sums was used and the assumptions of Equation 2.44 and 2.45 holds. These two parameters are separated in the equation above to make it clear that the reference line strength from one line database can, if desired, be mixed with a total integrated partition function from another line database. It is this \( S_{ls}(T) \) that goes into Equation 2.35. Though not all simplifications above are valid for calculations of all \( S_{ls}(T_0) \), the ratio to scale \( S_{ls}(T_0) \) to another temperatures is valid in local thermodynamic equilibrium.

### 2.2.1.3 For Non-Local Thermodynamic Equilibrium

The discussion on line strength above is related to cases when there is a local thermodynamic equilibrium. If a system is not in local thermodynamic equilibrium, then the emission coefficient and the absorption coefficient are different (see Equations 2.12 and 2.30). I recommend López-Puértaz and Taylor (2001) and Goussev (2002) for further reading on the subject of what causes the atmosphere to leave local equilibrium. Below follows a brief discussion on the implications for the atmospheric line absorption.

In non-local thermodynamic equilibrium, the number densities of the energy states are not directly related to the atmospheric temperature. Despite this, it is still convenient to describe the number density distribution of a molecule in non-local thermodynamic equilibrium using the same formalism that applies when the molecule is in local equilibrium. This can be achieved by combining Equations 2.38 and 2.45 for the energy state number distributions as

\[ n_j' = n g_j e^{-E_{e,j}/k_B T_{e,j}} e^{-E_{v,j}/k_B T_{v,j}} e^{-E_{r,j}/k_B T_{r,j}} e^{-E_{s,j}/k_B T_{s,j}} \cdots \sum_j g_j e^{-E_{e,j}/k_B T_{e,j}} e^{-E_{v,j}/k_B T_{v,j}} e^{-E_{r,j}/k_B T_{r,j}} e^{-E_{s,j}/k_B T_{s,j}} \cdots. \]  

(2.49)

while replacing the atmospheric temperature to each energy state \( (E_{e,j}, E_{v,j}, E_{r,j}, E_{s,j}, \cdots) \) with a corresponding “state temperature” \( (T_{e,j}, T_{v,j}, T_{r,j}, T_{s,j}, \cdots) \). Determining
2.2. Atmospheric Line Absorption

these local disequilibrium state temperatures is beyond the scope of my thesis, please see the references above for details.

Often the state distribution does not have to be considered to be as complicated as above. One common practice is to only consider one of the states of energy out of local equilibrium. For example, it is common in moderate non-local thermodynamic equilibrium that only the vibrational state has to be considered in disequilibrium. In particular, and simplifying the problem further, when mostly the higher energy vibrational energy states are out of equilibrium, then the state number distribution can be written

\[ n'_j = n_j e^{-\frac{(E_j - E_{v,j})}{k_B T_v} - \frac{E_{v,j}}{k_B T_v}} \frac{Q(T)}{} \]

(2.50)

because the largest contribution to \( Q(T) \) is anyways from the lower energy states (i.e., the exponents approach zero for larger \( E_j \), so \( Q(T) \) is mostly from the sums of the lower \( E_j \)). Simplified further, the ratio between the disequilibrium and the equilibrium energy state number density is in these cases

\[ r_j = \frac{n'_j}{n_j} = e^{-\frac{(E_j - E_{v,j})}{k_B T_v} - \frac{E_{v,j}}{k_B T_v}} \frac{1}{e^{-E_j/k_B T}} = e^{-\frac{E_{v,j}(T-T_v)}{k_B T_v}}. \]

(2.51)

Intuitively, the emission coefficient scales linearly with the number density of the higher energy state — this is the state that emits radiation. So Equation 2.35 has to be scaled with the ratio \( r_j \) to get the emission coefficient. That is

\[ S_{l,e}(T) = S_{l,e}(T) r_j. \]

(2.52)

From the same logic that lead to Equation 2.48, the scale factor for absorption in Equation 2.35 is found as

\[ S_{l,a}(T) = S_{l,a}(T) \frac{r_i - r_j e^{-h f_{ji}/k_B T}}{1 - e^{-h f_{ji}/k_B T}}. \]

(2.53)

To compute \( \alpha_a \) and \( \alpha_e \) for Equation 2.11 of the previous section, simply replace \( S_{l,i}(T) \) is Equation 2.35 with \( S_{l,a}(T) \) and \( S_{l,e}(T) \), respectively.

2.2.1.4 Zeeman Effect

The Zeeman effect polarizes radiation depending on the orientation and strength of the magnetic field. This is done by projecting the angular momentum of the energy level onto the magnetic field. Different projections along the magnetic field will then change the total energy of a level by a different amount. As a consequence, the energy of the radiation emitted and absorbed will also change depending on the projection so that the projection changes the central frequency of the transition and also the polarization of the radiation. For more detailed remarks see, e.g., Schadee (1978) and Paper I of this thesis. This subsection will describe the cause of the splitting, both from a classical and modern physics viewpoint. It will not go into any details on other physical effects.
2.2.1.4.1 Classical View of Splitting  The original description by Zeeman for the influence of magnetism on line frequencies was from classical physics and experimentation. Having measurements of the effect, Zeeman (1897) describes the splitting of lines for some molecules classically with the magnetic part of the Lorentz equation

\[ m\vec{a} = e\vec{v} \times \vec{H}, \quad (2.54) \]

and the assumption, also from Lorentz, that electrons are orbiting around molecules and are held in place with a spring-like force

\[ m\vec{a} = -kr. \quad (2.55) \]

In the above equations, \( m \) is the mass of the electron, \( e \) is the charge of the electron, \( \vec{a} \) is the acceleration of the electron, \( \vec{v} \) is the speed of the electron, \( \vec{r} \) is the position of the electron, \( k \) is the spring constant of the original transition, and \( \vec{H} \) is the magnetic field. The idea at the time of the spring-like force was that vibrations in \( \vec{r} \) causes the electric field to vibrate, releasing energy like a dipole antenna. The released energy is then the radiating field, or stream of photons.

Summing both forces, setting \( \vec{H} \) along the \( \hat{z} \)-axis, the movement of the particle can be found from

\[
\begin{align*}
\frac{d^2x}{dt^2} &= -kx + eH_z \frac{dy}{dt} \\
\frac{d^2y}{dt^2} &= -ky - eH_z \frac{dx}{dt}
\end{align*}
\]

This system of equations has the solution

\[
\begin{align*}
x(t) &= x(0) e^{-i\left(\sqrt{\frac{k}{m}} + \frac{eH_z}{4\pi m}\right)t} \\
y(t) &= y(0) e^{-i\left(\sqrt{\frac{k}{m}} + \frac{eH_z}{4\pi m}\right)t}
\end{align*}
\]

From the above, it can be seen that an external magnetic field changes the central frequency of the vibrations by

\[ \Delta f_Z = \frac{eH_z}{4\pi m} \quad (2.58) \]

from the zero magnetic field frequency of

\[ f_0 = \frac{1}{2\pi} \sqrt{\frac{k}{m}} \quad (2.59) \]

The change in frequency due to the magnetic field is also called frequency splitting, or Zeeman splitting, because of the multiple lines that are formed from the original line. As one example, a line in a 50\( \mu \)T magnetic field would in this case have a Zeeman splitting of about 700 kHz.

The method hints at why only some molecules experience the splitting and others do not: there must be 'free' electrons available to interact with the magnetic field; electrons are 'free' if their spin is not counteracted by the spin of another electron. If there are no available electrons, the molecule will not experience splitting.
2.2. Atmospheric Line Absorption

The original theory developed by Zeeman as above can explain the splitting of one line into two lines when the molecule is placed in an external magnetic field. The theory can also explain the splitting of one line into three lines, with a remaining central line, perhaps because part of the line is unaffected by magnetism. However, more than three split lines occur in nature. This is a problem for the theory by Zeeman that Equation 2.58 does not account for.

2.2.1.4.2 Modern View of Splitting Returning to the description of energy levels in the beginning Subsection 2.2.1, the Zeeman effect changes the energy of a level by adding a perturbation to Equation 2.37 such that

\[ \Delta E_Z = E_j + E_{Z,j} - E_i - E_{Z,i}, \]  

(2.60)

where \( E_{Z,j} \) and \( E_{Z,i} \) are the energy perturbation associated with the two energy levels. That is, the modern way to look at frequency splitting is

\[ f_Z = \frac{\Delta E}{h} + \frac{E_{Z,j} - E_{Z,i}}{h}. \]  

(2.61)

Notice the absence above of the “absolute value” signs of Equation 2.39 on the Zeeman components. Both positive and negative frequency shifts occur. The Zeeman component of the frequency is several orders of magnitude smaller than the otherwise central frequency, so the resulting line frequencies are not negative. For more details on the derivations below, I recommend Berestetskii et al. (1980).

The energy associated with one Zeeman state is

\[ E_Z = -\frac{eh|\vec{H}|}{4\pi m} gM \]  

(2.62)

where the factor \( eh/4\pi m \) is known as the Bohr magneton, which also occurs in Equation 2.58, and is usually written as \( \mu_0 \), i.e.,

\[ E_Z = -\mu_0|\vec{H}|gM, \]  

(2.63)

where \( M \) is the projection of the total angular momentum on the magnetic field, and \( g \) is a state constant, e.g., for molecular oxygen described by

\[ g = g_s \frac{J(J + 1) + S(S + 1) - N(N - 1)}{2J(J + 1)}, \]  

(2.64)

where \( g_s \) is a factor to account for relativistic effects (\( g \) and \( g_s \) are discussed for SO and \( O_2 \) by Christensen and Veseth, 1978, and Berdyugina and Solanki, 2002, discuss these for several other molecules). \( J \) is the total angular momentum number including spin, \( S \) is the total spin angular momentum number, and \( N \) is the total angular momentum number without spin. For clarity, \( M \) is an integer or half-integer such that \(|M| \leq J \), i.e.,

\[ M \in \{-J, -J + 1, -J + 2, \cdots, J - 2, J - 1, J\}. \]  

(2.65)
There are thus $2J + 1$ possible $M$ for a molecule with integer $J$ and $2J$ possible $M$ for a molecule with half-integer $J$. Molecular oxygen has integer $J$.

Getting from energy levels to frequency shift is straightforward (following derivations in, e.g., Berestetskii et al., 1980, who also explains the details to a greater extent) as

$$
\Delta f_Z = -\frac{\mu_0 |\vec{H}|}{h} (g'M' - g''M''),
$$

where the primes and the double primes are the respective upper and lower quantum states of the system, such that $M'$ is a projection of $J'$, and such that $M''$ is a projection of $J''$. Note that $M' - M'' \in \{-1, 0, 1\}$. Since we have $2J + 1$ different $M$ for molecular oxygen, there are $6j + 3$ ways to create $\Delta f_Z$, where $j$ is the smallest out of $J'$ and $J''$. At most, an absorption line of central frequency $f_{ji}$ is thus split into $6j + 3$ different lines, although some combinations of $M'$ and $M''$ can give the same $\Delta f_Z$ to overlap some of the split lines.

To understand Equations 2.63 and 2.64 it is necessary to treat the quantum numbers above as vectors and write that the change in energy state is

$$
E_Z = \vec{\mu} \cdot \vec{H},
$$

where $\vec{\mu}$ is the magnetic moment of the molecule due to spin, which is

$$
\vec{\mu} = -\frac{2\pi \mu_0}{h} g_s \vec{S},
$$

where the quantum number associated with $\vec{S}$ is one-half times the number of 'free' electrons. The above equation should be read so that the spin of the electrons along the magnetic field is responsible for the shifted energy levels. This is very useful to keep in mind in the simplification that follows below. Since only the magnetic component along the magnetic field is of interest, the above equation may be rewritten as

$$
\frac{2\pi \mu_0}{h} g_s \vec{S} = \frac{2\pi \mu_0}{h} g_s \vec{S} \cdot \vec{J},
$$

where $\vec{J}$ is the total angular momentum vector including spin, i.e.,

$$
\vec{J} \equiv \vec{N} + \vec{S}.
$$

The squares (dual $\vec{J} \cdot \vec{J}$) allow the extraction

$$
E_Z = -\frac{2\pi \mu_0}{h} \mu' \left( \vec{J} \cdot \vec{H} \right) = -\mu_0 |\vec{H}| \mu' M,
$$

since $hM/2\pi$ is the projection of $\vec{J}$ on $\vec{H}$. The intention is to show that $\mu'$ is $g$ from Equation 2.64, so we write

$$
\mu' = g = g_s \frac{\vec{S} \cdot \vec{J}}{\vec{J} \cdot \vec{J}}
$$

(2.72)
2.2. Atmospheric Line Absorption

Having defined $\vec{J}$ as the total angular momentum above, it follows that

$$\vec{S} \cdot \vec{J} \equiv \vec{S} \cdot \left( \vec{N} + \vec{S} \right) = \vec{S} \cdot \vec{N} + \vec{S} \cdot \vec{S},$$  \hspace{1cm} (2.73)

where $\vec{S} \cdot \vec{N}$ can be understood from

$$\vec{J} \cdot \vec{J} = \left( \vec{N} + \vec{S} \right) \cdot \left( \vec{N} + \vec{S} \right) = \vec{N} \cdot \vec{N} + \vec{S} \cdot \vec{S} + 2 \vec{S} \cdot \vec{N}.$$  \hspace{1cm} (2.74)

It is now straightforward to rewrite

$$\frac{\vec{S} \cdot \vec{J}}{\vec{J} \cdot \vec{J}} = \frac{\vec{J} \cdot \vec{J} - \vec{N} \cdot \vec{N} + \vec{S} \cdot \vec{S}}{2 \vec{J} \cdot \vec{J}},$$  \hspace{1cm} (2.75)

which can be written in terms of the absolute length of the vectors\(^1\)

$$\frac{\vec{S} \cdot \vec{J}}{\vec{J} \cdot \vec{J}} = \frac{J(J+1) - N(N+1) + S(S+1)}{2J(J+1)}.$$  \hspace{1cm} (2.76)

It is through the above derivation seen that

$$g = g_s \frac{\vec{S} \cdot \vec{J}}{\vec{J} \cdot \vec{J}} = g_s \frac{J(J+1) + S(S+1) - N(N+1)}{2J(J+1)}.$$  \hspace{1cm} (2.77)

The value of $g_s$ depends on the molecule in question and is a function of, e.g., relativistic effects (see, e.g., Veseth, 1976, 1977, for more details).

Not only the frequency change due to the magnetic field is important for Zeeman-split lines. The relative strength and the polarization of split lines are also important. This is discussed in Paper I.

2.2.2 Line Shape

Lines do not only influence the radiation at a single frequency but are rather broadened and influence a wider frequency range. To create the final spectroscopic response, all overlapping broadened lines must be added together. To describe the line broadening, several physical functions are used, some of which are described below. The described functions all broaden the line symmetrically around the line frequency. These functions are described by the line frequency and the relative width of the broadening. The relative width commonly used is the half-width at half-maximum\(^2\).

The normalization used herein is that the basic line shape functions integrated over frequency is unity, i.e.,

$$\int_{\infty}^{-\infty} F(f)df = 1,$$  \hspace{1cm} (2.78)

where $F(f)$ is any line shape function. Others may normalize the line shape to, e.g., $\pi$ because this turns out to be a common factor in line shape calculations.

\(^1\)The length of $\vec{J}$ is $\sqrt{J(J+1)}\hbar/2\pi$. Similar expressions hold for the other angular momentum vectors.

\(^2\)The half-width at half-maximum is formally defined as the absolute frequency change for which $F(f) = \frac{1}{2}F(f_0)$, where $F(f)$ is a distribution function centered around $f_0$. 
2.2.2.1 Natural Broadening

From Hilborn (1982) the natural line shape may be found from the natural decay rate, $t_s$, of Equation 2.41, as

$$F_N(f) = \frac{1}{\pi} \frac{1/2\pi t_s}{(f - f_0)^2 + (1/2\pi t_s)^2}, \quad (2.79)$$

where $1/2\pi t_s$ is the half-width at half-maximum natural broadening of the distribution, and $f_0$ is the line central frequency. The above is called the natural line shape because it is directly related to the natural lifetime of an energy level. Intuitively, as any function narrows in time it gets broader in frequency. This can be demonstrated in principle by the Heisenberg uncertainty $\Delta t \Delta f \geq C$, where $C$ is a constant, $\Delta t$ is the certainty in time, and $\Delta f$ is the certainty of the frequency change. Since a faster rate of decay is more certain in time, it is also more uncertain in frequency (and thus distributed over a broader frequency range).

If we want a more mathematical understanding of why lines cannot influence only their central frequency, it is straightforward to derive the natural line shape from the rate of decay discussed in Subsection 2.2.1. Considering a line with only one possible frequency, in time the wave should oscillate according to

$$E(t) = e^{i2\pi f_0 t}. \quad (2.80)$$

However, we already know that this cannot be the shape of the wave since the amplitude of the wave depends on the number of molecules in states that can emit at $f_0$ so Equation 2.42 shows that there is a dampening of the wave amplitude as a function of the natural lifetime of each state level. We therefore have to write the dampened waveform of the line as

$$E(t) = e^{-|t|/t_s} e^{i2\pi f_0 t}, \quad (2.81)$$

where I am adding the “absolute value” signs on the time associated with the decay because the decay is one-dimensional in time; intuitively, there is no way to know the distribution of energy states before some time zero. The Fourier transform of Equation 2.81 yields

$$\mathcal{F} [E(t)](f) \equiv \int_{-\infty}^{\infty} e^{-|t|/t_s} e^{i2\pi f(t - f_0)} df' = \frac{1}{1/t_s + i2\pi(f - f_0)} + \frac{1}{1/t_s - i2\pi(f - f_0)}, \quad (2.82)$$

with the real part identical to Equation 2.79.

2.2.2.2 Thermal Broadening

The molecules of the atmosphere are moving. This movement is directly linked to the kinetic energy of the atmosphere; kinetic energy in the equilibrium atmosphere is described by the atmospheric temperature. Emitted radiation will thereby be either
red-shifted or blue-shifted to some degree depending on the molecules’ speed relative to the observer due to Doppler shifting. Doppler shift is calculated as
\[ f = f_0 \left(1 + \frac{v}{c} \right), \]  
(2.83)
where \(v\) is the velocity of the molecule.

The atmosphere is mostly not going anywhere, so the average velocity is zero in wind-free conditions. Since it is only the velocity relative to the observer that is important, a centered one-dimensional Maxwell distribution describes the motion of the molecules statistically. This one-dimensional velocity distribution is
\[ D_M(v) = \sqrt{\frac{1}{\pi}} \sqrt{\frac{m}{2k_BT}} \exp \left( -\frac{mv^2}{2k_BT} \right), \]  
(2.84)
where \(m\) is the molecule’s mass. The integral \( \int_{v_i}^{v_j} D_M(v)dv \) returns the ratio of molecules with \(v_i < v < v_j\). The velocity distribution and Doppler shift functions will together act like a broadening function. Known as the Doppler broadening function, it can be written as
\[ D_M(f) = \sqrt{\frac{1}{\pi}} \sqrt{\frac{m}{2k_BT}} \exp \left( -\frac{mc^2}{2k_BTf_0^2} \right) \left[ f - f_0 \right]^2. \]  
(2.85)
Some simplifications can be made since from Equation 2.83
\[ dv = \frac{c}{f_0} df, \]  
(2.86)
and these simplifications are useful because it is inconvenient to always write
\[ \int_{v_i}^{v_j} D_M(f)df = \int_{f_i}^{f_j} \frac{c}{f_0} D_M(f)df \]  
(2.87)
for calculating the ratio of molecules emitting at \(f_i < f < f_j\), which is the quantity that is actually interesting for the line shape. The Doppler broadening function is thus commonly written as
\[ F_D(f) = \frac{c}{f_0} D_M(f) = \sqrt{\frac{1}{\pi}} \sqrt{\frac{mc^2}{2k_BTf_0^2}} \exp \left( -\frac{mc^2}{2k_BTf_0^2} \right) \left[ f - f_0 \right]^2. \]  
(2.88)
From the above equation, the half-maximum is found at
\[ f = f_0 \left(1 \pm \sqrt{\frac{2k_BT \ln 2}{mc^2}} \right). \]  
(2.89)
The half-width at half-maximum thermal broadening is then simply
\[ \Delta f_D = f_0 \sqrt{\frac{2k_BT \ln 2}{mc^2}}. \]  
(2.90)
Thermal broadening is the most easily understood broadening parameter. So when thermal broadening is dominant, then it is often straightforward to analyze spectral features to retrieve atmospheric parameters, even on planets other than Earth.
2.2.2.3 Pressure Broadening

As pressure increases, the rate of collisions between molecules increase. The lifetime of an energy level in vacuum may be longer than the collision interval of the molecules, but collisions can force transitions, which reduces the effective lifetime of energy levels. As the effective lifetime of an energy level is decreased by increased collisional rates, the line shape becomes broader for the same reasons that the natural lifetime of an energy state broadens the line. Since the pressure broadening is governed by collisions, both colliding molecule matters and some collisions can be more or less effective at dampening the state level.

Pressure broadening is from this picture very similar to the natural broadening of Equation 2.79. According to Rosenkranz and Staelin (1988), the Lorentz distribution that describes pressure broadening is in its complex form

\[ F_L(f) = \frac{1}{\pi} \frac{1}{f - f_0 - i\Delta f_p}, \tag{2.91} \]

where \( \Delta f_p \) is the half-width at half-maximum pressure broadening. This is called pressure broadening because

\[ \Delta f_p = [\gamma_0(T) + i\delta_0(T)] p, \tag{2.92} \]

where \( p \) is the pressure, \( \gamma_0 \) is a line specific pressure broadening parameter, and \( \delta_0 \) is a line specific pressure shift parameter. The imaginary part of the complex Lorentz distribution describes attenuation and the real part is associated with refraction or phase delay.

2.2.2.4 Combining Pressure and Thermal Broadening

To use a single line shape for the entire observed atmosphere is important for internal consistency in a radiative transfer model. Lacking internal consistency may cause problems when deriving, e.g., the altitude from which measured radiation originates. This is especially problematic from altitudes with similarly strong pressure broadening as thermal broadening. Both the Lorentz distribution and the Doppler broadening distribution are limited to being useful in their separate regions, as governed by which half-width at half-maximum broadening variable is largest.

The Voigt function fulfills the condition of internal consistency by being the convolution of the Doppler distribution and the imaginary part of the Lorentz distribution. The Voigt function is written

\[ F_V(f) = (F_D * \Im\{F_L\})(f) = \int_{-\infty}^{\infty} F_D(f')\Im\{F_L(f - f')\} df', \tag{2.93} \]

where \( \Im\{F_L\} \) denotes the imaginary part of \( F_L \).

Calculations of more specialized propagation sometimes require that both attenuation and phase delay are known. It is not possible to use the Voigt distribution for
these specialized cases. Instead, a more general method has to be used that returns not only the attenuation but also the phase delay. Using the Faddeeva function (see e.g., Heinzel, 1978) fulfills this last condition. It can be written as

\[ w(z) = \exp\left(-z^2\right)\text{erfc}(-iz), \]

(2.94)

where \( \text{erfc}(\cdots) \) is the complex error function, for mathematical completeness

\[ \text{erfc}(x) = 1 - \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n}{n!(2n+1)} x^{2n+1}, \]

(2.95)

and

\[ z = \frac{1}{\pi \Delta f_D F_L^\dagger(f)} \]

(2.96)

where \( F_L(f)^\dagger \) is the complex conjugate of Equation 2.91. There are presently no analytical solutions to the Voigt or Faddeeva functions, but numerical algorithms exists for both functions. For example, the algorithm by Zaghloul and Ali (2011) (which is available in \texttt{C++} under the MIT license in an implementation by Steven G. Johnson.)

It is possible to utilize the Faddeeva function to calculate the normalized line shape by

\[ F_V(f) + i F_{F/V}(f) = \frac{1}{\sqrt{\pi \Delta f_D}} w(z), \]

(2.97)

where \( F_{F/V}(f) \) is the Faraday-Voigt line shape, which describes the shape of the phase delay around a line, and \( F_V(f) \) is still the Voigt line shape.

There are line shape effects ignored by the line shape discussions so far. These include adding a speed-dependency on the broadening parameters and treating various collisional regimes differently, amongst other effects (see Hartmann et al., 2008, for a detailed discussion). Recently, the International Union of Pure and Applied Chemistry suggested using an altered line shape to address these effects but little to none of this has been incorporated in practice in the available major line databases to this date (see Ngo et al., 2013; Tran et al., 2013; Tennyson et al., 2014, for details and discussions on the suggested line shape), though preparations in the high-resolution transmission molecular absorption database (HITRAN Rothman et al., 2013) appears underway.

2.2.2.5 Line Mixing by Ordered Approximations

All discussion above focuses on transitions from one energy level to another giving rise to distinct lines with distinct line centers, broadening parameters, etc.. These transitions are easy to describe because they simply change the energy level in the emitter (absorber), e.g., from \( E_j \) to \( E_i \) by emitting (absorbing) a photon. There are however times when this is not the case, and when different energy levels interact.

I return to Hartmann et al. (2008) as a good book on the subject on collisional effects. They explain that the essence of simple line mixing is that there are other
ways for the emitter (absorber) to change from $E_j$ to $E_i$ than by direct emission (absorption). One of these is by collisions, which can impart or remove energy from the emitting (absorbing) molecule. If there are energy levels $E_j'$ or $E_i'$ sufficiently close to $E_j$ and $E_i$ that a collision can change $E_j$ into $E_j'$ or $E_i$ into $E_i'$, other paths are open for the emitter (absorber) to change from $E_j$ to $E_i$. Note that it is important that the path of the transition is still from $E_j$ to $E_i$ to keep the Maxwell-Boltzmann distribution valid. Two molecules with this path in the atmosphere of Earth are O$_2$ and CO$_2$. Since the photon emitted/absorbed is from the change of $E_j'$ to $E_i'$, but the population levels are those of $E_j$ and $E_i$, the process is commonly known as line mixing. Line mixing has been studied extensively. For a short historical overview, follow works in order by Anderson (1949); Baranger (1958); Fano (1963); Ben-Reuven (1966), which offer the theoretical development of pressure broadening.

Line mixing introduces a line shape that is not purely Lorentzian and additive at high pressures. One way to approximate the line shape still involves the Lorentzian, but with small perturbations. These perturbations depends on some power of the pressure, and are known as ordered approximations. For more details see Smith (1981), on whose work much of the discussion that follows below is based. The idea with the ordered approximations is that absorption being additive per line, as Equation 2.47, is valid even for lines that are mixed by just changing the line shape function, though all mixed lines must be included to not have negative absorption.

The first order O$_2$ model by Rosenkranz (1988) mixes the imaginary part of the refractive index with its real counterpart. In his work, the line shape becomes

$$F'(f) = (1 - iY) F(f),$$

where $Y$ is the first order line mixing coefficient. The first order mixing coefficient has temperature and pressure dependence as

$$Y = y' p \left( \frac{T_0}{T} \right)^x.$$  \hspace{1cm} (2.99)

The exponent, $x$, is set as 0.8 by the model for the 60 GHz oxygen band and the values of $y'$ for a subset of the strongest lines in the band can be found tabulated in Rosenkranz (1988) or, for a newer versions of first order coefficients, Tretyakov et al. (2005).

A second order model for O$_2$ is presented by Makarov et al. (2011). In this model the line shape changes as

$$F'(f) = (1 + G - iY) F(f - f'),$$

where $G$ and $f'$ are the new second order line mixing coefficients, and they also use a different temperature dependence as

$$Y = \left( y'_0 + y'_1 \left[ \frac{T_0}{T} - 1 \right] \right) p \left( \frac{T_0}{T} \right)^x.$$  \hspace{1cm} (2.101)
2.3. The Inverse Problem

\[ G = \left( g'_0 + g'_1 \left[ \frac{T_0}{T} - 1 \right] \right) p^2 \left( \frac{T_0}{T} \right)^{2x}, \]  

(2.102)

and

\[ f' = \left( \delta f'_0 + \delta f'_1 \left[ \frac{T_0}{T} - 1 \right] \right) p^2 \left( \frac{T_0}{T} \right)^{2x}, \]  

(2.103)

where \( x \) is still 0.8. The differences between these two models are small but noticeable in the far wings of a band. (It is important when using any ordered mixing model that the line parameters used together with the mixing model are those assumed when deriving the coefficients. If this is not the case, the errors from the mixing quickly accumulates, so to use any of the models above, also use the associated data.)

2.3 The Inverse Problem

There are many ways to turn a measurement of radiation into information about the state of a medium, i.e., solving the inverse problem. Most of these inverse methods rely on a statistical approach that connects a measurement and a numerical model of the measurement to an associated state of the medium. To understand these methods, I recommend the introducing chapters by Rodgers (2000) and will present just one inverse method from this work below: the Gauss-Newton Method.

In short, there are errors involved with measurements and such errors mean that there is an uncertainty involved in determining the state of the medium. For a moderately non-linear relationship between the state of the medium and the measurement\(^3\), one way to approach the state of the medium is to iteratively solve

\[ \vec{x}_{i+1} = \vec{x}_a + S_a J_i^T (J_i S_a J_i^T + S_i)^{-1} \left[ \vec{y} - F(\vec{x}_i) + J_i (\vec{x}_i - \vec{x}_a) \right]. \]  

(2.104)

Here, \( \vec{x}_i \) represents the estimated state of the medium after \( i \) iterations. This means it is a vector consisting of the temperature profile, the wind profile, the magnetic field profile, the pressure profile, the volume mixing ratio profiles of all molecules in the medium, all the absorption line parameters of interest, and so on and so forth. (But only for the part of the medium interacting with the radiation, and often only the variables for which the state information is meaningful have to be included in \( \vec{x}_i \).) The other variables are: \( \vec{x}_a \) is the a priori assumption on the medium, \( S_a \) is the covariance of the a priori, \( J_i \) is the Jacobian matrix as

\[ J_i = \frac{\partial F(\vec{x}_i)}{\partial \vec{x}_i}, \]  

(2.105)

\( F(\vec{x}_i) \) is the result of the radiative transfer solution with model inputs \( \vec{x}_i \), \( S_i \) is the error covariance matrix of the measurements, and \( \vec{y} \) is the corresponding measurement. Note that

\[ \vec{I} = F(\vec{x}), \]  

(2.106)

\(^3\)Rodgers defines moderate non-linearity as meaning that the state of the medium cannot be found by linear approximations of the numerical model, but that uncertainty of the state of the medium is nevertheless linear around the solution.
as the modeled radiation from one of Equations 2.10 or 2.28 for a discrete set of layers, and that $\vec{x}$ then contains inputs for these layers. The covariance matrices, $S_a$ and $S_\epsilon$, are best determined/guessed from data and contain the statistical assumptions made about the measurement error and the uncertainty of the state of the medium. There are plenty of steps involved in determining $\partial I/\partial \vec{x}$, but these are mostly trivial once the formalism of Sections 2.2.1 and 2.2.2 is clear, though it does require a bit of work to get the details right.

There are two complications that are noteworthy enough to clarify, before leaving the subject of partial derivations to create the Jacobian matrix, because they both have relatively simple and practical solutions that should not be missed. The first is that the line shape partial derivation can be found from Equation 2.97 using

$$\frac{\partial}{\partial x} w(z) = 2 \left( z w(z) - \frac{1}{\sqrt{\pi}} \right) \frac{\partial z}{\partial x}$$

following, e.g., Heinzel (1978), such that only the partial derivation with regard to $z$ is necessary for any line shape derivative. The second is that the derivative of a matrix exponent (c.f. Equation 2.20) must be solved numerically, for instance using the method by Brančík (2006).
Chapter 3

Modeling

The bulk of my work has been in coding computer models of the theoretical descriptions in the previous chapter. Most of this work is detail-oriented and therefore not publishable in peer-reviewed journals. My code is nevertheless available to all via the web in the GPL-licensed Atmospheric Radiative Transfer Simulator (ARTS) software package. This chapter will give examples of simulations running ARTS for special scenarios of the theoretical descriptions of the previous chapter. There is again a propensity towards molecular oxygen absorption and radiative transfer. First is a brief section introducing the software, then follows the examples for generic radiative transfer and for absorption by the Zeeman effect.

3.1 Atmospheric Radiative Transfer Simulator

The first official version of ARTS was announced with Buehler et al. (2005), though development started long before. The most recent major publication was for the release of ARTS 2.0 by Eriksson et al. (2011a). More publications both using and developing ARTS together with its modules are available through www.radiativetransfer.org (at the time of writing). The Q-package (Qpack) retrieval toolbox by Eriksson et al. (2005) was released at the same time as ARTS, offering a way to directly use these simulations for retrievals/inverse calculations.

ARTS handles three-dimensional radiative transfer through planetary atmospheres in Stokes formalism. It is modular and allows for the combination of several modules to calculate the absorption. The previous chapter touches on only a fraction of the theoretical descriptions of these modules. An ARTS simulation starts by setting up the simulated scenario. The user is asked to define the assumptions they make about the atmosphere’s physical properties, the sensor characteristics, considerations for the absorption, and a few other things. General control files — the type of file that controls an ARTS simulation and where all user assumptions must be made clear — are provided for a number of scenarios to make it easy to get started. The model then simulates the radiative transfer following either the scalar or polarized solutions.
of the radiative transfer equations (with alterations when scattering is accounted for that I will avoid for I have not worked much with scattering). There are detailed descriptions on how to get started using ARTS — and on what theory it applies — made available by Eriksson et al. (2011b,c,d) and attainable together with the source code.

3.2 Basic Radiative Transfer Simulations

This section will present the consequence on radiative transfer for some observational geometries of transfer through Earth’s atmosphere by simulations using ARTS. The section is not interested in variations or statistics but just in providing example simulations, so everything except the sensor position and line of sight is kept constant between simulations.

The atmosphere in all of these simulations is from subarctic winter conditions using the associated temperature, pressure, and volume mixing ratio profiles from Anderson et al. (1986), in which the temperature range is between 200 and 260 K throughout the profile. The magnetic field conditions are from around Kiruna, Sweden, where magnetic field strength is a bit higher than 50 μT (using the model by Finlay et al., 2010). The simulated frequency range is between 50 and 850 GHz because this is the frequency range in which I have built most of my experience. The frequency gridding is dense near molecular oxygen line centers and sparse almost everywhere else, so many features not related to molecular oxygen will not be properly represented in the plots. For simplicity, only the unpolarized total radiation will be shown.

The absorption of the atmosphere is by molecular nitrogen (with the continua absorption model from Rosenkranz, 1993, which is mostly important in frequency ranges between stronger absorption features), molecular oxygen (with line parameters around 60 GHz and 120 GHz from Tretyakov et al., 2005, and line parameters between 368 GHz and 834 GHz from Rothman et al., 2013), water (with the full absorption model from Rosenkranz, 1998, which contains strong absorption features around 180 GHz, 320 GHz, 380 GHz, and is the strongest feature at low altitudes in the frequency range above 400 GHz), and some trace gases (which are simulated using line parameters from Rothman et al., 2013).

In short, the simulations are simplified and do not represent any real instrument observation, but at the same time they are not absurd for the broad case. To keep this section brief, many details are skimmed over — depending on application and interest, there are plenty of details to pursue and the reader is referred to the appended papers for pursuits of some of these details, and to the plethora of literature available through peer-reviewed journals for the pursuit of other details.

3.2.1 Zenith Observation from Ground

This simulation places the sensor at surface altitudes and have its line of sight pointing parallel to the normal of the planet. The simulated brightness temperature and
temperature Jacobian for the full frequency range is shown in Figure 3.1. The first plot in the figure shows the brightness temperature — this is the radiation vector $\vec{I}$ of Equation 2.106 in brightness temperatures — and the second plot shows the partial derivative of the simulation in units of brightness temperature over the atmo-

![Figure 3.1: Example of ground-based radiation spectra in sub-THz frequency range observing parallel to the surface normal vector on Earth. The upper plot shows the simulated brightness temperature and the lower plot shows the Jacobian with regards to temperature.](image-url)
spheric temperature — this is the corresponding Jacobian matrix $J$ for $\vec{x} \rightarrow \vec{T}$ as per Equation 2.105.

Brightness temperature is associated with the source emitting it. In Subsection 2.1.1.3 it is told that if the absorption is high then the temperature of the medium is responsible the emission of the observed radiation and if the absorption is low, then the background radiation is most important for the observation. In zenith observations, the background radiation is from the emissions of the Universe itself — the cosmic background radiation at 2.7 K. The atmosphere is much warmer at 200-260 K. The large difference between these numbers makes an intuitive analysis of the brightness temperatures possible. The radiation in frequency ranges of brightness temperatures around 200-260 K are (almost purely) from the medium. These frequency ranges have strong absorption and therefore the radiation is from the lowest parts of the atmosphere. The temperature Jacobian of Figure 3.1 shows this as strong peaks at low altitudes when the brightness temperature is high. In frequency ranges where the brightness temperature is less than 200 K, part of the radiation will be from space. This means that the absorption is relatively weak, and that the atmospheric emission is spread over larger altitude ranges. In Figure 3.1, frequency ranges of low brightness temperature have also got a temperature Jacobian distributed over a wider altitude range.

To observe radiation from higher altitudes requires low opacity. It also requires something to observe. Both conditions can be achieved, for instance by taking measurements near the center of weak absorption lines, which is what was done in Paper III, or by observing emissions from species that are uncommon at lower altitudes but common at higher altitude. Figure 3.2 shows a zoom in of Figure 3.1 for the simulated radiation from the weaker absorption line in Paper III. It also shows the temperature and the magnetic field Jacobian matrices — the latter is $J$ for $\vec{x} \rightarrow |\vec{H}|$ as per Equation 2.105. I will leave discussing the magnetic strength Jacobian to the limb example geometry subsection.

It should be clear from Figure 3.2 that the interpretation of the temperature Jacobian is much more complex in the zoomed in frequency range than in the simple examples given above for the full frequency range. There is still a sharp peak at low altitudes. This is because the absorption line is part of the 60 GHz molecular oxygen absorption band and at lower altitudes the pressure-broadened absorption of other lines of the band is important. The peak is not as sharp as for other frequency ranges, however, which lets some radiation from higher altitudes through to the ground. It is in fact intuitive to view the brightness temperature plot of the figure as showing mostly radiation from low altitudes in the wings of the plot (i.e. at 10 MHz and more away from the line center), and the differences between the radiation close to the line center and the radiation in the wings as radiation that originates from high altitudes.
3.2. Basic Radiative Transfer Simulations

Figure 3.2: Zoom on 53.07 GHz line from Figure 3.1. Upper plot shows the simulated brightness temperature, the lower left plot shows the Jacobian with regards to temperature, and the lower right plot shows the Jacobian with regards to magnetic field strength.

### 3.2.2 Nadir Observation from Space

This simulation places the sensor at satellite altitudes (above the model atmosphere) and have its line of sight pointing anti-parallel to the normal of the planet’s surface. The simulated brightness temperature and temperature Jacobian for the full frequency range is shown in Figure 3.3.

In nadir geometry, the background radiation is from surface emission (in this case a blackbody emission of about 260 K). This is the reason why the brightness temperature range is much more narrow for the nadir geometry than for the zenith.
Figure 3.3: Example of satellite-based radiation spectra in sub-THz frequency range observing anti-parallel to the surface normal vector on Earth. Plot order is the same as for Figure 3.1.

geometry. High opacity features will in nadir geometry be from radiation at higher altitudes, and low opacity features will have radiation from the surface and closer to the ground. The higher the altitude, the lower the pressure and thereby the less the pressure broadening becomes, so absorption is reduced in the wings as a function of altitude. This is why the temperature Jacobian contains several features reminiscent
3.2. Basic Radiative Transfer Simulations

of line shapes. Central parts of the line absorption is reduced primarily by the loss of molecules at higher altitudes and so these frequency ranges are often sensitive up to stratospheric and even mesospheric altitudes in nadir geometry. One absorption line sensitive to mesospheric altitudes is the 61.15 GHz molecular oxygen line, which Figure 3.4 zooms in on, showing the brightness temperature spectra and the same two types of Jacobian matrices as was shown in Figure 3.2. (To repeat, I will leave all discussion on the magnetic strength Jacobian to the next subsection.)

Figure 3.4: Zoom on 61.15 GHz line from Figure 3.3. Plot order is the same as for Figure 3.2.

The multiple wiggles in the center of the brightness temperature of Figure 3.4 is from the Zeeman split lines at high altitudes. These are not present in Figure 3.2.
because that line is from energy levels with higher angular momentum than the line in Figure 3.4 and therefore experience a much finer splitting between different lines, making them indistinguishable from just broadened spectra. The temperature Jacobian of this simulation peaks at altitudes between 50-70 km near the line center, with slightly higher and lower altitudes as a function of frequency. Away from the line center, the altitude peak is lower at about 30-50 km, with lower altitudes the further from the line center we get, though since the line is in the center of the molecular oxygen absorption band, the decrease in altitude with increasing frequency stagnates further from the line center where the band is important. The high altitude peak is why the Special Sensor Microwave Imager/Sounder (SSMIS; Kunkee et al., 2008; Swadley et al., 2008) observe near the center of oxygen lines.

### 3.2.3 Limb Observation from Space

This simulation places the sensor at satellite altitudes (above the model atmosphere) and have its line of sight pointing perpendicular to the normal of the planet at 60 km altitude — 60 km is called the tangent altitude in this observation geometry. The simulated brightness temperature and temperature Jacobian for the full frequency range is shown in Figure 3.5.

In limb as in zenith geometry, the background radiation is 2.7 K. When the tangent altitude is high, then pressure broadening is low and only the frequencies in vicinity of an absorption line is affected by it. This creates the jagged shape seen in the figure, where only the Doppler broadening is important. In this jagged shape, there are several smaller peaks and a lot of these peaks are from trace gases.

As a generalized simplification, high altitude limb observations are not done best by covering a wide frequency range\(^1\). Instead, zooming in on just one or a few of the narrow absorption lines is better. Far from the lines, there is not much information on the atmosphere available as can be seen in the temperature Jacobian of Figure 3.5. Figure 3.6 shows such a zoom in on the 368.50 GHz molecular oxygen line. Similar to as before, its temperature and magnetic strength Jacobian are both included.

The brightness temperature zoom shows a plateau with wiggles on top. The plateau-shape is because the low pressure combined with the multiple Zeeman split lines. This makes the drop-off in absorption with frequency sudden at the thermal broadening of the outermost split line, and with space as background the brightness temperature drops almost immediately as the absorption. The wiggles are there because the Zeeman effect pattern creates regions of higher and lower absorption between Zeeman split lines. In the temperature Jacobian, the intermittently higher and lower absorption shows that the radiation from the central parts of the line is from different altitudes. The temperature Jacobian also shows that there is close to no information

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\(^1\)One exception, for example, is when the chemistry of the high altitude is being studied, because then a wide frequency range can give the state distribution of the molecules involved by measuring several emission lines. The state distribution could be required to estimate the volume mixing ratio of chemically active molecules.
3.2. Basic Radiative Transfer Simulations

Figure 3.5: Example of satellite-based radiation spectra in sub-THz frequency range observing perpendicular to the surface normal vector on Earth at 60 km altitude. Plot order is the same as for Figure 3.1.

about the atmospheric temperature in the far wings of the line. The large negative numbers near the edge of the plateau are perhaps of most importance; these numbers say that if the atmospheric temperature is increased then the brightness temperature there will decrease. So somewhat intuitively, knowing the line shape makes determination of the atmospheric temperature at the tangent altitude possible.
The magnetic strength Jacobian plot will require some more explanations. With its switching of positive and negative numbers as a function of altitude inside the bounds of the brightness temperature plateau, it says that the shape of the plateau itself will change if the magnetic field is changed. This makes intuitive sense as the line centers of the Zeeman split lines shift frequency as the magnetic field change. What is most interesting is the strong positive peak off the edge of the plateau. As a numerically simplified exercise, if we assume an increased magnetic field strength of 1 $\mu$T then the brightness temperature will increase by about 0.3 K at most in some frequency ranges and less in others. The same number for the other two zoomed

\footnote{The simplification is in the assumption that a change in the magnetic field strength can happen in only one layer so we do not have to care about the altitude. In practice, a change in the magnetic field strength can happen in multiple layers.}

Figure 3.6: Zoom on 368.50 GHz line from Figure 3.5. Plot order is the same as for Figure 3.2.
in geometries are 0.1 K for nadir geometry and 0.001 K for zenith geometry. If a change in brightness temperature is important for a measurement or not depends on the noise levels of the instrument taking the measurement, and the uncertainty of the magnetic field itself. A high noise sensor or a relatively unchanging magnetic field on a mission interested in temperature does not have to bother with magnetic strength errors. However, we suggest a mission taking measurements of the emissions of molecular oxygen in the atmosphere of Mars as way to measure the Martian crustal magnetic field in more details in Paper VI, so there are applications other than just noise reduction from knowing the magnetic strength Jacobian, and sensor technology is on the level where even small perturbations in magnetic field strength influence measurements.

3.3 Model of Atmospheric Line Absorption

This section will provide some figures on how calculations of atmospheric absorption works. It will omit even more details than the previous section on modeling radiative transfer.

Applying Equations 2.60 and 2.83, Figure 3.7 has been created for many Zeeman split absorption lines. This figure shows the Zeeman components and their relative strength for one atmospheric scenario.

One key point of this figure is that the higher the angular momentum is, the greater the number of split lines becomes. For sufficiently high angular momentum, the split lines can no longer be discerned from an overall spectra. Another key point is the splitting of the line into different components (\(\sigma_+\), \(\sigma_-\)). These are used to set up the polarized propagation matrix as a function of the angles between the magnetic field and the propagation path. For more details see the theory chapter above or Paper I, and sources therein, as appended below.

For a single set of atmospheric parameters (1 Pa, 200 K, 50 \(\mu\)T, and with a local line of sight and an orientation of the magnetic field that neither favors nor disfavors any particular polarization state by much), I have prepared Figure 3.8 to show the propagation matrix and its associated transmission matrix. Perturbations on temperature and magnetic field are shown as separate plots. This figure, as all figures in this chapter, is mostly conceptual.

The shape of the propagation matrix in Figure 3.8 is the same as in Equation 2.24. In that equation, frequency dependency is implicit though here it is shown explicitly around the central line. The title of the plots describe the atmospheric scenario. The low and high magnetic field and temperature plots have had their parameters changed by 5 \(\mu\)T and 20 K, or 10% respectively, but retains the standard atmospheric scenario in the other parameters. The absorption increases substantially if the magnetic field is zeroed, but a change in magnetic field by 10% is less important for the absorption.

---

Field strength at one layer is probably accompanied by a change in in the magnetic field strength of adjacent layers.
Figure 3.7: Examples of how different Zeeman effect components looks for some molecular oxygen absorption lines in a low pressure, 50 µT and 200 K environment.

than a change by 10% in temperature. The differences are still noticeable in the figure. Increasing either the temperature or the magnetic field strength widens the shape of the frequency distribution, though the change in shape of the frequency distribution of the absorption is not the same. Oppositely but for similar reasons, lowering the temperature or magnetic field strength narrows the shape of the frequency distribution in different ways. The scenario without any magnetic field considered at all is by far the narrowest in frequency. As such its peak absorption is much higher and in this particular scenario it has a transmission of only 4%, whereas the other plots have all around 80% or more transmission. In practice, a layer thickness of 10 km might be too thick for the absorption line experiencing no magnetic field whereas it is more acceptable for absorption lines experiencing the magnetic field.
3.3. Model of Atmospheric Line Absorption

Figure 3.8: The propagation and transmission matrices of the 61.15 GHz molecular oxygen absorption line. The transmission matrix is from \(\exp(-Kr)\) for \(r = 10\) km to enhance the transmission. See the text for details. The example of no magnetic field applies to all absorption lines, though the absorption and thereby the transmission will be numerically higher or lower depending on the line of choice. The Zeeman pattern strongly depends on the line as seen in Figure 3.7. Also note the difference in scale for the propagation matrix marked “No Magnetic Field”.
This chapter briefly describes two applications for the theory and modeling described in previous chapters. The example for Earth is for unpublished work on the retrieval of temperatures up to the top of the mesosphere using a meteorological sensor. The example for Mars expands on the idea of retrieving the crustal magnetic fields from Martian atmospheric molecular oxygen by showing how different polarization components are simulated, with particular focus on circular polarization as this applies to Paper VI.

4.1 Mesospheric Temperature Retrieval

As mentioned in the previous chapter, the Special Sensor Microwave Imager/Sounder (SSMIS; Kunkee et al., 2008; Swadley et al., 2008) measures near the center of molecular oxygen absorption lines. Its observation geometry is at 45° off-nadir, so Figure 3.4 does not give an accurate depiction of what it can observe. The off-nadir geometry means slightly higher altitudes are observed (because absorption increases with the path length), but the channels of SSMIS have a wide frequency distribution, and are not only measuring a single absorption line, so the altitude sensitivity distribution is also wider than in the temperature Jacobian of Figure 3.4.

We (primarily myself and Patrick Eriksson) worked to set up ARTS and Qpack to handle temperature retrievals from SSMIS measurements following up on the model comparison we did for SSMIS in Paper IV. Our goal for now is to be able to derive temperature profiles globally from the top of the troposphere to the top of the mesosphere for the available data. This work is still considered to be in a preliminary stage, but temperature profiles can be retrieved globally. We are at the stage of trying to validate the derived temperature profiles. So far we have found that our profiles are reliable at high latitudes but that results for equatorial latitudes are less good. At equatorial latitudes, the magnetic field is weaker resulting in a more narrow line shape as shown in figure 3 of Paper IV. An offset in the central line frequency in the model, or a drifting local oscillator in the sensor, can therefore cause a large
difference in the brightness temperature near the equator but only a small offset near the (magnetic) poles. The details of this are still pending further investigation. So with the lack of detailed validation in mind, an example of three years of temperature retrievals over Kiruna, Sweden, is included as shown in Figure 4.1.

![Temperature retrievals from SSMIS measurements over Kiruna, Sweden.](image)

Figure 4.1: Temperature retrievals from SSMIS measurements over Kiruna, Sweden. Top row are retrieved temperatures and bottom row is the a priori temperature profiles as based on MSISE-90 (Hedin, 1991). The thin lines at about 12 km and at about 75 km indicate the minimum and the maximum altitudes of a measurement response of over 95%.

These temperature profiles are using SSMIS measurements taken from one satellite. This SSMIS unit takes measurements of the radiation from over Kiruna about four times a day. There are three other satellites in orbit around Earth carrying an SSMIS unit spanning back a decade that we ignore for Figure 4.1. Note that the differences between the retrieved temperature profiles and the a priori temperature profiles range more than 100 K. The a priori profiles differs a lot from the retrieved profiles during the winter, but are more accurate during summer.

That the a priori profiles are less accurate in the winter than in the summer at polar latitudes is somewhat expected and a prime reason to perform temperature retrievals for high altitude measurements. At stratospheric altitudes and above, Kiruna
is sunny all day during the summer season resulting in fairly predictable temperatures. During the winter seasons, however, the dynamics is complicated at stratospheric altitudes. Kiruna is affected by the polar vortex and is located close to the edge of its influence. Temperatures in and around this vortex are very different, and this shows as large variations during winter in Figure 4.1. Another important effect in polar winters is sudden stratospheric warming events. Although rare, when these events do occur they rapidly increase the stratospheric and mesospheric temperatures. The strong increase in temperatures seen around January 2012 in the figure is likely from a sudden stratospheric warming event. Validation is required before more detailed analysis of these profiles than this becomes interesting.

4.2 Mars Crustal Magnetic Field Retrieval

Both Papers V and VI are about retrieving Martian crustal magnetic fields using the Zeeman effect. This section aims to extend the discussion of those papers with an introduction on the choice of polarization. The simulations showed here are based on the same inputs as the simulations in Paper VI for a tangent altitude of 40 km in a region of moderately strong magnetic fields near the Martian equator (the same location as used in the example of figure 3 of Paper VI). Figure 4.2 shows the simulated brightness temperatures around the 368.50 GHz absorption line for some azimuthal angles in the tangent point.

Figure 4.2 gives that the expected brightness temperature should be around 80 K for this particular setup. The linear polarization components are negligibly small, and the circular polarization signal is at about 1% of the full signal as strongest and much weaker far from the line center. That circular polarization is larger than linear polarization is clear from the physics of the Zeeman effect and can be understood from looking at Figure 3.7. Circular polarization is from combining the oppositely signed $\sigma_+ / \sigma_-$ components, and linear polarization is from combining the $\sigma_{\pm}$ and $\pi$ components. Overlap of the components means lower level of polarization, and the least overlap of components happens for oppositely signed $\sigma$ components, since they have their strength split opposite in frequency. In Paper V, we focused on linear polarization because we did not know if the magnetic field was so small-scaled on Mars that a change in angle between the magnetic field and the propagation path of the radiation could cause strong circular depolarization. Paper VI focuses on circular polarization because it turns out that the previous concern had no practical impact given the available knowledge of the magnetic field.

Figure 4.3 shows the magnetic strength Jacobian for the two circular polarization components. The change in sign with altitude shows that there is some depolarization due to changes in the magnetic field orientation throughout the geometry of the transfer. The change in sign at the line center is because circular polarization shifts the weighted line center, and this shift gets larger if the magnetic field strength is increased.
Comparing the magnetic strength Jacobian of Figure 4.3 with the magnetic strength Jacobian of Figure 3.6, the numbers are of similar magnitude. The main differences for Earth to Mars is that the frequency distribution is significantly wider for Earth than for Mars because magnetic field strength is much larger. This means that it is more difficult to retrieve magnetic strength on Mars than on Earth, because if less of the spectra is influenced by the magnetic field strength, then fewer channels of a spectrometer taking a measurement can be used for the retrieval.

Figure 4.3 does not address the concern of finding out the angle between the magnetic field and the propagation path. Switching azimuthal angle by 180° changes left circular polarization into right circular polarization and vice versa. This could be addressed by measuring $V$ rather than the radiation of either of the circular polarization. In Paper VI, we instead set up a measurement scheme to observe a tangent point from multiple directions that efficiently emulates $V$ from the radiation of a single circular polarization. This difference is why Paper VI presents an error analysis for
the different magnetic components rather than for the total magnetic field strength.
Chapter 5

Summaries of Appended Publications and Conclusions

Below follows a summary of the publications included in this doctoral thesis. After this follows a simple concluding remark on the entirety of my work.

5.1 Appended Works

Each of the appended works have been introduced, implicitly or directly, in the preceding chapters. The abstracts of each of the appended works are available just a few pages ahead for more detailed summaries.

5.1.1 Paper I: Zeeman Model in ARTS

The article contains the essential changes made to ARTS to include the Zeeman effect. It briefly compares ARTS and other Earth atmospheric radiative transfer models treating the Zeeman effect. The essence of these differences are that we treat polarization in Stokes formalism in ARTS, and that the full 3D geometry of the atmosphere that was already implemented in ARTS can be used to allow for a magnetic field that changes along the path of the radiation. The article demonstrates the effectiveness of the ARTS Zeeman module by comparing model results with satellite measurements by Odin-SMR, showing a good qualitative agreement between the model and the instrument measurement. The paper itself gives an overview of the Zeeman effect in ARTS, which is complemented by the theory of this “kappa” in Chapter 2 and by the modeling examples of Chapter 3.

5.1.2 Paper II: Extension for Low Altitudes

The original Zeeman effect module implementation did not consider line mixing and so it was limited to use at higher altitudes. There are available models of line
mixing, and modern versions of these were implemented together with the Zeeman effect module and presented in the article. This allows for use of the same propagation model at both high and low altitudes, achieving a desired internal consistency in the propagation model. This paper is a brief note explaining the model extension, which uses the theory under Subsection 2.2.2.5: Line Mixing by Ordered Approximations.

5.1.3 Paper III: Validation by Ground-based Measurements

The ground-based Temperature Radiometer (TEMPERA; Stähli et al., 2013) in Bern, Switzerland, takes measurements of molecular oxygen emissions between 52.4 GHz up to 53.2 GHz. This is in the weakly absorbing part of the molecular oxygen absorption band, which means that the radiation near the center of the covered lines is from Zeeman-affected transitions at high altitude, and that off-center radiation is from lower altitudes. The line we focused on in Paper III is used in example Figure 3.2, and discussed in the connected text. For reasons explained in the work itself and in the theory, the brightness temperature measurements will change as a function of the azimuthal angle of observation because this changes the observed polarization. TEMPERA was set up to take measurements along different azimuthal angles for this study in order to examine the polarization of the Zeeman effect at mesospheric altitudes.

My contribution to this work is with the Zeeman effect module of ARTS. The article found that the simulations with the Zeeman module agree with the change in the measurements found for different azimuthal angles. As far as we know, this is the first time such an agreement has been demonstrated by ground-based instruments, which validates the implementation of the Zeeman effect module and opens up for more detailed research taking such measurements into account, for instance in temperature retrievals in the mesosphere from ground stations.

5.1.4 Paper IV: Model Comparison for SSMIS

In meteorological numerical weather applications, there is a vast volume of data to process. To a large extent, satellite data are directly assimilated into numerical weather forecasting models. In order to cope with the large volume of data produced by different satellites, fast and parametrized radiative transfer models are often used in this process. Met Office uses RTTOV as their radiative transfer model, and in this paper we compare RTTOV with the ARTS Zeeman module for SSMIS. Chapter 4 and Figure 4.1 shows the atmospheric altitudes where SSMIS can be helpful in retrieving temperature profiles.

The comparison shows that the models agree well for the two lower altitude mesospheric channels. The two highest altitude channels had lesser agreements near the equator and mid-latitudes, but agree better closer to the poles. Interestingly, if we reduce ARTS to a two-dimensional magnetic field (where the angles and the magnetic strength are constant throughout the path of the transfer), then the agreements
between ARTS and RTTOV improves a lot. An improvement is expected, since RTTOV uses a two-dimensional magnetic field, however the level of improvement was unexpectedly large.

5.1.5 Paper V: Remote Sensing of Planetary Magnetism

The fifth paper describes a method for detecting Zeeman-polarized lines on Mars, and by this example on other planets, that can used to return information on the strength of the magnetic field. In essence, the described method takes the polarization state of the radiation into account, not as a function of splitting but by relative differences in intensities of perpendicular polarization components.

In addition, the paper identifies the problems of using a single polarization sensor when measuring Zeeman species in an atmosphere that is poorly defined. This is done by showing that a measurement of Mars radiation from Herschel, which leaves a significant residual when fit to the modeled atmosphere, can also be understood as a magnetic residual. However, the residuals in the Herschel measurements are larger than expected if the magnetic field was the primary cause of them.

5.1.6 Paper VI: Martian Magnetism Retrieval Estimations

The last appended work is just submitted and has not undergone peer review yet. It expands on the ideas of Paper V by emulating knowledge of the polarization change of the radiation by the magnetic field through multiple measurements. It simulates these measurements and calculates the expected retrieval errors of the horizontal components of the magnetic field for modern sensor technology. The end of Chapters 4 expands on the ideas of Paper VI by explaining some of the basic design ideas that the paper takes for granted. The paper suggests a method of measurements that can find the horizontal components of the Martian magnetic field at 200 nT certainty at every 4 km of altitude from close to the ground up to around 70 km. As the paper is still under review, I will not discuss it further here.

5.2 Concluding Remarks

My thesis has been about the implementation and some applications of the Zeeman effect in planetary atmospheric radiative transfer. The implementation of a Zeeman effect module in the Atmospheric Radiative Transfer Simulator is presented in Papers I and II. These two works present the mathematical considerations taken in the modeling. This Zeeman module has been applied in Papers III and IV for measuring radiation from Earth’s atmospheric molecular oxygen. We find a good qualitative agreement between simulations and measurements from both ground- and space-borne platforms, with quantitative agreements that are within expected uncertainties. The temperature profiles retrieved in Figure 4.1 deserves mentioning as another application of importance to my thesis, even though the work to validate
these profiles are still underway. Finally, Papers V and VI presents tentative simulations for using the Zeeman effect on Mars molecular oxygen for measurements and quantifications of the magnetic field from crustal sources on Mars. The work for this thesis might in the future help with more systematic retrievals of mesospheric temperatures on Earth, and also to map the crustal magnetic fields of Mars at higher accuracy than today.


References


A treatment of the Zeeman effect using Stokes formalism and its implementation in the Atmospheric Radiative Transfer Simulator (ARTS)

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A treatment of the Zeeman effect using Stokes formalism and its implementation in the Atmospheric Radiative Transfer Simulator (ARTS)

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A R T I C L E   I N F O

Article history:
Received 13 February 2013
Accepted 6 September 2013
Available online 16 September 2013

Keywords:
Zeeman effect
Atmospheric radiative transfer
Polarization
Stokes formalism

A B S T R A C T

This paper presents the practical theory that was used to implement the Zeeman effect using Stokes formalism in the Atmospheric Radiative Transfer Simulator (ARTS). ARTS now treats the Zeeman effect in a general manner for several gas species for all polarizations and takes into account variations in both magnetic and atmospheric fields along a full 3D geometry. We present how Zeeman splitting affects polarization in radiative transfer simulations and find that the effect may be large in Earth settings for polarized receivers in limb observing geometry. We find that not taking a spatially varying magnetic field into account can result in absolute errors in the measurement vector of at least 10 K in Earth magnetic field settings. The paper also presents qualitative tests for O2 lines against previous models (61.15 GHz line) and satellite data from Odin-SMR (487.25 GHz line), and the overall consistency between previous models, satellite data, and the new ARTS Zeeman module seems encouraging.

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1. Introduction

The Zeeman effect [1] occurs when an external magnetic field interacts with a molecule or an atom of total electron spin different from zero. Such an interaction will split an original energy level into several sub-levels [2]. One molecule in the atmosphere of Earth with total electron spin different from zero is O2 for which the Zeeman effect plays a crucial role in radiative transfer in the microwave region at lower pressures [3]. Simplistically, the Zeeman effect can be regarded as several lines shifted from a central frequency with lines polarized in a quasi-symmetric manner around that central frequency. When line broadening parameters are much larger than the frequency shift, Zeeman affected radiative transfer may be physically indistinguishable from non-Zeeman affected radiative transfer. For an early review on the quantum physics of the problem see Hill [4], for a more recent review see Schadee [5] and for a detailed textbook discussion see, e.g., Berestetskii et al. [6] in the Landau and Lifshitz series on theoretical physics. For instructions on determining important parameters for the Zeeman effect see, e.g., Veseth [7] and Christensen and Veseth [8].

There are (at least) two different approaches for polarized radiative transfer simulations. We will call these the coherency formalism and the Stokes formalism, and we...
refer to Appendix A for a short description of these. Lenoir [2,3] was the first to describe the Zeeman effect on radiative transfer for O₂ microwave lines using coherency formalism for the atmosphere of Earth. Lenoir’s approach has been incorporated into models by Rosenkranz and Staelin [9], Hufford and Liebe [10], Pardo et al. [11], von Engeln [12], Schwartz et al. [13], and Han et al. [14], usually to make temperature retrieval for specific instruments possible. Except for von Engeln [12], all of these authors seem to consider the magnetic field as constant in strength and direction throughout the propagation path (a magnetic vector rather than the full magnetic field).

There are data available from instruments with sufficient microwave spectral resolution to observe the Zeeman and direction throughout the propagation path (a magnetic vector). There is a need to consider the magnetic field as constant in strength and direction throughout the propagation path (a magnetic vector). Some works include Rees et al. [17] and Berdyugina and Solanki [18]. The solar physics community uses the Zeeman effect to measure the magnetic field of stars. These measurements are usually done at shorter wavelengths and therefore for a different set of molecules and atoms than those usually considered in radiative transfer in planetary atmospheric sciences.

The Atmospheric Radiative Transfer Simulator (ARTS) [19,20] handles microwave radiative transfer in any atmospheric and weak magnetic field. ARTS operates using Stokes formalism, can operate in full 3D and run simulations on various planets in the solar system. Polarization in the model was previously mainly a product of the ice cloud and surface scattering modules [21,22]. All molecular absorption/emission were assumed to be scalar before the addition of the Zeeman module. Now the Zeeman module may also be used to model the polarized radiative transfer in ARTS. ARTS can be found at http://www.sat.ltu.se/arts/ and is both free of cost and open-source.

We will in this paper describe the implementation of the Zeeman effect in ARTS. This will be done by providing the practical theory of the Zeeman effect using Stokes formalism in Section 2. We will show examples of how ARTS handles O₂ lines in the mesosphere of Earth in Section 3 as well as compare our model with previous models and data. Section 4 contains a short discussion on the results of Section 3, an outlook on what we plan to do with the newly implemented Zeeman module in the future and a short conclusion.

2. Theory

2.1. Introduction

The radiative transfer equation in local thermodynamic equilibrium without scattering is (see, e.g., [23–25] or [26])

\[
\frac{d \vec{T}}{ds} = -\mathbf{K}(\vec{T} - \vec{B}),
\]

where \(\vec{T} = (I, Q, U, V)^T\) is the Stokes measurement vector as defined by, e.g., Eriksson et al. [20], \(s\) is the path, \(\mathbf{K}\) is the propagation matrix and \(\vec{B}\) is the source function, usually \([8, 0, 0, 0]^T\) with \(8\) as the Planck function. Note that other terms are in use in the literature to describe \(\mathbf{K}\). These include, e.g., extinction matrix and absorption matrix. The propagation matrix for a single line of a single species due to attenuation without the Zeeman effect is simply

\[
\mathbf{K}_{i,j,n,m} = a_{i,j,n,m} \mathbf{A}_i,
\]

where \(\mathbf{A}_i\) is the unity matrix, \(a_{i,j,n,m}\) is the line absorption coefficient, \(j\) is the total angular momentum quantum number, \(N\) is the total angular momentum number without spin, \(\nu_s\) denotes the upper level, double prime denotes the lower level of the line transition and \(i\) is the species. The absorption coefficient for a single line of a single species can be calculated from

\[
a_{i,j,n,m}(\nu) = n_i s_{i,j,n,m}(\nu) F(\nu),
\]

where \(n_i\) is the molecular number density of molecule \(i\) in the atmosphere, \(s_{i,j,n,m}\) is the line strength of the \(j \rightarrow j'\) and \(N \rightarrow N'\) transitions, \(F\) is some line shape function and \(\nu\) is the frequency.

2.2. Introducing the Zeeman effect

The equation for the propagation matrix for one \(j \rightarrow j'\) and \(N \rightarrow N'\) line using Stokes formalism in a Zeeman affected case will be

\[
\mathbf{K}_{i,j,n,m}(\nu) = \mathbf{K}_i(\nu) + \mathbf{K}_0(\nu),
\]

where

\[
\mathbf{K}_i(\nu) = \frac{n_i}{2} \sum_{M} s_{i,j,n,m} \sum_{M,M'} \mathbf{S}_{M,M'} F(\nu, \nu_0 + \Delta \nu_0) \mathbf{P}_{M,M'}
\]

is due to attenuation and

\[
\mathbf{K}_0(\nu) = n_i \sum_{M,M'} s_{i,j,n,m} \sum_{M,M'} \mathbf{S}_{M,M'} F(\nu, \nu_0 + \Delta \nu_0) \mathbf{P}_{M,M'}
\]

due to what is called the magneto-optic effect. The terms in the propagation matrix are cumulative, such that for all species and allowed transitions

\[
\mathbf{K}(\nu) = \sum_{j,i,n,m} \mathbf{K}_{i,j,n,m}(\nu).
\]

In Eqs. (4) and (5), \(s_{M,M'}\) is the relative line strength of the Zeeman sub-levels, \(M\) is the projection of \(\vec{J}\) on the magnetic field, \(F_{\nu, \nu_0}\) are line shape functions, \(\nu_0\) is the frequency of the non-Zeeman affected line center, \(\Delta \nu_0\) is the frequency shift due to the Zeeman effect, and \(\mathbf{P}_{M,M'}\) are the polarization rotation matrices using Stokes formalism. The sub-indices \(A\) and \(B\) stand for the attenuation and the magneto-optic effect respectively. The factor \(J\) in Eq. (4), is by the convention that

\[
\sum_{M,M'} s_{M,M'} = 1, \quad \det \left( \sum_{M,M'} \mathbf{P}_{M,M'} \right) = 2, \quad \det \left( \sum_{M,M'} \mathbf{P}_{M,M'} \right) = 0.
\]

The frequency shift, the relative line strength, the polarization rotation matrices and the line shapes will be discussed in Sections 2.3, 2.4, 2.5 and 2.6, respectively.

There are discrete molecular energy levels associated with the combination of quantum numbers \(J\) and \(N\). A transition between two such sets of numbers emits or absorbs radiation with the difference in energy between these levels. Various nomenclature are used in the
literature for the allowed types of transitions. For \( \Delta J = 1, 0, -1 \), Lenior [3] use \( ^N \) whereas the spectroscopic community seems to use \( R, Q, P \) [5]. We will simply use \( \Delta J \) when the change of \( J \) demands reference. For \( \Delta M = 0, \pm 1 \) there seems to be only one accepted notation with \( \pi \) representing \( \Delta M = 0 \) and \( s \) representing \( \Delta M = \pm 1 \). We will conform to this notation system. The angular momentum quantum number \( J \) is limited to \( |N - S| \leq J \leq N + S \) [6], where \( S \) is the total electron spin quantum number.

The projection of the total angular momentum \( \vec{J} \) on the local magnetic field vector \( \vec{H} \) can take the form \( M = -J, -J + 1, \ldots, J - 1, J \) [3]. Transitions of the types \( \Delta J = 0, \pm 1 \) and \( \Delta M = 0, \pm 1 \) are the only allowed transitions, though there exists an exception for the special case of \( \Delta M = 0 \) that is not allowed [6]. An illustration of an example transition is given in Fig. 1 showing the allowed \( \Delta M \) sub-levels.

In practice, databases like, e.g., HITRAN [27,28], AFGL-86 [29] and IGRF-11 [30] can be consulted to find the parameters necessary to describe the Zeeman effect.

### 2.3. Frequency shift

Zeeman splitting refers to the shift in the upper and lower energy levels due to the external magnetic field interacting with the molecule. The energy shift of a level is

\[
\Delta \varepsilon = -g_M \mu_B \varepsilon 
\]  

(8)

where \( H \) is the magnitude of the local magnetic field, \( \mu_B \) is the Bohr magneton and \( g_M \) is the Landé factor [6]. According to Lenior [3] the factor \( g \) is

\[
g = g_S [J(J+1) + SS + 1] - NN(N+1) 
\]  

(9)

where \( g_S \) is a particle dependent constant. Lenior [3] used \( g_s = 2.00232 \), the value for a free electron. It might be helpful to not use this simplification. See Table 1 for constants of \( g_s \) that take relativistic effects and coupling between the spin and the electrons angular momentum into account. We will note here that the difference in \( g_s \) only becomes important for sensors with a very high frequency resolution (i.e. a few kilohertz for Earth conditions).

Since \( J \) is \( N \) for cases when \( S = 0 \), following Eq. (8) it is clear that the Zeeman effect only occurs for molecules with \( S \neq 0 \). It is important to note that Eq. (8) for the level \( J = 0 \) is reduced to \( \Delta \varepsilon = 0 \) but that there is still Zeeman splitting if the other level has \( \Delta \varepsilon = 0 \).

To get the Zeeman affected frequency shift, we have to compute the difference between the change of energy in the upper and lower levels. In other words, we use

\[
\Delta \varepsilon_0 = \frac{\mu_B g_M \varepsilon}{h} (M - g'M')
\]  

(10)

to calculate the frequency shift of each Zeeman sub-level, where \( h \) is the Planck constant [6]. Prime and double prime denote the upper and lower level quantum numbers respectively.

### 2.4. Relative line strength

The relative line strength, \( S_{MM'} \), of the Zeeman sub-levels is found in Schadee [5] but are here renormalized as in Berestetskii et al. [6]. The equations for the relative line strength depending on \( \Delta J \) and \( \Delta M \) can be found in Table 2. We would also like to point out that the relative line strengths of Table 2 agree with Lenior [3] for the special cases presented therein. An example of the relative frequency shift versus the relative line strength for the Zeeman sub-levels can be found in Fig. 2.

![Fig. 1. An example of a Zeeman affected transition that is similar to the transition of the strong O$_2$ 187.95 GHz line. Note that \( \Delta M \) is along \( \vec{H} \) as shown by \( M \) being a projection of \( \vec{J} \) on \( \vec{H} \) in the figure—the implications of this directionality and how it affects polarization is discussed in the text and is also shown in Fig. 3.](image_url)

### Table 1

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the transition with \( \Delta M \) (middle panel) has a larger range of frequency shifts for its sub-levels than orientations 90°. A geometric property.

levels that involve a change in the angular momentum component. See Fig. 3 for a simple visualization of \( \theta \). The latter point is important to explain why, e.g., Rees et al. [17] and Jefferies et al. [31] that describe the attenuating polarization rotation matrix of Eq. (4) that can change all of the Stokes vector components, and that
describe the magneto-optic polarization rotation matrix of Eq. (5) that can only affect the last three of the Stokes vector components. See Fig. 3 for a simple visualization of the polarization vectors and propagation direction vector \( \vec{R} \). Note that the polarization rotation matrix dependencies in show the contribution to the polarization rotation matrix due to the attenuation \( A \) and the magneto-optic effect \( B \), with the indices representing the main contributing Stokes parameter. Eqs. (11) and (12) agree with our intuitive description above, and Eqs. (13) and (14) will rotate the polarization. The latter point is important to explain why, e.g., \( B_1 \), which only affects linear polarization, is said to be from \( V \), which is the circular polarization parameter of the Stokes vector. \( B_1 \) is strongest when \( \vec{R} \) is along \( 90° \), which cancels all other magneto-optic effects and implies that

2.5. Polarization rotation

The polarization induced by the Zeeman effect may be understood from the example of a local magnetic field oriented 90° to the propagation path. Since \( M \) is the projection of \( \vec{J} \) on \( \hat{H} \), it makes intuitive sense that sub-levels that involve a change in the angular momentum \( M \) are associated with linearly polarized radiation in the direction of \( \hat{H} \), and this is indeed the case. As stated in Section 2.4, these sub-levels will account for half of the transition's angular momentum. For this transition but that frequency shift is relative to the largest split of the three examples. We see that the transition with \( \Delta M = 0 \) (lowest panel) has the largest split. We further see that the transition with \( \Delta M = 0 \) and larger \( J \) (middle panel) has a larger range of frequency shifts for its sub-levels than the transition with \( \Delta M = 0 \) and lower \( J \) (upper panel), but that the individual sub-levels are also farther apart for the latter.

According to Berestetskii et al. [6], \( \alpha \) and \( \sigma_\perp \) each account for half of the relative line strength. For this normalization to be consistent with Eqs. (4) and (5) the \( \alpha \) component therefore carry a factor of 3 in Table 2, whereas the \( \sigma_\perp \) components carry a factor of 1 in Table 2. That the factor is twice as large as for the \( \alpha \) component than for the \( \sigma_\perp \) components can, in a simplified manner, be viewed as a geometric property.

Fig. 2. Representation of normalized relative line strength versus relative frequency shift for three different \( O_3 \) transitions. (These are the transitions used for radiative transfer in Figs. 4–7, in the upper panel \( \omega_2 = 118.75 \) GHz, in the middle panel \( \omega_2 = 66.15 \) GHz, and in the lower panel \( \omega_2 = 482.26 \) GHz.) Note that the relative line strength is normalized per transition but that frequency shift is relative to the largest split of the three examples. We see that the transition with \( \Delta M = 0 \) (lowest panel) has the largest split. We further see that the transition with \( \Delta M = 0 \) and larger \( J \) (middle panel) has a larger range of frequency shifts for its sub-levels than the transition with \( \Delta M = 0 \) and lower \( J \) (upper panel), but that the individual sub-levels are also farther apart for the latter.

\[
\Phi_{\alpha \perp} = \begin{bmatrix}
1 - 2 \cos^2 \theta \\
\sin 2 \theta \\
0
\end{bmatrix}
\]

(11)

and

\[
\Phi_{\alpha} = \begin{bmatrix}
- \sin \theta & - \cos \theta \\
0 & \sin \theta
\end{bmatrix}
\]

(12)

describe the attenuating polarization rotation matrix of Eq. (4) that can change all of the Stokes vector components, and that

\[
\Phi_{\alpha \perp} = \begin{bmatrix}
0 & 0 & 0 \\
0 & 0 & 0 \\
- \cos \theta & \sin \theta & 0
\end{bmatrix}
\]

(13)

and

\[
\Phi_{\alpha} = \begin{bmatrix}
0 & 0 & 0 \\
0 & 0 & 0 \\
- \sin \theta & 0 & 0
\end{bmatrix}
\]

(14)

describe the magneto-optic polarization rotation matrix of Eq. (5) that can only affect the last three of the Stokes vector components. See Fig. 3 for a simple visualization of the polarization vectors and propagation direction vector \( \vec{R} \).
the medium acts like a Faraday rotator by allowing one type of circular polarization to traverse the medium faster than the other, causing a phase delay that in turn rotates the linear polarization. Similar phase delays exist for linear polarization, as can be understood from $B_H$ and $B_V$. We offer our own derivation of the polarization matrix for both the attenuation and the magneto-optic effect in Appendix A.

### 2.6. Line shape

It is conventional to define the line shape functions $F_{\alpha}(\nu, \Delta_0 + \Delta \nu)$, where

$$\nu = \frac{\nu_0 + \Delta \nu - \nu}{\Delta \nu}$$

represents the frequency difference from the line center in units of Doppler broadening width ($\Delta_\nu$), and

$$a = \frac{\nu}{4\Delta \nu}$$

represents the ratio between pressure broadening width ($\nu$) and Doppler broadening width. From, e.g., Jefferies et al. [31] and Landi Degl’innocenti [32] we find a developed and an applied theory on the line shapes of the attenuation and the magneto-optic effect. Following their examples, the line shape of attenuation around the central frequency is the Voigt function

$$F_{\alpha}(\nu, 0) = \frac{a}{\pi} \int_{-\infty}^{\infty} \frac{e^{-y^2}}{(\nu - y)^2 + a^2} \, dy$$

and the line shape for the magneto-optic effect around the central frequency is the Faraday-Voigt function

$$F_{\alpha}(\nu, a) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{(\nu - y)e^{-\nu^2}}{(\nu - y)^2 + a^2} \, dy$$

We find from, e.g., Samporna et al. [33] that we can use a renormalized Faddeeva function

$$w(z) = \frac{e^{-z^2}}{\sqrt{\pi}} \int_{-\infty}^{z} e^{-y^2} \, dy,$$

where $z = \nu + i\alpha$ to describe both the line shape functions.

### 3. Model and results

This section will show and discuss the qualitative differences that the ARTS Zeeman module offers for radiative transfer simulations when active. The section will also show qualitative tests of how the ARTS Zeeman module compares to previous models and satellite measurements.

The atmospheres used for all the figures and comparisons herein are from AFGL 1986 [29]. The atmospheres are numerically defined up to 120 km — everything above is ignored and considered vacuum. The only molecule from which lines are considered in our calculations is O$_3$. The magnetic field used is from IGRF-11 [30] and we do not take secular variations into account. We use the algorithm by Zaghloul and Ali [34]$^1$ to estimate a solution to the Faddeeva function in all simulations below.

Radiative intensities presented in this section are all in Rayleigh–Jeans brightness temperature $T_B$. The Stokes formalism as defined by Eriksson et al. [20] implies that $I$ is the total intensity, that the horizontal linear polarization can be read from $I_{1-V}$, vertical linear polarization can be read from $I_{V}$, $-45^\circ$ linear polarization from $I_{-1+U}$, $45^\circ$ linear polarization from $I_{1-U}$ and that the left circular polarization can be read from $I_{1+V}$.

#### 3.1. Properties of the model

A simple comparison between non-$J$ and Zeeman affected radiative transfer for various tangent altitudes above (65 N, 133 E) is shown in Fig. 4. Fig. 4 mainly demonstrates the effect of the Zeeman module in ARTS for one magnetic field, satellite position, viewing direction, atmosphere and so on, and the results are not general. We see that there is almost no difference between non-$J$ and Zeeman affected $I_{1-V}$ brightness temperature $T_B$. Contrary to this, we also see that there is a huge difference between non-$J$ and Zeeman affected $I_{1-Q}$. In other words, it is clear that the Zeeman splitting affects different types of polarization in different ways. Theory states that $-45^\circ$ polarization and $45^\circ$ polarization should give roughly similar resulting $T_B$, and this is indeed the case. For circular polarization there is a distinguishable power skewness to the right of the central frequency for $I_{1-V}$ and to the left of the central frequency for $I_{1+V}$. The asymmetric $T_B$

---

$^1$ Reimplemented in C by Steven G. Johnson under the MIT License (attainable through http://ab-initio.mit.edu/faddeeva).
frequency skewness is to be expected from the quasi-symmetry of circular polarization in $s^7$ due to its mirrored frequency shift and relative line strength.

We think that it is important to note the possibility of varying the local magnetic field vector along the propagation path in ARTS and how this affects radiative transfer as compared to using a non-varying local magnetic field vector, which contrasts the ARTS Zeeman module to the most previous Zeeman capable radiative transfer models.

Fig. 4. Comparison between a Zeeman module and a non-Zeeman module affected line. The direction of $\vec{H}$ at the tangent point is northward and the angle between $\vec{R}$ and $\vec{H}$ is approximately 100°. Frequency shift is given with respect to the O$_2$ 118.75 GHz line. Dashed lines represent the case when the Zeeman effect is ignored and solid lines represent Zeeman affected radiances. This figure is discussed further in the text.

Fig. 5. Tangent point limb sounding radiative transfer model comparison between a varying local magnetic field and a constant local magnetic field $\vec{H}$ from the tangent point. Dashed lines represent the tangent point $\vec{H}$ simulations and solid lines use a full IGRF-11 field. The tangent point of this plot is at (0°N, 0°E) and 80 km. The azimuth angle of $\vec{R}$ at the tangent is given in the legends. Blue approximates $\theta$ at 90° and red approximates 0°. The O$_2$ line is the 118.75 GHz line. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this paper.)

Fig. 6. Qualitative comparison between the implemented model in ARTS (solid lines) and the forward model as used by von Engeln [12] (dotted lines) in mid-latitude summer atmospheric conditions for the $N = N' = J = 9$ and $J' = 10$ line. Different colors indicate different tangent altitudes. There is a qualitative overlap between the models with some differences, likely due to the use of slightly different atmospheres. However, there are very clear differences at 90 and 100 km. It seems that the two models disagree about where the outermost peaks should occur. For more about this figure see the text. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this paper.)

3.2. Qualitative rest results

We have qualitatively compared our model to the simulation results in Fig. 5.6 of von Engeln [12]. The results of this comparison can be found in Fig. 6. We find that our models qualitatively agree well for all but the outermost lines at 90 and 100 km tangent point heights. We do not understand the reason for this discrepancy. Comparing our results with results of another model [10], Fig. 2 of Hartmann et al. [16], however, we find that the consistently concave shape is reproduced in ARTS but not by von Engeln [12]. This second comparison strengthens our belief that the implementation in ARTS is valid.

A qualitative comparison with data from Odin-SMR, see Fig. 7, shows that the implemented Zeeman module more accurately describes the breadth of the line absorption in real sub-millimeter wave limb sounding data than a similar run without the Zeeman module. This qualitative comparison makes it clear that, e.g., temperature retrieval at lower pressures using O$_2$ lines must take the Zeeman effect into account.

4. Summary, conclusions and outlook

This paper has presented a practical approach to the theory of the Zeeman effect in Stokes formalism in the atmospheric sciences. Furthermore, we have presented important features of the implemented ARTS Zeeman module, we have shown that the ARTS Zeeman module see that it is preferable to define $\vec{H}$ as part of a field. Failing to do so may introduce absolute errors in $T_b$ of at least 10 K. During the run described above, the magnetic field in ARTS changed about 1.5 μT in strength, $\theta$ changed with about 11° and $\eta$ changed with about 29°.
constituting a physical meaning. In Stokes formalism the propagation is a real $4 \times 4$-matrix, with each element carrying its own physical meaning. Both formalisms carry many innate symmetries, as is clear from the physics (e.g. polarization rotation), and they of course describe the same physical processes.

To our knowledge the Zeeman effect has so far only been described in terms of coherency formalism in the Earth atmospheric sciences. We therefore think it prudent to show the steps necessary to translate between the coherency formalism and the Stokes formalism for the Zeeman effect. The radiative transfer equation without scattering for local thermodynamic equilibrium using Stokes formalism can be found in Section 2.1 as Eq. (1). Equivalently, the radiative transfer equation using coherency formalism [3] is

$$\frac{dS}{ds} = - \left( GS + SG^\dagger \right) + \left( G + G^\dagger \right) B,$$

(1)

where $G$ is the complex propagation matrix, $S$ is the radiative coherency matrix containing information equivalent to that in the Stokes vector, and $B$ is the Plank function. Note that $\dagger$ symbolizes the complex transpose.

From Lenior [3], we find that the propagation matrix is $G_m = A_m + iB_m$, where the subindex $m$ denotes a local magnetic field vector coordinate system throughout this section. These coherency matrices are

$$A_m = \begin{bmatrix} A_1 & iA_2 \\ -iA_1 & A_2 \end{bmatrix} \text{ and } iB_m = \begin{bmatrix} B_1 & B_2 \\ -B_1 & iB_2 \end{bmatrix},$$

where $A_m$ is the attenuation matrix that is Hermitian ($A_m = A_m^\dagger$) and $iB_m$ is the magneto-optic effect matrix that is anti-Hermitian ($iB_m = -iB_m^\dagger$). The attenuation matrices for $\sigma$ and $\sigma_2$ can be found in Lenior [3]. Due to how we have defined $A_m$ and $B_m$ above, if the values in $A_m$ and $B_m$ only depend on $\nu$ (see Fig. 3) then $A_m = f(\nu) B_m^\dagger$, where $f(\nu)$ is real ($A_m$ and $B_m$ remain similar in form but their effective values follows separate functions of frequency). Note that $*$ represents the element-wise conjugate. We will treat the attenuation and the magneto-optic effect separately in the derivation below.

The transformation from coherency formalism to Stokes formalism ($S \Rightarrow \mathbb{S}$) is

$$S = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \Rightarrow \mathbb{S} = \begin{bmatrix} S_{11} + S_{22} \\ S_{11} - S_{22} \\ 2S_{12} \\ 2(S_{21} - S_{12}) \end{bmatrix},$$

(2)

where the components are in energy and not amplitude of the wave (see, e.g. Mishchenko et al. [25] and von Engeln [12] to find these definitions). When looking in more detail at this transformation it becomes clear that

$$S = a_1 I + a_2 Q + a_3 U + a_4 V$$

(3)

where

$$a_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad a_2 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad a_3 = \begin{bmatrix} 1 & \ast \\ -\ast & 1 \end{bmatrix}.$$
form a given complex coherency propagation matrix, $G_n$, into the Stokes propagation matrix, $K_m$, of Eq. (1). We see that this is equivalent to stating that

$$G_n \cdot S \cdot G_n^t = K_m \cdot \bar{T},$$

which can be divided into two parts, the attenuation

$$A_n \cdot S \cdot \Delta \alpha_m = K_{a,m} \cdot \bar{T}$$

and the magneto-optic effect

$$i(B_n \cdot S - B_m) = K_{e,m} \cdot \bar{T},$$

where it is clear that $K_m = K_{a,m} + K_{e,m}$ and we must remember that $K_m$ is always real but $G_n$ is not always real. It is quite tedious, but straightforward, to use Eq. (A.3) to solve the above expressions for $K_m$. We get the attenuation propagation matrix

$$K_{a,m} = \begin{bmatrix} A_1 + A_2 & A_1 - A_2 & 0 & 2A_3 \\ A_1 - A_2 & A_1 + A_2 & 0 & 0 \\ 0 & 0 & A_1 + A_2 & 0 \\ 2A_3 & 0 & 0 & A_1 + A_2 \end{bmatrix}$$

(A.4)

and the magneto-optic effect matrix

$$K_{e,m} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 2B_1 & 0 \\ 0 & -2B_1 & 0 & -B_1 + B_2 \\ 0 & 0 & B_1 - B_2 & 0 \end{bmatrix}$$

(A.5)

The above expressions assume that the main axis is determined from the local magnetic field vector rather than from an external sensor. This is quite inconvenient from a modeling standpoint as it makes linear polarization difficult to track along the propagation path. It is therefore necessary to rotate Eq. (1) from the local magnetic field vector coordinate system to a sensor dependent coordinate system using

$$L \cdot \bar{T} = K_m \cdot \bar{T} \cdot L^{-1} = K_m \cdot L^{-1} \cdot B,$$

where $L$ is the same as in Fig. 3. The above notations ensure that $K_m$ acts in the magnetic coordinate system on $\bar{T}_n = L^{-1} \cdot \bar{T}$, and that the result $d'_{\bar{T}_n} = L^{-1} \cdot d'_{\bar{T}}$ also acts in the magnetic coordinate system. The propagation matrix we use in ARTS to always remain in the sensor determined coordinate system is thus derived from Eq. (A.6). We get that

$$K = L \cdot K_m \cdot L^{-1},$$

(A.8)

with $K_m = K_{a,m} + K_{e,m}$ as above.

References


A note on modelling of the oxygen spectral cross-section in the Atmospheric Radiative Transfer Simulator – Zeeman effect combined with line mixing in the Earth’s atmosphere

Authors:
R. Larsson

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A note on modelling of the oxygen spectral cross-section in the
Atmospheric Radiative Transfer Simulator – Zeeman effect combined
with line mixing in the Earth’s atmosphere

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(Received 18 July 2013; accepted 21 April 2014)

A new module to the Atmospheric Radiative Transfer Simulator is presented that
models the strong oxygen spectral band at 60 GHz. The module handles the line
mixing effect and works with or without additionally calculating the Zeeman effect. It
is shown how the module may be internally reduced to calculations of the Zeeman
effect at higher altitudes, and to calculations of the line mixing effect at lower altitudes.
The article ends with a short discussion on what is being done to validate the module,
and what may be done to refine the theoretical description of line mixing in the
simulator.

1. Introduction

In analysis of remote-sensing data, from both ground-based and satellite-based sensors, a
common approach to retrieve the atmospheric state is to emulate the observation in a
model, adopting the atmospheric state that produces the best fit between observation and
model as the retrieved state. In order to simulate observations well, such a model is
required to handle a wide range of physics, including, e.g., sensor specific setups,
representing atmospheric states adaptively, and being able to simulate relevant species’
spectral properties. This work focuses on the last point and, specifically, on how to
represent the oxygen spectral cross section of the strong 60 GHz band. The goal is to
allow simulations of the fully polarized oxygen spectra, regardless of observation geo-
metries in the Earth’s atmosphere.

Calculations of the oxygen spectral cross-section in the Earth’s atmosphere is quite a
complicated task. At higher altitude, the Zeeman effect becomes evident and magnetic
corrections are necessary on a line-by-line basis (Lenoir 1967, 1968). At lower altitude,
pressure corrections due to the line mixing effect are equally necessary for the entire band
(Baranger 1958; Fano 1963; Ben-Reuven 1966). In order to account for both regions, we
need a method that allows the pressure corrections to be void at high altitudes, and also
makes the magnetic corrections void at lower altitudes. This method should preferably be
continuous in the intermediate region to allow for better retrievals and reduce the risk of
biases in the model.

Several models work to address these issues. One well known model is from Liebe
(1981). In this model, the atmosphere is divided in two parts: the pressure region and the
magnetic region. These regions are treated differently to speed up calculations. Essentially, Liebe (1981) parameterizes the most important components of the lines to
estimate the spectrum in the respective regions. Another well-known model is from Rosenkranz and Staelin (1988). These authors consider the addition of phase to the problem of radiative transfer, and how calculations of the Zeeman effect cannot be done by scalar approximations because of the phase. The line shape in their work is a modified Lorentz function that adopts a modified broadening width to account for the Doppler broadening. The line shape of this work may then be modified by first-order line mixing according to Rosenkranz (1988). A couple of more recent models are presented in the work by Schwartz, Read, and Van Snyder (2006), made to analyse observation from the Microwave Limb Sounder, and in the work by Han et al. (2007) for fast estimations of observations by the Special Sensor Microwave Imager/Sounder. The above models are all similar to how the Zeeman effect and line mixing calculations are now done in the Atmospheric Radiative Transfer Simulator (ARTS). The main differences are that ARTS uses the Stokes vector rather than the complex intensity matrix as its theoretical basis for polarization, that the ARTS line mixing module uses the updated methodology presented by Makarov, Tretyakov, and Rosenkranz (2011), and that the ARTS Zeeman module is generalized to more oxygen transitions by using the work done by Schadee (1978). Another difference is the broad set of modules available for specialized simulations.

ARTS was released by Buehler et al. (2005), together with readily available tools to retrieve atmospheric parameters from e.g. satellite measurements by Eriksson, Jiménez, and Buehler (2005). At its release, the simulator handled line-by-line calculations and had the option to add continuum models (Kuhn et al. 2002), as well as simple cloud models (Sreerekha, Buehler, and Emde 2002). The code is written intentionally modular to easily allow for new and varied applications. For instance, building on the initial version, modules to handle particle scattering (Emde et al. 2004; Davis, Emde, and Harwood 2005), and work to efficiently model sensors (Eriksson et al. 2006) were also made available. The current official release is version 2.0 (Eriksson et al. 2011), which includes a module for faster absorption calculations (Buehler, Eriksson, and Lemke 2011), as well as the previously mentioned modules. These stable versions of ARTS have been extensively used for active retrievals, and for more experimental work (see e.g. Golchert et al. 2005; Buehler et al. 2006; Davis et al. 2007; Harlow 2007; Pietranera et al. 2007; Sreerekha et al. 2008; Rydberg et al. 2009; Kottayil et al. 2012; Jiménez et al. 2013). The development of ARTS is still moving forward with several generalizations to allow for simulations of atmospheres other than the Earth’s (Rezac and Mendrok 2012), as well as the newly included Zeeman module (Larsson et al. 2014). ARTS is both free of cost and an open source. It can be accessed from http://www.sat.ltu.se/arts/.

A new ARTS module, which calculates line mixing on the fly, and its compatibility with the Zeeman effect is described and discussed in the following sections.

2. Theory

2.1. General background

The classical way to model line-by-line atmospheric radiative transfer is to assume that polarization effects are negligible and that the atmosphere is homogeneous for sufficiently thin layers. It is under these conditions that it is possible to solve the one-dimensional scalar radiative transfer equation,

$$\frac{df}{dr} = -\alpha(I - B),$$  \hspace{1cm} (1)
for the outgoing radiation in one dimension, by knowing the incoming radiation. This solution is

\[ I_1 = I_0 \exp(-ar) + B[1 - \exp(-ar)]. \] (2)

In the equations above, \( I \) is the intensity of the radiation at any point along the one-dimensional distance vector \( r \), \( \alpha \) is the absorption of the atmosphere, and \( B \) is the Planck emission from the atmosphere. Indices ‘0’ and ‘1’ refer, respectively, to the incoming and outgoing radiations. The assumption of homogeneity in the layer of the atmosphere along the one-dimensional path means that both \( \alpha \) and \( B \) are constants in the last equation. For more details on how the above equations are treated in ARTS see the description by Buehler et al. (2005). For inhomogeneous media, e.g. clouds, Eriksson et al. (2011) and sources therein describe how the above equations are altered in ARTS.

Allowing for the full Stokes vector does not alter the basic setup but accounts for polarization. The transfer equation simply becomes vectorized (see e.g. Del Toro Iniesta 2003),

\[ \frac{\partial I}{\partial r} = -K(I - B), \] (3)

where \( K \) is the 4 \times 4 propagation matrix, \( I = [I, Q, U, V]^T \) is the Stokes vector as defined by Eriksson et al. (2011), and \( B = [B, 0, 0, 0]^T \) is the vectorized Planck emission. The fully polarized equivalent of Equation (2) then reads

\[ I_1 = \exp(-Kr)I_0 + [1 - \exp(-Kr)]B, \] (4)

where \( I \) is the 4 \times 4 identity matrix. Note that both setups are allowed in ARTS, depending on the computational time and case of interest for the user. However, in order to compute the Zeeman effect it is necessary to use the vectorized equation.

The remainder of this work will focus on the spectral line shape model necessary to compute \( K \), which can itself be found by adding every line’s contribution together

\[ K = \sum_I n_g S_I \times \left\{ \frac{1}{2} \sum_{M'} \left[ S_M, M' \cdot F_A(v, v_I + \Delta v_z) \Phi_A(r, H) \right] \\
+ \sum_{M', \ell} \left[ S_M, M' \cdot F_B(v, v_I + \Delta v_z) \Phi_B(r, H) \right] \right\}, \] (5)

where \( I \) is a line, \( n_g \) is the number of molecules of the gas, \( S_I \) is the strength of the line, \( M \) is the projection of \( J \) along the magnetic field (\( J \) is the total angular momentum number including spin), \( S_{M, M'} \) is the relative strength of a split Zeeman line, \( F_A \) is the line shape of the attenuating part of the refractive index, \( v \) is the frequency, \( v_I \) is the central frequency of the line, \( \Delta v_z \) is the frequency shift of one Zeeman line, \( r \) is the propagation direction vector, \( H \) is the magnetic field vector, \( \Phi_A \) is the polarizing influence of the attenuation, \( F_B \) is the line shape of the phase changing part of the refractive index, and \( \Phi_B \) is the polarizing influence of the phase. This equation is explained in detail in another work (Larsson et al. 2014). The necessary input for the above equation can be found in the
works of Rothman et al. (2005, 2009), Christensen and Veseth (1978), Anderson et al. (1986), and Finlay et al. (2010). Note that if the ARTS Zeeman module is not in use, then $K$ is reduced to $\sum_i \left[n_a S_i F_i(v, v_i)\right]$ 1 in the simulator.

2.2. Line mixing line shape

The implemented line shape can be found by rewriting the line shape in Makarov, Tretyakov, and Rosenkranz (2011) to account for the Doppler broadening as

$$F(z) = F_A + iF_B = \left(1 + gp^2 - iy_p\right) \ w(z),$$

where $g_l$ is a second-order line shape correction, $y_l$ is a first-order phase correction, $p$ is the pressure, and the Faddeeva function

$$w(z) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\exp(-y^2)}{z-y} dy,$$

with $z = v' + ia$,

$$v' = \frac{v - v_l - \Delta v_\omega - \delta v p^2}{\Delta v_D}, \quad a = \frac{\Delta v_p}{\Delta v_D},$$

where $\delta v_l$ is the second-order frequency correction, $\Delta v_D$ is the Doppler broadening half width, and $\Delta v_p$ is the pressure broadening half width. Note that the work by Makarov, Tretyakov, and Rosenkranz (2011) does not directly address what happens with the imaginary part of Equation (6). This led to the adoption of $F_B = \Re[w(z)]$ in ARTS, where $\Re$ denotes the imaginary part.

The real part of the Faddeeva function is the Voigt shape function that describes the imaginary part of the refractive index around a line as a convolution of the Lorentz function and the Doppler broadening function (see e.g. Sampoorna, Nagendra, and Frisch 2007). The imaginary part of the Faddeeva function is the Faraday–Voigt shape function that describes the real part of the refractive index around a line (see e.g. Jefferies, Lites, and Skumanich 1989). These shapes are necessary to describe both line mixing and the Zeeman effect. Hence, to follow the idea of a full spectral model for the strong 60 GHz oxygen band, solid – and preferably fast – calculations of the Faddeeva function is a necessity. There exists a plenitude of suggested solutions to compute the Faddeeva function, including the works by e.g. Humlíček (1982), Wells (1999), and Zaghloul and Ali (2011). An implementation of the last of these solutions is included in ARTS.

As the Voigt shape function reduces to the Doppler broadening function for low pressures, and to the Lorentz function at high pressures, it already partly constitutes a solution to an internally consistent line shape function at high and low pressures. What is then needed is just to show that both line mixing and Zeeman splitting are clearly dominant at their respective regions.

It turns out to be a straightforward theoretical exercise to show this reductive property of the line shape of Equation (6). The line mixing parameters are all pressure dependent so that these disappear at low pressures; i.e. when $p \to 0$ in Equations (6) and (8), $\delta v p^2 \to 0$, $gp^2 \to 0$, and $iy_p \to 0$. It is, thus, seen that the line shape is reduced to the Faddeeva
function without any pressure corrections as \( p \to 0 \), and it follows that the calculations are purely of the Zeeman effect.

As mentioned, at high pressures the Faddeeva function reduces to the Lorentz shape function, such that the attenuating part of Equation (6) is

\[
F_A \approx \frac{(1 + g(p^2))\Delta \nu_p}{(v - v_l - \Delta \nu_z - \delta \nu p^2)^3 + \Delta \nu_p^2} + y_p \frac{v - v_l - \Delta \nu_z - \delta \nu p^2}{(v - v_l - \Delta \nu_z - \delta \nu p^2)^2 + \Delta \nu_p^2}.
\]

Because \( \Delta \nu_p \gg \Delta \nu_z \) at high pressures, it can safely be said that \( \Delta \nu_z \) is insignificant compared to \( v_l \) to the shape. All Zeeman split lines are at approximately the same relative frequency, and thus it follows that the calculations are purely of the line mixing effect.

3. Results

Some simple demonstrative plots showing the transition of influence on the diagonal element of \( K \) between the line mixing effect and the Zeeman effect can be found in Figure 1(a)–(c). These plots show the full theory of Equation (6) by tracking the Zeeman

![Figure 1](image-url)

Figure 1. Demonstration of the transition between line mixing and Zeeman dominant pressure regions for the diagonal element of the propagation matrix. These plots were generated from ARTS using the Tropical scenario by Anderson et al. (1986) for a simulated downward looking satellite sensor above \((0°, 0°)\). In all three subplots, the blue line is generated using both Zeeman and line mixing modules in ARTS, the pink line is generated using only the line mixing module, the red line is generated using only the Zeeman module, and the green line is generated using pure line-by-line calculations. The pressure in the descending order in these plots are around 50, 500, and 5000 Pa.
effect at low pressure \((p \leq 50 \text{ Pa})\), by overlapping the line mixing and Zeeman effect at intermediate pressures \((p \approx 500 \text{ Pa})\), and by tracking the line mixing effect at high pressure \((p \geq 5000 \text{ Pa})\).

4. Discussion and conclusions

The short theoretical explanation above shows that ARTS, with an internally consistent method to calculate the 60 GHz band spectral cross section, now handles both high and low pressure conditions without special care for the intermediate pressures. This is demonstrated by Figure 1. The method uses a more modern approach to line mixing than the commonly used first-order correction (see e.g. Liebe, Rosenkranz, and Hufford 1992; Tretyakov et al. 2005) at high pressure, and at low pressure the method calculates the highly resolved and polarized spectra associated with the Zeeman effect. Due to the modularity of ARTS, the user may select to calculate only one of the effects if fastness of calculations is necessary. However, some questions remain open to study.

First and foremost is the question of validation. One of the applications to verify the model is to work with retrieved Odin-SMR (Murtagh et al. 2002) data in limb sounding of oxygen. Another potential application is to work with data from the instrument presented by Stähli et al. (2013) in order to retrieve atmospheric parameters for two lines around 53 GHz. In both applications first results are promising, but the modelling works are in such an early stage that no conclusion on the model validity can be drawn at this moment.

Another problem is that the method is not easily generalized to other gases that experience line mixing, to the parameterization of other line databases, and to the atmospheres of other planets than Earth. As explained in e.g. the work by Tretyakov et al. (2005), the first-order method is parameterized differently for different background atmospheres since pressure broadening of a single line is a function of the other atmospheric species. This problem also holds true for the second-order method. There exist more general methods. One example is the Energy-Corrected Sudden (ECS) method described by Rodrigues et al. (1999) for several CO\(_2\) bands, and by Makarov, Tretyakov, and Boulet (2013) for the 60 GHz O\(_2\) band. ECS is currently under consideration for implementation in ARTS to offer comparison with the second-order line mixing method, and hopefully allow line mixing to be modelled more readily at other planets. There are some problems facing its full implementation, including how to make the calculations fast and how to let it reduce to modelling the Zeeman effect at low pressure. The advantages of this method is that it is closer to the theory presented by e.g. Ben-Reuven (1966). Because of this, it is the hope of the author that using ECS with the renormalization procedure of Niro, Boulet, and Hartmann (2004) will make the method more easily adaptable to simulations of different planetary atmospheres than the ordered correction methods.

Acknowledgements

I am thankful to the greater ARTS community for development and distribution of the model.

References


Zeeman effect in atmospheric $O_2$
measured by ground-based
microwave radiometry

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Zeeman effect in atmospheric O2 measured by ground-based microwave radiometry

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Received: 18 November 2014 – Published in Atmos. Meas. Tech. Discuss.: 5 January 2015
Revised: 19 March 2015 – Accepted: 7 April 2015 – Published: 23 April 2015

Abstract. In this work we study the Zeeman effect on stratospheric O2 using ground-based microwave radiometer measurements. The interaction of the Earth magnetic field with the oxygen dipole leads to a splitting of O2 energy states, which polarizes the emission spectra. A special campaign was carried out in order to measure this effect in the oxygen emission line centered at 53.07 GHz. Both a fixed and a rotating mirror were incorporated into the TEMPERA (TEMPERature RAdiometer) in order to be able to measure under different observational angles. This new configuration allowed us to change the angle between the observational path and the Earth magnetic field direction. Moreover, a high-resolution spectrometer (1 kHz) was used in order to measure for the first time the polarization state of the radiation due to the Zeeman effect in the main isotopologue from ground-based microwave measurements. The measured spectra showed a clear polarized signature when the observational angles were changed, evidencing the Zeeman effect in the oxygen molecule. In addition, simulations carried out with the Atmospheric Radiative Transfer Simulator (ARTS) allowed us to verify the microwave measurements showing a very good agreement between model and measurements. The results suggest some interesting new aspects for research of the upper atmosphere.

1 Introduction

The Zeeman effect is a phenomenon which occurs when an external magnetic field interacts with a molecule or an atom of total electron spin different from 0. Such an interaction will split an original energy level into several sub-levels (Lenoir, 1967). In the atmosphere, oxygen is an abundant molecule which in its ground electronic state has a permanent magnetic dipole moment coming from two parallel electron spins. The interaction of the magnetic dipole moment with the Earth magnetic field leads to a Zeeman splitting of the O2 rotational transitions. In this state, each rotational level with quantum number \( N \) is split into three levels of total quantum number \( J(J+1) \) following a Hund’s coupling case (Pardo et al., 1995). This effect was studied by Gautier (1967) and Lenoir (1967, 1968) in the 60 GHz band of the main isotopologue \(^{16}\text{O}_2\). It is established, from these works, that the Earth’s magnetic field splits the different Zeeman components over a range of a few megahertz around the center of each rotational line. The shape of each component is governed by a pressure broadening mechanism up to 60 km of altitude and by a Doppler mechanism above (Pardo et al., 1995).

Zeeman splitting of millimeter-wavelength emissions of oxygen molecules must be taken into account for altitudes above 45 km in the terrestrial atmosphere when modeling the radiative transfer of these molecules. Temperature soundings of the atmosphere at high altitudes are not possible without including this effect (Von Engeln et al., 1998; Von Engeln and Buehler, 2002; Stähli et al., 2013; Shvetsov et al., 2010).
The observation of this effect for $^{16}$O has also been possible from satellite measurements. Hartmann et al. (1996) observed the Zeeman broadening of the oxygen emission line of the $9^+$ line in the 61.1509 ± 0.062 GHz frequency range using the Millimeter-Wave Atmospheric Sounder on the NASA space shuttle during the ATLAS missions. Comparison of satellite measurements and radiative transfer models including the Zeeman effect have also been addressed (Han et al., 2007, 2010; Schwartz et al., 2006). Han et al. (2007) used spectral passband measurements from the Special Sensor Microwave Imager/Sounder (SSMIS) on board the Defense Meteorology Satellite Program F-16 satellite to measure the oxygen magnetic dipole transitions ($7^+, 9^+, 15^+$, and $17^+$; Rosenkranz, 1993). These measurements were used to validate a fast model developed from the radiative transfer model of Rosenkranz and Staelin (1988). Moreover, the measurements were also used together with data from the Microwave Limb Sounder (MLS) on board the Aura spacecraft for assimilation in a numerical weather prediction (NWP) model (Hoppel et al., 2013). Schwartz et al. (2006) also reported a comparison of another radiative transfer model with measurements of the 118 GHz oxygen line from MLS.

In this work we present an experiment in which the Zeeman broadening of the oxygen emission line at 53.0669 GHz is observed and the polarization state of the radiation due to this effect is detected for the first time using a ground-based microwave radiometer.

The measurements were possible using a fast Fourier transform (FFT) spectrometer with 1 GHz of bandwidth to measure the whole oxygen emission line centered at 53.07 GHz and a narrow spectrometer (4 MHz) to measure the center of the line with a very high resolution (1 kHz). These measurements have been compared to a model which includes the Zeeman-splitting effect. The incorporation of this effect to the forward model will allow extension to the temperature retrievals beyond 50 km. This improvement in the forward model will be very useful for the assimilation of brightness temperatures in NWP models. It is also important to note that ground-based measurements of the atmosphere with good temporal resolution complement satellite measurements, which are temporally limited by their satellite’s orbital parameters.

The paper is organized as follows: in Sect. 2, the instrumentation and the measurements are briefly outlined. The Zeeman effect theory and the modeling are presented in Sect. 3. Section 4 presents the results of this study. Firstly the simulations using a model are addressed and secondly the tropospheric correction performed to the radiometer measurements and the results obtained during this campaign are presented. Finally, the conclusions are given in Sect. 5.

2 Instrumentation and measurements

The TEMPERA (TEMPERature RAdiometer) radiometer is a microwave radiometer that provides temperature profiles from the ground to around 50 km (Stähli et al., 2013). This is the first microwave radiometer that measures temperature in the troposphere and stratosphere at the same time. The instrument is a heterodyne receiver at a frequency range of 51–57 GHz. Figure 1 shows a picture of TEMPERA, which is operated in a temperature-stabilized laboratory in the ExWi building of the University of Bern (Bern, Switzerland; 575 m above sea level; 46.95° N, 7.44° E). In this lab a styrofoam window allows views of the atmosphere over the zenith angle range from 30 to 70°. The instrument mainly consists of three parts: the front end to collect and detect the microwave radiation and two back ends consisting of a filter bank and a digital FFT spectrometer for the spectral analysis. The radiation is directed into the corrugated horn antenna using an off-axis parabolic mirror. The antenna beam has a half power beam width (HPBW) of 4°. The signal is then amplified and downconverted to an intermediate frequency for further spectral analysis. A noise diode in combination with an ambient hot load is used for calibration in each measurement cycle. The noise diode is calibrated regularly (about once a month) using a cold load (liquid nitrogen) and a hot load (ambient). The receiver noise temperature $T_N$ is in the range from 475 to 665 K. More details about the calibration with TEMPERA can be found in Stähli et al. (2013).

For tropospheric measurements the instrument uses a filter bank with four channels. By switching the local oscillator frequency with a synthesizer, it is possible to measure at 12 frequencies. In this way TEMPERA covers uniformly the range from 51 to 57 GHz at positions between the emission lines. Tropospheric retrievals are not addressed in this paper and more details about this measurement mode can be found in Stähli et al. (2013) and Navas-Guzmán et al. (2014).

The second back end is used for stratospheric measurements and contains a digital FFT spectrometer (Acqiris AC240) for the two emission lines centered at 52.5424 and 53.0669 GHz. The FFT spectrometer measures the two emission lines with a resolution of 30.5 kHz and a bandwidth of 960 MHz. The receiver noise temperature $T_N$ for the receiver–spectrometer combination is around 480 K. An overview of the technical specifications is given in Table 1. An example of FFT measurements is shown in Fig. 2 (upper panel). This figure shows the brightness temperature on
Table 1. Specifications of TEMPERA.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optical system</td>
<td>Corrugated horn antenna with parabolic mirror, HPBW = 4°</td>
</tr>
<tr>
<td>Receiver type</td>
<td>Uncooled heterodyne receiver, filter bank; digital FFT spectrometer</td>
</tr>
<tr>
<td>RF frequency range</td>
<td>Filter bank: 51–57 GHz, FFT spectrometer: 52.4–53.2 GHz</td>
</tr>
<tr>
<td>Receiver operation</td>
<td>Single sideband mode</td>
</tr>
<tr>
<td>Receiver noise temperature</td>
<td>475–665 K</td>
</tr>
<tr>
<td>Filter bank</td>
<td>Four filters, bandwidth 250 MHz and 1 GHz</td>
</tr>
<tr>
<td>FFT spectrometer</td>
<td>Bandwidth 1 GHz, resolution 30.5 kHz, 32 768 channels</td>
</tr>
<tr>
<td>Mixer (FFT back end)</td>
<td>I/Q</td>
</tr>
<tr>
<td>Calibration</td>
<td>Hot load, noise diode</td>
</tr>
</tbody>
</table>

Figure 1. TEMPERA at the laboratory at ExWi, Bern (Switzerland).

16 January of 2012 for the oxygen emission line centered at 53.07 GHz. The red box indicates the influence of the Zeeman effect by the broadened line shape in the center with a kind of a plateau (round line shape around the line center: ±1 MHz).

A second spectrometer was installed in TEMPERA in order to measure with a higher resolution the narrow spectral region where a broadening in the oxygen emission line is produced due to the Zeeman effect. This narrow-band software defined ratio (SDR) spectrometer consists of 4096 channels which cover a bandwidth of 4 MHz with a resolution of 1 kHz. An example of a monthly mean brightness temperature spectrum centered at 53.07 GHz measured with the SDR spectrometer is shown in Fig. 2 (lower panel).

Moreover, a set of two auxiliary mirrors was installed on the roof of the ExWi building in the University of Bern (Fig. 3). A rotating mirror allows one to observe the atmosphere under different azimuth angles and with a fixed elevation angle, while the fixed mirror directs the radiation from the rotating mirror into TEMPERA radiometer.
main goal of using these auxiliary mirrors is to measure the Zeeman-broadened oxygen line under different angles relative to the Earth’s magnetic field.

A special campaign was carried out in autumn of 2013 in order to detect the Zeeman effect with TEMPERA. Three months of measurements (September–November 2013) were performed using these auxiliary mirrors and the SDR spectrometer. A special measurement cycle was designed for TEMPERA during this period. Periodic cycles of almost 5 min were performed. This whole cycle consisted of 13 subcycles, each one starting with a hot load calibration in combination with a noise diode for 10 s followed by other 10 s of atmospheric measurements in one azimuth direction. A total of 13 azimuth angles were scanned ranging from 71.5 to 191° in steps of 10° during the whole cycle. The elevation angle was fixed at 60° during all the measurements since it was found as the angle at which the intensity of the emission lines was highest (Stähli et al., 2013).

Figure 3. Secondary mirror installed on the roof of the ExWi building at the University of Bern.

3 Zeeman effect theory and modeling

3.1 Theory

The Zeeman effect (Zeeman, 1897) occurs because the spin of unpaired electrons couples to the external magnetic field, changing the internal energy of the molecule. A transition between two of these altered energy levels can change the frequency dependence of the absorption spectrum. The Zeeman energy change is calculated by

\[ \Delta E = -g \mu_B M |H|_z, \]

where \( g \) depends on the line and molecule (see, e.g., Christophersen and Veseth (1978) for molecular oxygen), \( \mu_B \) is the Bohr magneton, and \( M(J_J) \) is the projection of \( J \) on the magnetic field.

The quantum numbers necessary can be found in most databases, e.g., HITRAN (Rothman et al., 2013). There are \( 2J + 1 \) possible \( M \) for a state level (these are \( M = -J, -J+1, \ldots, J \)), and \( M \) can only change by 0 or ±1. A transition without changing the value of \( M \) is called a \( \pi \) transition, and a transition with changing \( M \) is called a \( \sigma \) transition. The total line strength is not altered by the effect but will be distributed among the new lines. Each line “produced” by this procedure then undergoes the same broadening mechanisms (thermal and pressure) to create the absorption spectrum.

In addition to splitting the line, the change in energy level depends on the direction of the magnetic field and the propagation path of the radiation, which means that the absorption also depends on the polarization of the radiation. The main polarization occurs along the magnetic field in the plane perpendicular to the propagating radiation. If \( H \) is entirely in this plane, then the radiation will be linearly polarized along \( H \) for \( \sigma \) transitions and linearly polarized perpendicular to \( H \) for \( \pi \) transitions. If \( H \) is parallel/anti-parallel to the path of the propagating radiation, then the \( \sigma \) and \( \pi \) transitions will circularly polarize the radiation in opposite ways, and \( \pi \) transitions do not affect the radiation at all. The polarization effect will generally scale between the two cases above as a function of the angle that \( H \) forms with the direction of the propagating radiation.

3.2 Modeling

The first official release of the Atmospheric Radiative Transfer Simulator (ARTS) was by Buehler et al. (2005) as a flexible/modular code base for radiative transfer simulations. Since then, ARTS has been under continual development. One key release is version 2.0 by Eriksson et al. (2011), which describes the ARTS scripting potential and a few of the modules. Presently, ARTS is at version 2.2; the latest version includes, among other new features, a module that calculates the Zeeman effect presented by Larsson et al. (2014).

In short, ARTS calculates each of the three polarization components individually before adding their absorption contributions to a Stokes vector propagation matrix. The polarization of the radiation is internally kept in a universal coordinate system defined by the sensor through all of the propagation. The line shape should return both its imaginary and real part to account for dispersion-caused polarization rotation. The input magnetic field is either static or three 3-D-gridded fields, one field for each coordinate: \( x \), \( y \), and \( z \). This propagation matrix is then sent to the radiative transfer calculator, which solves the vector radiative transfer equation (as
4 Results

4.1 Brightness temperature simulations incorporating the Zeeman effect

Brightness temperature spectra have been simulated using the ARTS model which was described in the previous section. ARTS was set with all the information about instrumental aspects and location of TEMPERA in order to simulate the same measurement conditions. The brightness temperature was calculated for 13 azimuth angles (71.5° : 10° : 191.5°) and a fixed elevation angle (60°) and to simulate the atmospheric conditions of 15 October 2013 (Figs. 5 and 6). The altitude of the platform was set at 12 km in order to avoid any tropospheric effect in the spectra. On 15 October 2013, the total intensity of the magnetic field over Bern at the altitude of 50 km was 46.547 nT with a declination of 1°21′44″ and an inclination of 62°46′16″ (www.ngdc.noaa.govgeomag/ magfield.shtml). Figure 5 shows the calculated brightness temperature spectra for a linear horizontal polarization of the oxygen emission line centered at 53.07 GHz in a range of 5 MHz. From these simulations we can observe that the spectra are almost identical for most of the frequency range plotted here and differences are only observed in the central part when the observational azimuth angle is changed. In the narrow central frequency range we can observe that both the shape and the intensity of the spectra changes for the different observations. For the higher azimuth angles the brightness temperature spectra are lower and the shape is flatter, while for lower angles the spectra are higher and the shape is less flat. The maximum difference in brightness temperature between the most intensive spectrum (91.5°) and the least intensive (191.5°) is 2.5 K. Figure 6 shows linear vertical polarization. We observe a similar pattern for linear vertical polarization as for linear horizontal polarization, with the peak strength of the signal changing mainly in the center of the line as a function of the azimuthal angle. However, the change is much smaller for linear vertical polarization, which only has a maximum difference of 1 K between the most and least intense spectra. Also, the change with azimuthal angle is inverted compared to linear horizontal polarization. For the linear vertical polarization the most intensive spectrum corresponds to the observational angle of 181.5° while the least intensive corresponds to 91.5°. This behavior is clearly associated with the polarization nature of the Zeeman effect, since the polarized state of the observed radiation changes when the angle between the propagation path and the direction of the Earth magnetic field is varied. It is also interesting to note from Figs. 5 and 6 that the differences between horizontal and vertical polarization are very small when close to the 181° azimuth angle. This is in good agreement with theory, as this direction corresponds to measurements of radiation which has been propagated along the magnetic field towards TEMPERA. This parallel propagation results in minimal differences among linear polarizations.

The brightness temperature has also been simulated without considering the Zeeman effect in the ARTS model. These simulations correspond to the dashed lines shown in Figs. 5 and 6. We found that when the Zeeman module is not active there is no difference in the spectra for different observational angles. Moreover, the spectrum presents higher brightness temperature values and it does not show any broadening in the center of the oxygen emission line.

In order to compare the simulated spectra from ARTS with the measurements, the effects of the different optical components of TEMPERA on the polarization state of the radiation,
as well as the vertically polarized observing antenna, have to be considered. A full characterization of the polarization state of the radiation can be done by means of the Stokes vector, \( s \), which is defined as

\[
s = \frac{1}{2} \sqrt{\mu} \begin{bmatrix} I \\ Q \\ U \\ V \end{bmatrix} = \begin{bmatrix} E_v^* E_h + E_h^* E_v \\ E_h^* E_v - E_v^* E_h \\ E_v^* E_h - E_h^* E_v \\ E_h^* E_v + E_v^* E_h \end{bmatrix},
\]

where \( \epsilon \) and \( \mu \) are the electric and magnetic constants, respectively, \( \langle \cdot \rangle \) indicates time average, and \( E_v \) and \( E_h \) are the complex amplitudes for vertical and horizontal polarization, and the last two components, \( U \) and \( V \), correspond to linear \( \pm 45^\circ \) and circular polarization, respectively. The Stokes components are converted to brightness temperature by inverting the Planck function (Eriksson et al., 2011); this new Stokes vector of brightness temperatures is denoted as \( s' \).

The calculus of the measured brightness temperature \( T_{b0} \) considering the sensor polarization response can be expressed as (cf. Eriksson et al. (2011), Eq. 19)

\[
T_{b0} = \mathbf{p} L(\chi) s',
\]

where \( \mathbf{p} \) is a row vector of length 4 which describes the sensor polarization response. In the case of TEMPERA, whose antenna is vertically polarized, the vector \( \mathbf{p} \) is [1, 0, 0, 0]. The rotation of the Stokes reference frame due to the reflection in the different mirrors and the rotation of the external mirror is considered using the transformation matrix \( L(\chi) \), which allows one to obtain a consistent definition between the polarization directions for atmospheric radiation and sensor response. This matrix is defined as (Liou, 2002)

\[
L(\chi) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos 2\chi & \sin 2\chi & 0 \\ 0 & -\sin 2\chi & \cos 2\chi & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.
\]

The rotational angle \( \chi \) has been calculated using the GRASP software package (www.ticra.com/products/software/grasp). This software package allows design and analysis of complex reflector elements using physical optics, physical theory of diffraction and the method of moments. Figure 7 shows the setup of this simulation, where we can see the different TEMPERA components (horn antenna, parabolic mirror and the two auxiliary mirrors, the fixed and the rotating mirror) and the ray tracing of an electric field which is propagated from the antenna to the atmosphere. The calculated angle \( \chi \) can be expressed as \( \chi = \psi + \psi_{\text{effect}} \) where \( \psi \) is the observational azimuth angle defined in our experiments (\( \phi = \pm 71.5^\circ \text{ or } 191.5^\circ \)) and \( \psi_{\text{effect}} \) is \( 141.5^\circ \). Once the sensor polarization response and the rotation of the polarized radiation have been characterized, the effective brightness temperature can be calculated as (Eriksson et al., 2006)

\[
T_{b0} = [1100] L(\chi) s'.
\]

Figure 8 shows the effective brightness temperature spectra calculated for the case simulated in ARTS (15 October 2013) in Figs. 5 and 6. For these spectra we can appreciate again the same pattern as in the ARTS simulations, with almost the same intensity on the wings of the oxygen emission line and some differences in the central frequencies when the azimuth angle is changed. The highest brightness temperature is found at 71.5°, while the lowest is found at 191.5°. The latter position corresponds to the maximum broadening found when the direction of observation is almost antiparallel to the direction south–north. The maximum difference between the most and the least intense spectra is 2.5 K.
Figure 7. Simulation of the propagation of a vertical electric field from the TEMPERA antenna to the atmosphere and passing through the different mirrors using the GRASP package software.

Figure 8. Simulated effective brightness temperature, taking into account that the radiation passed through the different TEMPERA components.

In order to study the difference in the broadening of each azimuth observational spectrum due to the Zeeman effect, we have calculated the ratio among each spectrum to the averaged spectrum from all the observational angles. Figure 9 shows these ratios for the different azimuth angles. Azimuthal behavior with a ratio below unity in the center of the line also has a ratio above unity in the wings, which means that the line experienced more than average broadening. The opposite is also true: azimuthal behavior with values above unity in the center means less than average broadening. The different ratios show a clear azimuth dependence, indicating that the highest broadening is found when the azimuth angle is 191.5° while the smaller broadening is found at 71.5°.

4.2 Tropospheric correction of SDR spectrometer

A ground-based microwave radiometer measures a superposition of emission and absorption of radiation at different altitudes. The received intensity at ground level can be expressed in the Rayleigh–Jeans limit (\( h\nu \ll kT \)) as a function of the brightness temperature. In these conditions the radiative transfer equation is given by

\[
T_b(\nu, z_0) = T_0 e^{-\tau(\nu, z_0)} + \int_{z_0}^{z_1} T(z) e^{-\tau(\nu, z)} \alpha(\nu, z) dz,
\]

where \( T_b \) is the brightness temperature at frequency \( \nu \), \( T_0 \) is the brightness temperature of the cosmic background radiation, \( T(z) \) is the physical temperature at height \( z \), \( z_0 \) is the Earth surface, \( z_1 \) is the upper boundary in the atmosphere, \( \alpha \) is the absorption coefficient, and \( \tau \) is the opacity. The opacity is defined as

\[
\tau(\nu, z) = \int_{z_0}^{z} \alpha(\nu, z') dz'.
\]
The contribution of the troposphere to the brightness temperature measured with a microwave radiometer at ground level is very important and it could be very different depending on the observational direction or on the period of measurements. After oxygen, water vapor and liquid water (clouds) are the most important components in the atmosphere, the emissions of which have relevance in the microwave spectrum. It is very important to correct our measurements for any tropospheric effect in order to ensure that the changes observed in our measurements for different observational directions come from the stratosphere (Zeeman effect) and not from the troposphere.

Since the tropospheric portion of the pathlength provides a relatively spectrally flat signal the microwave radiative transfer equation can be rewritten as

\[ T_b(z) = T_b(z_{\text{trop}})e^{-\tau} + T_{\text{trop}}(1 - e^{-\tau}), \]  

(9)

where \( T_b(z_{\text{trop}}) \) is the brightness temperature as observed from the tropopause, \( \tau \) is the tropospheric zenith opacity, and \( T_{\text{trop}} \) is the effective temperature of the troposphere.

From this equation the opacity can be calculated as

\[ \tau = -\ln \left( \frac{T_{\text{trop}} - T_b(z_0)}{T_{\text{trop}} - T_b(z_{\text{trop}})} \right). \]  

(10)

Since the atmospheric opacity is dominated by the contribution from the troposphere, the stratospheric contribution is considered negligible and the cosmic background radiation, \( T_{\text{bg}} \), is in practice used instead of \( T_b(z_{\text{trop}}) \) in Eq. (10). This means that the calculated \( \tau \) actually is approximately the total atmospheric opacity and hence includes the minor contribution from altitudes above the troposphere (e.g., absorption by stratospheric \( \text{O}_2 \) and \( \text{H}_2\text{O} \)) (Forkman et al., 2012).

The contribution of the stratospheric O\(_2\) and H\(_2\)O) (Forkman et al., 2012).

\( T_{\text{trop}} \) has been estimated using a linear model between the weighted tropospheric temperature and the ground temperature (Ingold et al., 1998). The weighted tropospheric temperature was calculated using radiosonde measurements. Radiosondes are launched twice a day at the aerological station of MeteoSwiss in Payerne (40 km west of Bern). One year of radiosonde data was used and the linear fit found between \( T_{\text{trop}} \) at 53 GHz and the ground temperature \( T_z \) was \( T_{\text{trop}} = 0.8159 T_z + 47.21 \text{ K} \). The constant term \( T_{\text{trop}} \) is independent of frequency and has a value of 2.7 K (Gush et al., 1990). The term \( T_b(z_0) \) is measured using the wings of the oxygen emission line centered at 53.07 GHz for every azimuth angle. The simultaneous measurements performed with the FFT spectrometer allow us to measure in the wings of the oxygen emission line, where most of the contribution to the brightness temperature comes from the troposphere. In the frequency range of interest, the tropospheric attenuation increases with increasing frequency. In order to account for this, we determine the correction factor at each frequency using a linear fit between the frequency ranges highlighted in red in Fig. 10.

Once all the terms are calculated, the brightness temperature corrected for tropospheric effects can be obtained as

\[ T_b(z) = T_b(z_0) - T_{\text{trop}}(1 - e^{-\tau}) \frac{e^{-\tau}}{e^{-\tau}}. \]  

(11)

It is interesting to note that for the correction presented in this section we have used the scalar radiative transfer equation, since this tropospheric correction is independent of polarization state. This assumption is valid if scattering can be neglected, which should hold in the absence of strong precipitation.

### 4.3 Stratospheric brightness temperature measurements

As already described in Sect. 2, a special campaign of microwave radiometer measurements has been performed for 3 months in autumn 2013 in the ExWi building of University of Bern. During this campaign, TEMPERA was set up with a special configuration in order to be able to observe the Zeeman effect from ground-based measurements. Radiometer measurements in different azimuth angles (13 angles) were carried out in order to scan the atmosphere under different angles between the propagation path and the local Earth magnetic field. Figure 11 shows mean monthly brightness temperature spectra obtained for different azimuth angles in October 2013. All the measurements were corrected for tropospheric effects following the procedure described in the previous section. Figure 11a shows the whole range (4 MHz) measured with the SDR spectrometer. From this plot we observe that the mean spectra for the different azimuth angles show almost identical values outside of the narrow central region. However, differences in the intensity and
in the shape are observed in the very narrow range centered on 53.067 GHz. Figure 11b shows a zoom of the spectra in the central frequency range (±0.25 MHz), while higher brightness temperature and less flat shapes are observed in lower azimuth angles.

These results are in good agreement with the simulations performed including the Zeeman effect with ARTS (Sect. 4.1). However, we can notice that there is an offset in the baseline between model and data, the shape of the center line (±2 MHz) is not altered. Thus the main conclusions of Zeeman polarization measurements and the ARTS module validation are solid.

Figure 12 shows a direct comparison of the brightness temperature spectra from SDR measurements (solid lines) and from ARTS model (dashed lines) for two observational azimuth angles (91.5° and 181.5°). An offset correction has been applied to the simulated spectra in order to compare with the measurements. Although the absolute values are not exactly the same for the modeled and measured spectra in the center of the oxygen emission line we can clearly observe that the behavior of the spectra for the two azimuth angles are the same. The spectra show a higher broadening for the highest azimuth angle for both measurements and simulations. In order to compare the measurements with the model in a more quantitative way, we have compared the ratio of the maximum mean brightness temperature of each spectrum to the mean value for all the spectra at the central frequencies (range of ±0.25 MHz). Equation (12) indicates explicitly the expression of these calculations:

\[
\frac{T_{\text{mean}}(\text{max})}{T_{\text{mean}}(\text{max})} = \frac{\text{mean}[T_{\text{b}}(\nu_1 - \nu_2, \psi)]}{\text{mean}[\sum_{n=1}^{n} T_{\text{b}}(\nu_1 - \nu_2, \psi_i)]} \tag{12}
\]

where \(\nu_1\) and \(\nu_2\) indicate the frequency range which corresponds to an interval of 0.5 MHz centered at 53.067 GHz. \(\psi\) is the observational azimuth angle for a specific position and \(n_1\) is the total number of positions scanned by TEMPERA (13 positions).

Figure 13 shows these ratios calculated with the ARTS model simulating the conditions of 15 October 2013 and the ones obtained from the mean monthly spectra (October 2013)
measured by TEMPERA. We can observe that, in general, there is a very good agreement between the measurements and the model. Both simulations and measurements show higher ratio values (> 1), which indicate a smaller broadening regarding the averaged spectrum for the smallest azimuth angles and a larger broadening (ratios < 1) for the largest angles. The relative differences between both ratios are lower than 1% for all the azimuth angles. We observe that the ratios for some azimuth angles are almost identical while some discrepancies are observed for other ones. The errors for the TEMPERA measurements have been estimated by evaluating the uncertainties associated with the different terms of the tropospheric correction (Eq. 11). The error bars shown in Fig. 13 have been calculated using error propagation theory and they presented values very similar (± 0.01) for all the observational angles. The errors associated with the simulations were obtained by evaluating the ratio of the simulated spectra plus Gaussian white noise. The calculated uncertainties presented values much smaller than the ones found for the measurements (maximum value of 4.6 × 10^-5). It is important to note that the differences found between measurements and simulations are within the measurement uncertainties. From this comparison we can conclude that the agreement between measurements and model is clear. These results show the polarized state of the radiation due to the Zeeman effect, which is revealed for a different broadening in the spectra when the angle of the Earth’s magnetic field and the observational path is changed.

5 Conclusions

This work presents an experiment in which the Zeeman broadening of the oxygen emission line at 53.0669 GHz is observed and the polarization state of the radiation due to this effect is detected for the first time using a ground-based microwave radiometer. A special campaign was carried out in order to detect this effect with the TEMPERA radiometer. The installation of a fixed and a rotating mirror in front of TEMPERA allowed us to measure under different angles between the observational path and the Earth’s magnetic field direction. A total of 13 azimuth angles were scanned ranging from 71.5° to 191.5°. In addition, the use of a narrow spectrometer (4 MHz) allowed us to measure the center of the oxygen emission line with a very high resolution of 1 kHz.

The brightness temperature spectra for the different azimuth angles were simulated using the ARTS model. This forward model applies a vector radiative transfer code which includes the Zeeman effect. ARTS was set up with all the information about instrumental aspects and location of TEMPERA in order to simulate the same measurement conditions. These simulations showed almost identical spectra for most of the frequency range (4 MHz) and differences were only observed in the central part when the observational azimuth angle was changed. The spectra considering linear horizontal polarization showed lower values of brightness temperature and flatter shapes for the highest azimuth angles, while for lower angles the spectra showed higher values and the shapes were less flat. The maximum difference in brightness temperature between the most intensive spectrum (91.5°) and the least intensive (191.5°) was 2.5 K. For the linear vertical polarization the effect in the central frequencies was smaller, with a maximum difference of brightness temperature of 1 K between the most and the least intensive spectra; the azimuthal order was the inverse. These results are an evidence of the polarized nature associated with the Zeeman effect, which shows changes in the polarized state of the observed radiation when the angle between the propagation path and the direction of the Earth’s magnetic field is varied.

In order to compare the ARTS simulations with the measurements the effects on the polarization state of the radiation due to the different optical components of TEMPERA radiometer were taken into account using the GRASP software package. The effective brightness temperature calculated after this correction showed that the most intense and least-broad spectrum was found at 71.5° and the least intense spectrum at 191.5°. The maximum difference between both spectra was 2.3 K.

Similar behavior to the simulations was observed for the measured spectra from the TEMPERA radiometer. A direct comparison of the ratios of the maximum brightness temperature of each spectrum to the mean value for all the spectra at the central frequencies showed a very good agreement between the model and the measurements. Both simulations and measurements showed a smaller broadening for the smallest azimuth angles and a larger broadening for the largest angles. The small discrepancies found for some azimuth angles were always within the measurement uncertainties.
This comparison is so far the most stringent test of the implementation of the Zeeman effect in ARTS. The comparison provides an effective test for the first three components of the Stokes vector. The third component, $U$, affects the end result through the rotation in Eq. (5). For example, if $U$ were treated to be 0, this would give a clear degradation of the match between ARTS and TEMPERA in Fig. 11. ARTS is presently compared to a Zeeman forward model developed especially for handling circularly polarized radiation, providing a test for the last Stokes component.

The inclusion of the Zeeman effect in the ARTS model will allow extension of the upper limit of temperature profiles from ground-based microwave radiometers beyond 50 km. Preliminary results of the temperature retrievals including the Zeeman effect show higher values of the measurement response at higher altitudes, indicating a possible extension of several kilometers of the temperature profiles. This new retrieval setup and a detailed validation of the temperature profiles will be presented in a separate paper.

It has also the potential for improving the temperature retrieval for stratospheric and mesospheric T sounders onboard satellites. A related application is the assimilation of Zeeman affected brightness temperatures into NWP models, where ARTS can help to assess the accuracy of the more approximative, but much faster, radiative transfer tools applied for that purpose.

Acknowledgements. This work has been funded by the Swiss National Science Foundation under grant 200020-146388 and MeteoSwiss in the framework of the GAW project “Fundamental GAW Parameters by Microwave Radiometry”.

References


Modeling the Zeeman effect in high-altitude SSMIS channels for numerical weather prediction profiles: comparing a fast model and a line-by-line model

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Bibliography:
Modeling the Zeeman effect in high-altitude SSMIS channels for numerical weather prediction profiles: comparing a fast model and a line-by-line model

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Received: 9 June 2015 – Published in Atmos. Meas. Tech. Discuss.: 2 October 2015
Revised: 8 February 2016 – Accepted: 11 February 2016 – Published: 3 March 2016

Abstract. We present a comparison of a reference and a fast radiative transfer model using numerical weather prediction profiles for the Zeeman-affected high-altitude Special Sensor Microwave Imager/Sounder channels 19–22. We find that the models agree well for channels 21 and 22 compared to the channels’ system noise temperatures (1.9 and 1.3 K, respectively) and the expected profile errors at the affected altitudes (estimated to be around 5 K). For channel 22 there is a 0.5 K average difference between the models, with a standard deviation of 0.24 K for the full set of atmospheric profiles. Concerning the same channel, there is 1.2 K on average between the fast model and the sensor measurement, with 1.4 K standard deviation. For channel 21 there is a 0.9 K average difference between the models, with a standard deviation of 0.56 K. Regarding the same channel, there is 1.3 K on average between the fast model and the sensor measurement, with 2.4 K standard deviation. We consider the relatively small model differences as a validation of the fast Zeeman scheme for these channels. Both channels 19 and 20 have smaller average differences between the models (at below 0.2 K) and smaller standard deviations (at below 0.4 K) when both models use a two-dimensional magnetic field profile. However, when the reference model is switched to using a full three-dimensional magnetic field profile, the standard deviation to the fast model is increased to almost 2 K due to viewing geometry dependencies, causing up to ±7 K differences near the equator. The average differences between the two models remain small despite changing magnetic field configurations. We are unable to compare channels 19 and 20 to sensor measurements due to limited altitude range of the numerical weather prediction profiles. We recommend that numerical weather prediction software using the fast model takes the available fast Zeeman scheme into account for data assimilation of the affected sensor channels to better constrain the upper atmospheric temperatures.

1 Introduction

The main isotopologue of molecular oxygen’s ground-state millimeter-wavelength band around 60 GHz is used by several satellites to remotely measure temperature. This is because the band’s radiometric signal is strong due to molecular oxygen’s high and fairly constant volume mixing ratio (~ 21%) at all altitudes below about 80 km (see e.g., Anderson et al. (1986) for the O₂ volume mixing ratio in the US Standard Atmosphere). Some examples of sensors utilizing this band for temperature soundings are the Advanced Microwave Sounder Unit (AMSU-A), the Special Sensor Microwave Imager/Sounder (SSMIS; Kunkee et al., 2008), and the Microwave Limb Sounder (MLS; Schwartz et al., 2006). All the lines of the millimeter band experience magnetic
solving and polarization from the Zeeman effect (Zeeman, 1897; Lenoir, 1967, 1968). In the atmosphere of Earth, this magnetic splitting is larger than the Doppler broadening, but only at higher altitudes is the magnetic splitting larger than the pressure broadening. As a simplistic and intuitive guideline for Earth, Doppler broadening in the 60 GHz band is about 50 to 70 kHz, magnetic splitting is in the range of 0.5 to 2 MHz, and pressure broadening by air is in the range of 10 to 20 kHz Pa⁻¹ (see e.g., Rothman et al., 2013, for air pressure broadening). Measured signals with significant weight at altitudes above what corresponds to 25 to 200 Pa (around 60 to 45 km) are therefore altered by the magnetic field. As a comparison, numerical weather prediction schemes usually profile up to 2–10 Pa (around 80 to 65 km). The Zeeman effect must thus be taken into account by the radiative transfer schemes used as forward models for numerical weather prediction assimilations at the top of the modeled profiles. This has been pointed out by Lenoir (1967, 1968), Liebe (1981), Rosenkranz and Staelin (1988), Hartmann et al. (1996), Han et al. (2007), Kobayashi et al. (2009), and Stähli et al. (2013), among others.

The Radiative Transfer model for Television Infrared Observation Satellites Operational Vertical Sounder (RTTOV) is designed for operational usage as a fast radiative transfer scheme (Saunders et al., 1999). In previous versions (RTTOV-8 and older), the Zeeman effect was included as transmission offsets based on Liebe (1981) but Kobayashi et al. (2009) showed that this scheme introduced unacceptable errors for retrievals of atmospheric parameters. It was concluded that the old method for Zeeman effect calculations in RTTOV is worse for assimilations than simply ignoring the Zeeman effect altogether. This is problematic as the uppermost atmospheric levels are the least constrained part of the numerical weather prediction models. The errors at the uppermost regions of the numerical weather prediction profiles can be ~5 K, with the top of the profile having even larger errors of up to 10 or 20 K, but the magnitude of the errors depends on latitude and season. The variability of the upper atmosphere is also large and depends on season and latitude. As a rough global estimate from available data sets from experimental satellites (from Remsberg et al., 2008), the variability between 65 and 80 km altitude (10 and 1 Pa) in the atmosphere is around 15 K. Inaccurate modeling of the radiation from these parts of the profile does not help to constrain the temperatures enough in the assimilation schemes. A new and fast Zeeman effect radiative transfer scheme designed by Han et al. (2007, 2010) has been implemented in RTTOV since version 10.

The Atmospheric Radiative Transfer Simulator (ARTS) is designed to be a reference radiative transfer model (Buehler et al., 2005; Eriksson et al., 2011). The ARTS Zeeman module implementation is described by Larsson et al. (2014) and has been validated by Navas-Guzmán et al. (2015). This work focuses on comparing ARTS with the new RTTOV scheme for the higher altitude SSMIS channels that are covered by numerical weather prediction profiles, and it is partly based on previous technical work presented by Larsson (2014). SSMIS is a conical scanner flying at an inclination of around 100° at about 800 km altitude. It scans with a sensor zenith angle of ~5° relative to the surface and covers a 2200 km wide swath ahead of the satellite. For the upper atmospheric sounding channels that we are interested in, the swath is divided into 30 pixels with approximately 25 ms integration time each. Between scans, SSMIS uses what remains of its 1.9 s scan cycle to calibrate against hot and cold loads. Model comparisons as this have proven valuable in the past for other spectral regions (see Buehler et al., 2006), as they allow us to quantify differences between the fast and the reference model schemes. Besides for numerical weather prediction applications, it is also important to quantify model discrepancies for climatological studies, where statistical methods are used to identify trends that can be small compared to an individual measurement’s noise equivalent brightness temperature.

The next section describes the way both models treat the Zeeman effect, and it also describes how we conduct our comparison. Later sections present the model comparisons, and conclude this work with some remarks on future prospects.

2 Method

We focus our efforts on SSMIS channels 19 through 22, which are sensitive to circular polarization of four O₂ lines between 60 and 64 GHz, and have weighting functions with peaks that range in altitudes between 40 and 80 km (see Han et al., 2007). These channels are described by Swadley et al. (2008). Channel 19 has a local oscillator at 63.283248 GHz, with an intermediate frequency of 285.271 MHz, and a 3 dB passband width of 1.35 MHz. Channels 20–22 are all on the same local oscillator at 60.792668 GHz, with the same first intermediate frequency of 357.892 MHz. Here the channels start to differ. Channel 20 simply has a 3 dB passband of 1.35 MHz, whereas channel 21 has a secondary intermediate frequency of 2.0 MHz applied before placing a 3 dB passband of 1.3 MHz, and channel 22 has a secondary intermediate frequency of 5.5 MHz applied before placing a 3 dB passband of 2.6 MHz. For each channel we have prepared five sets of brightness temperature data. One of these sets are measurements from SSMIS on board DMSP-18 taken on 25 September 2013 between 00:00 and 06:00 (UTC). The other four data sets are forward simulations in ARTS and RTTOV using the atmospheric profiles derived from Met Office’s numerical weather prediction for the SSMIS measurements. The four simulated sets are (1) ARTS with a three-dimensional magnetic field, (2) RTTOV with a two-dimensional magnetic field (i.e., independent of altitude), (3) ARTS with the same two-dimensional magnetic field as RTTOV, and (4) ARTS without any magnetic field at all. The following subsections describe necessary components of our forward simulations.
and discuss a few error sources when comparing the data sets to one another.

2.1 Model descriptions

This subsection describes how the models treat the Zeeman effect. Sources to the broader transfer schemes are cited, but not reviewed in detail.

2.1.1 RTTOV

RTTOV is a fast radiative transfer model used in numerical weather prediction data assimilation schemes. It achieves its speed by precalculations of coefficients for several predictors, based on a training set of monochromatic transmission, that translate the atmospheric profiles into polychromatic transmission for select channels at some atmospheric profile levels. Coefficients for these predictors have been determined for many operational instruments, and the model is widely used. The transmission is used to calculate the sensor-measured intensity using

\[ I = \sum_i B(T_{i,f}) \Delta \tau_i(\cdots), \]

where the index \( i \) is for each simulated layer of the atmospheric profile, \( n \) is the number of layers constructed from the profile, \( B(T_{i,f}) \) is the Planck function for the center of the polychromatic channel, \( T_{i,f} \) is the temperature of the \( i \)th layer, and \( \Delta \tau_i(\cdots) \) is the difference in the transmission to space across the layer. The triple dots indicate inputs to the transmission prediction scheme. For more information on the predictors, see Saunders et al. (1999).

There is no polarization in RTTOV as it models scalar radiative transfer. However, in deriving the RTTOV coefficients, the polarized nature of the Zeeman effect (and of other effects) is dealt with in monochromatic calculations of the polarization state of the entire transmission. The output of these calculations is the coefficient for the polarization component that is relevant for the polychromatic channel. The effective transmission from a level is thus

\[ \tau_{i,f} = P_{i,f} \Delta \tau_i(\cdots), \]

where \( \dagger \) indicates the conjugate transpose of the matrix, \( x \) indicates evaluation for the transmission of the wanted polarization component, and, counting upwards along the radiation path,

\[ P_{i,f} = T_{i,f} T_{i-1,f} \cdots T_{i-k,0}, \]

where \( T_{i,f} \) is the polarized transmission across the \( i \)th layer. For Eq. (1), \( \Delta \tau_i = \tau_{i+1} - \tau_i \). The transmission from the \( n+1 \) level is taken as unity when considering \( \Delta \tau_0 \). The work by Han et al. (2007) discusses the Zeeman implementation in detail and gives the predictors (in their Table 2). RTTOV uses a two-dimensional magnetic field consisting, for the entire radiation path, of just one magnetic field magnitude and one angle relative to the viewing direction of the instrument. These magnetic parameters are combined with the layer temperature to form the predictors.

2.1.2 ARTS

ARTS is a monochromatic line-by-line radiative transfer model that calculates absorption from a spectral line database for every level of the atmospheric profile. The intensity as seen by a simulated sensor in ARTS is from solving

\[ I_{\text{out}} = \exp\left(-K_{i,0}\right) I_{\text{in}} + \left(1 - \exp\left[-K_{i,0}\right]\right) B(T_{i,f}) \]

for each layer, where \( K_{i,0} \) is the polarized propagation matrix for the \( i \)th layer, \( r_i \) is the distance the radiation transfers through the layer, \( I_{\text{in}} \) is the incoming polarized radiation, and \( B(T_{i,f}) \) is the source function column vector (here \( B(T_{i,f}) = 0, 0, 0^T \), where \( B(T_{i,f}) \) is the Planck function). For details on the ARTS calculations see Eriksson et al. (2011).

The Zeeman module of ARTS calculates the Zeeman-affected propagation matrix at every atmospheric level by splitting lines into their polarized components as a function of the local magnetic field orientation. The propagation matrices are then averaged over the layer and used in Eq. (4). Both three-dimensional and two-dimensional magnetic fields are accepted as input. If the magnetic field is three-dimensional this means that there is a unique magnetic vector per level, whereas the two-dimensional magnetic field is similar to the RTTOV definition. In either case, ARTS keeps the polarization of the propagation matrices stored throughout the modeled transfer. By the end of the simulation, the polarized polychromatic sensor response is calculated from the monochromatic simulations and the channels’ spectral responses. For more details on the ARTS Zeeman module see the work by Larsson et al. (2014). Navas-Guzmán et al. (2015) recently and successfully simulated ground-based observations of molecular oxygen microwave radiation using the ARTS Zeeman module for several observational directions at high spectral resolution, which validates the ARTS implementation of the Zeeman effect for linear polarization.

2.2 The atmospheric profile inputs

There were a total of 8300 atmospheric profiles used for the simulations in this work. The profiles are derived from Met Office’s numerical weather prediction model. For a description of the Met Office numerical weather prediction profiles at high altitude and a list of assimilated data, see Long et al. (2013). The profiles are abstractly shown in Fig. 1. Note that there is an unfortunate visual illusion in Fig. 1 that there is a discontinuity between the temperature at the 10 Pa level (65 km) and the temperature at higher pressure levels. One major problem we encounter is that the channels of SSMIS
are sensitive to altitudes that are above the numerical weather prediction profiles’ top at 10 Pa. The weighting functions of channels 21 and 22 are mostly covered by the 10 Pa level but the weighting functions of channels 19 and 20 are not covered. To work around the problem of insufficient high-reaching pressure levels of the Met Office profiles, we assume that all higher altitude pressure levels have the same temperature as the 10 Pa level. This assumption is simple and inaccurate, as the lapse rates at high altitudes are generally large, but it is another work altogether to deal with the temperature field above the top of the numerical prediction profiles in a way that minimizes errors. One reason to use a constant temperature extrapolation for this work follows from the fact that RTTOV predicts optical depths on preset coefficient levels. When presented with an atmosphere that has insufficiently high-reaching pressure levels, RTTOV does this after assigning the temperature of the supplied atmospheric top to all the overlying coefficient levels, which is an extrapolation at constant temperature across the overlying layer of gas. The radiative transfer integration is performed subsequently on the supplied levels, but includes the source function and the absorption for the overlying layer of gas by, in effect, moving the supplied top at fixed temperature across this layer to represent the space boundary. Since the radiation of both channels 21 and 22 is mostly emitted at an altitude range covered by the Met Office atmospheric profiles, forcing a constant temperature above the top emulates the behavior of RTTOV when it is directly supplied by the Met Office profiles for these channels. This still means that the simulated results of channels 19 and 20 are unrealistic. We therefore favor the low-altitude channels 21 and 22 in this comparison work but include a brief discussion on how the models differ for the higher channels 19 and 20. This discussion focus on qualitative differences between the models that are apparent for the channels despite the otherwise unrealistic simulations. As one more note on the atmospheric profiles, we assume, for simplicity, that there is a constant molecular oxygen volume mixing ratio for the entire profile even though this is not the case above ~ 80 km.

Version 11 of the International Geomagnetic Reference Field (IGRF-11; Finlay et al., 2010) is used for the ARTS simulations with a three-dimensional magnetic field. The two-dimensional magnetic field values at the altitude corresponding to 5 Pa (around 70 km) have been extracted from IGRF-11 for both ARTS and RTTOV for those simulations. These extracted values are mapped in Fig. 2, which also shows the global coverage of the data sets. The argument for using a two-dimensional magnetic field is that the magnetic field does not change much along the path of a transfer. If this argument is good for SSMIS observations, then the difference in brightness temperature as a function of magnetic field extraction altitude will be small for the simulations.

2.3 Spectroscopic considerations

The RTTOV simulations have been performed with the prediction coefficients derived by Han et al. (2007) in this study. ARTS uses line center frequencies from the Jet Propulsion Laboratory spectroscopy database (http://spec.jpl.nasa.gov/). There is a mismatch between the input line centers to ARTS and RTTOV by exactly 8.4, 8.1, 8.9, and 8.2 kHz referring to Table 1 in Han et al. (2007) for the 7+, 9+, 15+, and 17+ O2 lines, respectively. ARTS always uses the higher frequency. The line centers given by, e.g., Tretyakov et al. (2005) are 2.2, 1.9, 5.1, and 7.4 kHz below the line centers used by ARTS, but were derived for use at low altitudes where pressure broadening is more important than exactness of line centers. Nevertheless the model input spectroscopy is similar and should be compared with the frequency stability of SSMIS reported by Kunkee et al. (2008) (80 kHz for channels 19, 20, and 21; 120 kHz for channel 22). Since the frequency instabilities are larger than differences in the lines’ central frequencies between the models, we do not think that line center accuracy is crucial for the comparison with SSMIS data, but it can still introduce biases between the models. The channels’ spectral response and a few examples of the simulated spectra from ARTS can be seen in Fig. 3. (Note that from code review at the Met Office for the derivation of RTTOV’s coefficients, we find that it appears that round-off levels of 100 kHz have been used for the line centers. The resulting differences in line centers between ARTS and RTTOV are still small compared to SSMIS frequency stability. They are instead 16, 32, 14, and ~26 kHz for the 7+, 9+, 15+, and 17+ lines, respectively.)

From Fig. 3, we see that channels 19 and 20 are in the center of the broadened lines, and that channels 21 and 22 are in the line shape’s wings near the equator (weak mag-
Table 1. Mean and standard deviations of our comparison for the four SSMIS channels. The left two columns with data are a direct comparison between the SSMIS data set and the corresponding full model simulations. The rightmost column shows the Zeeman effect by turning the effect on and off in ARTS. The remaining columns compare RTTOV simulations with ARTS simulations using three-dimensional and two-dimensional magnetic fields. SD denotes standard deviation. n/a denotes data that are not applicable. Noise levels are from Kunkee et al. (2008).

<table>
<thead>
<tr>
<th>Channel</th>
<th>SSMIS cf.</th>
<th>RTTOV cf.</th>
<th>Zeeman</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Full ARTS</td>
<td>3-D mag. ARTS</td>
<td>2-D mag. ARTS</td>
</tr>
<tr>
<td>19</td>
<td>n/a</td>
<td>n/a</td>
<td>−0.336 K</td>
</tr>
<tr>
<td></td>
<td>SD</td>
<td></td>
<td>1.8305 K</td>
</tr>
<tr>
<td>Noise</td>
<td></td>
<td></td>
<td>2.7 K</td>
</tr>
<tr>
<td>20</td>
<td>n/a</td>
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<tr>
<td>22</td>
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<td>−1.156 K</td>
<td>−0.528 K</td>
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<td>SD</td>
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</tr>
<tr>
<td>Noise</td>
<td></td>
<td></td>
<td>1.3 K</td>
</tr>
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Figure 2. Magnetic field used in our simulation mapped on a two-dimensional surface showing the strength of the field in the left panel. The right panel contains the angle between the magnetic field vector and the radiation’s propagation path. (This figure appears in Larsson (2014) and is republished with rights from EUMETSAT.)

netic field strengths), but that channel 21 is on the edge of the strongly Zeeman-affected part of the line when the magnetic field is stronger (i.e., near the poles). It is clear from this figure in combination with Fig. 2 that the increased magnetic field strength at higher latitudes causes a stronger broadening of the line. Since the SSMIS channels measure so close to the line centers, resulting errors from line center mismatches have been studied using the same simulations as shown in Fig. 3. The results of these tests are in Fig. 4, which shows ARTS simulations with uniformly shifted line centers (emulating a channel frequency shift). We see that the effect of the channel frequency shift is large for channels 19 and 20 near the equator ($\Delta T_b \approx \pm 2$ K at $\pm 50$ kHz shift looking westward) and that the effect here strongly depends on the observational geometry ($\Delta T_b \approx \pm 2$ K at 50 kHz shift when instead looking eastward). Closer to the North Pole, the effect is still noticeable but is fairly constant with observational geometry ($\Delta T_b \approx 0.1$ K at $\pm 50$ kHz). There is a noticeable effect on channel 21 of $\Delta T_b \approx \pm 0.5$ K at $\pm 50$ kHz for the polar simulations and $\Delta T_b \approx \pm 0.2$ K at $\pm 50$ kHz for equatorial simulations. Channel 22 is only weakly affected by a shifting channel center, with $|\Delta T_b| < 0.05$ K even at $\pm 150$ kHz shift. Note that Figs. 3 and 4 only represent two locations on the globe and that the absolute effect of a shifting channel center changes over the globe.

Finally, we have prepared weighting functions for an example of one orbit (the orbit is from 1 January 2012 around 13:30 UTC) and for two measurement pixels (or observational geometries that are relative to the motion of the satellite). These are shown in Fig. 5. With respect to each channel, the weighting function of channel 22 is almost constant over the orbit and observational geometry is not im-

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important. Channel 21 is similarly little influenced by observational geometry but in the polar region (the reader should be reminded that this is where the magnetic field is stronger) the weighting function is “smeared” and the channel is influenced by much greater altitudes (though the influence is not very strong). Both of the weighting functions of channels 19 and 20 change with geographical location and with observational geometry. It can be seen that the observational geometry is important by the broadened weighting function in the westward-facing pixel as compared to the along-the-track pixel around the first pass at $-30^\circ$ latitude, which is not as evident during the second pass (comparing the then eastward-facing pixel to the along-the-track pixel). Again, remember that Fig. 5 only shows an example of one orbit and that the weighting function will be different for other orbits and for other observational geometries.

2.4 Are there layering issues?

Since ARTS averages optical properties and RTTOV averages atmospheric properties to create the layer transfer, we must quantify the errors introduced by this model discrepancy. We do this by artificially decreasing the maximum layer thickness ($\tau_l$ of Eq. 4) for ARTS. We find that using an atmospheric layering of 50 m for a few of the profiles instead of using the same layering thickness as RTTOV only changes our results by $\sim 2 \times 10^{-4}$ K. The layering thickness is therefore not an issue for ARTS. We cannot test this for RTTOV directly without altering the predictor coefficients, but it is shown by Han et al. (2007) that using a sparsely layered approach or using a 1 km altitude grid does not alter the simulated brightness temperature much. From these observations we argue that there is no issue with the layers in the present study.

3 Results and discussions

The results of our comparison are summarized in Table 1. Channel-by-channel, the table shows the mean differences between the compared data sets, their corresponding standard deviations, and the channels’ noise equivalent temperatures. Figures 6 to 9 show the data sets in spread plots and as global distribution maps for channels 19 to 22. Figure 10 shows SSMIS measurements cf. the simulations for channel 21, and Fig. 11 shows SSMIS measurements cf. the simulations for
experiences a Zeeman effect that is less than 0.1 K. The magnetic field is considered, but most of the rest of the planet experiences around 1 or 2 K. The simulations for channel 19, 20, and 22 have a mean difference showing |ΔTb| < 0.34 K. This is about the same size as the average Zeeman effect in ARTS at $\Delta T = -0.44$ K. There is a large increase in the standard deviation of the differences from 0.33 K in the two-dimensional magnetic field comparison to the three-dimensional magnetic field comparison, which has a standard deviation of 1.8 K. There is a still larger increase in standard deviation to 2.9 K if the Zeeman effect is ignored.

Figure 6 shows the channel 19 comparison of RTTOV with ARTS, which was run using both a full three-dimensional magnetic field and an identical two-dimensional magnetic field setup as used by RTTOV. From Table 1, it can be seen that the mean brightness temperature differences between the models are small on average regardless of magnetic field setup, with both comparisons’ mean difference showing |ΔTb| < 0.34 K. This is about the same size as the average Zeeman effect in ARTS at $\Delta T = -0.44$ K. There is a large increase in the standard deviation of the differences from 0.33 K in the two-dimensional magnetic field comparison to the three-dimensional magnetic field comparison, which has a standard deviation of 1.8 K. There is a still larger increase in standard deviation to 2.9 K if the Zeeman effect is ignored.

From the global distribution maps shown in Fig. 6, we see that the largest discrepancies for channel 19 between RTTOV and ARTS with a three-dimensional magnetic field are located all across the equator, with a brightness temperature differences of up to 7 K systematically distributed in higher and lower brightness temperature regions; most warmer regions are located to the south of the equator and most colder regions are located to the north of the equator when the satellite is moving southward. When the satellite is moving northward, the resulting warm–cold region distribution seems to change across the swath. By remembering Fig. 2, which shows the two-dimensional magnetic field, we can by eye correlate these larger brightness temperature differences with areas of relatively weak magnetic field strength and with a magnetic field angle that is close to being parallel with the radiation path. We use Fig. 13 to focus on equatorial differences between the channels in this study. For channel 19, this figure shows that the differences between three-dimensional ARTS and RTTOV range over 7 K near the equator, but that the same range for differences between two-dimensional ARTS and RTTOV is only around 1 K. We note that a large change over the swath is consistent with the changing weighting functions of channel 19 in Fig. 5, which close to the equator can be quite broadened by changing the observational geometry. Thus, if the satellite had been moving northward over Eurasia, instead of over the Pacific Ocean, we cannot expect to see the same type of regional discrepancies since the magnetic field angle is changed by the viewing geometry. Looking only at the comparison of RTTOV and ARTS simulations with a two-dimensional magnetic field for channel 19, we find brightness temperature differences between the models of up to 1 K. There appears to
be a weak positive bias of around 0.3 K in the equatorial regions and a weak negative bias of around 0.6 K closer to the poles. We cannot identify the reason for these discrepancies clearly but the line center frequency differences of around 20 kHz between the models can explain some of these differences.

For channel 20 in Fig. 7, most of the same features are available as for channel 19 in Fig. 6, with a few modifications. From Table 1, the average brightness temperature differences between models are small, with both comparisons showing a mean of $|\Delta T_b| < 0.17$ K. The average model to model difference is thus much smaller than the average Zeeman effect in ARTS, which is $\Delta T_b \approx -2.2$ K. The standard deviation of the model to model differences changes in the same way for channel 20 as it does for channel 19. RTTOV simulations minus ARTS simulations with a three-dimensional magnetic field have a much larger standard deviation of 1.7 K than the standard deviation of 0.27 K for RTTOV simulations minus ARTS simulations with a two-dimensional magnetic field. For channel 20 the ARTS Zeeman effect standard deviation of 2.0 K is relatively close to the three-dimensional model to model standard deviation. From Fig. 13, it can be seen that the equatorial differences between three- and two-dimensional ARTS and RTTOV are similar to the differences for channel 19. One interesting difference is that while channel 19 has a fairly even equatorial bias when it compares two-dimensional ARTS to RTTOV simulations, this is not the case for channel 20. Instead, the eastern hemisphere experiences a positive bias of about 0.5 to 0.7 K and the western hemisphere sees close to no biases.

The errors that remain in the comparison with RTTOV and ARTS simulations with a two-dimensional magnetic field for channel 20 are similar to those for channel 19 of up to $\sim 1.5$ K. Because both line centers for channel 20 are shifted in frequency with the same sign, we can compare the remaining discrepancies in Fig. 7 to the channel frequency shift presented in Fig. 4. As a test not presented in any figures of this work, we ran ARTS with changed line center frequencies of 30 kHz for the lines influencing channel 20. This altered spectroscopy reduces the mean difference between the models by half, but the standard deviation still remains fairly unchanged. This means that there are still unidentified discrepancies between the models for channel 20.

### 3.1.2 Channels 21 and 22

Common to both the lower peaking channels 21 and 22 is that the reduction to a two-dimensional magnetic field in ARTS is numerically noticeable but much smaller than for channels 19 and 20. It is possible in Fig. 8, for channel 21, to see this difference qualitatively in the global distributions near magnetically strong regions. One example is above Siberia where there is a region with two-dimensional ARTS simulations that are $\Delta T_b \approx 0.1$ K warmer than RTTOV. The three-dimensional ARTS simulations are instead $\Delta T_b \approx -0.2$ K to RTTOV. It is also possible to see a systematic 1 K gradient over the swaths near the equator in the comparison of RTTOV and three-dimensional ARTS in Fig. 13 for channel 21. This systematic gradient is reduced to a fraction of a Kelvin for differences between two-dimensional ARTS and RTTOV. Similarly to channels 19 and 20, these swath discrepancies
should change when SSMIS is scanning northward or southward. Still, since the Zeeman effect is weak for channel 21 at the equator, most model differences there (the average bias is around 1.7 K in Fig. 13) are due to other reasons than the Zeeman effect.

Focusing only on two-dimensional magnetic field simulations for channel 21 (Fig. 8; right column), the polar regions agree fairly well between ARTS and RTTOV, with $|\Delta T_b| < 0.6$ K, barring a $-1$ K region above Antarctica close to 0° E longitude. These $< 0.6$ K differences are possible to understand from the 30 kHz line shifts identified for channel 20 above. Similarly to channel 20, however, introducing the line center shifts only reduces the model to model discrepancies, without much change in the standard deviation. (We remind the reader that channels 20, 21, and 22 measure the same two lines as are shown in Fig. 3; therefore, effects on one of the channels should be similar to the others.) Since channel 21 weighting functions of Fig. 5 are stretched to higher altitudes near the poles, it is possible that some model differences have been missed or exaggerated in our study due to our constant temperature profiles at these higher altitudes. It is deemed unlikely that this has had a big impact on our results because the largest differences between the models are found across the equator, where the channel 21 weighting function is covered by our physical profile. Also, the standard deviation of the model to model difference is about 0.56 K. In relation to the sensor noise equivalent temperature of 1.9 K, the model to model standard deviation is small, so any effect of the stretched weighting function on our comparison is also small. From Fig. 12, the Zeeman effect is up to 8 K $T_b$ at the strong magnetic regions for channel 21, whereas the models compare to within 0.6 K in these regions. This means that the models are still fairly close to one another in the strong magnetic field regions compared to the size of the Zeeman effect. Instead of at the poles, the largest model differences are found close to the equator, where differences of almost 3 K appear. We cannot explain these large differences from the channel shifts of Fig. 4.

For channel 22, there seems to be no correlation between magnetic field parameters and model to model differences. This is not surprising considering that the Zeeman effect is not very important for channel 22, with an average effect of $\Delta T_b = 0.13$ K that has a standard deviation of only 0.088 K. The mean differences between the models are $\Delta T_b \approx -0.53$ K with a standard deviation of 0.24 K, regardless of magnetic field setup in ARTS. Concerning channel 21,
Figure 7. Channel 20 comparison of RTTOV and ARTS simulations as for Fig. 6.

Figure 8. Channel 21 comparison of RTTOV and ARTS simulations as for Fig. 6 but with a fixed color scale.
we find from Fig. 13 that near the equator there is a larger than average negative bias. For channel 22 it averages at $\Delta T_b \approx -0.75$ K. Another region of interest is the South Pole, where the largest model to model differences occur – it is not shown in any plots that Antarctica is the warmest region in our simulations with atmospheric temperature of around 280 K for channel 22. From the scatter plots of Fig. 9, we see that there are beginnings of deviation between the models at higher temperatures, which show the Antarctica deviations. One potential cause for these discrepancies is therefore that the RTTOV coefficients were derived using transmission coefficients from simulations with an atmospheric training set that also had highest temperatures around 280 K at the peak of the weighting function of channel 22. It has previously been identified as a problem by Buchler et al. (2006) for water spectroscopy models that RTTOV coefficients derived for atmospheric input close to the limits of the training set can cause accuracy issues in RTTOV. In other regions, the model to model differences are small and appear to oscillate around 0 K.

3.2 Models to measurements

Direct comparison of simulated measurements with the SS-MIS data set is only possible for channels 21 and 22 because the higher altitude channels 19 and 20 are not covered by the altitude levels of the numerical weather prediction profiles. We want to remind the reader that the Met Office numerical weather prediction model profiles are believed to be inaccurate at higher altitudes. All such inaccuracies are retained in the following comparisons of models to measurements.

The comparisons for channel 21 between SS-MIS measurements, with regards to RTTOV simulations and with regards to ARTS simulations with a three-dimensional magnetic field, are found in Fig. 10. We find that the mean value of SS-MIS measurements minus RTTOV simulations is $-1.3$ K, and the mean value of SS-MIS measurements minus ARTS simulations is $-0.34$ K. ARTS agrees better than RTTOV with SS-MIS. Both comparisons have a standard deviation of around 2.4 K, and the noise equivalent temperature of the sensor is 1.9 K (Kunkee et al., 2008). So even if ARTS appears to be better, RTTOV simulations are close to SS-MIS measurements given the sensor’s noise and RTTOV is close to ARTS given the simulations to measurement standard deviations.

One key point that we want to take note of is that the noise of channel 21 is a lot smaller than the standard deviation of simulations to measurement. This is a similarity between our study and the one performed by Han et al. (2007). They found that RTTOV agrees with SS-MIS at a root mean square of 2.3 K at a mean difference of $-0.95$ K for channel 21. Han et al. (2007) use retrieved temperature profiles by the limb-scanning SABER instrument on board the TIMED satellite. This should mean that their temperature profiles are reasonably accurate, since limb scanners have a high signal-to-noise ratio. Still, they found, as we do, that the standard
deviation of the simulations to measurement are consistently larger than the noise of the sensor.

Looking in more details at the global distribution maps, we see that the largest discrepancies for both models are available closer to the poles, with a tendency for warmer brightness temperature differences (up to about 7 K) in the south and colder brightness temperature differences in the north (down to about −7 K). The weighting function of channel 21 is shifted upwards for stronger magnetic field (see Fig. 5 at high absolute latitudes). This upwards shift places a significant part of the weighting function at pressure levels where we have set the temperature to a constant value (above the 10 Pa/65 km level). Clearly a better method for extending the temperatures above 10 Pa is required. Across the equator the models are closer to SSMIS measurements. RTTOV agrees better with SSMIS measurements near the equator, with an average difference of around −1 K, than ARTS simulations, which has an average difference of 2 K to the SSMIS measurements. Looking at the equator in more details in Fig. 13, we cannot determine if ARTS or RTTOV equatorial behavior is best there for channel 21. Both models compare to SSMIS with much larger effects over the swath at the equator than how the models compare to one another. Swath effects are about 3 K large between models and measurements. We remind the reader that these swath effects are 1 K between three-dimensional ARTS and RTTOV. ARTS has on average slightly smaller swath effects – reduced by about 20% judging by differences in the absolute averages of the a regression coefficient in the linear fit of \( y = ax + b \) that is plotted – than RTTOV but there is a large variation in these swath effects.

There are some similarities between the channel 21 and the channel 22 comparisons of model simulations and SSMIS measurements as found in Fig. 11. In average, ARTS still agrees better than RTTOV with SSMIS measurements, with the respective differences to measurements being \( \Delta T_b \approx −0.63 \) K for ARTS and \( \Delta T_b \approx −1.3 \) K for RTTOV as seen in Table 1. Both models have approximately 1.4 K standard deviation to the measurements, which is similar to the sensor equivalent noise temperature of 1.3 K (Kunkee et al., 2008). Since the model-to-measurement standard deviation retains atmospheric input errors, this means that the models have a good agreement with the measurements. There are still a few dominating features visible in the global distribution maps. These features are all in the Southern Hemisphere, with a region above West Antarctica that has a −7.5 K bias compared to both models, and two regions with a 3 K bias to the observations, one located just north of the cold Antarctica anomaly and another located towards the east of it.

We note that RTTOV and SSMIS agree better for channel 22 in our study than in the study by Han et al. (2007).
They found approximately the same average difference between RTTOV and SSMIS as we did ($\Delta T_b = -1.3$ K), but the standard deviation in their test was much larger at 2.2 K compared to 1.4 K in ours. The temperature profiles are more accurate for limb sounding, so their uncertainties should reasonably be below or similar to ours. One possible explanation is that there are measurements with colder brightness temperatures included in the study by Han et al. (2007) than compared to our study. These lower brightness temperatures were consistently underestimated by RTTOV, which should increase the standard deviation.
The swath dependencies around the equatorial crossings of this study. The first row shows the map of the data. Color-coding is the same in this map as in the other plots where the swath from one orbit has its own colors; black circles are not used because they are more than 5° from the equator (5° was just arbitrarily chosen as the limit). The y axis label in the other plots overlap with labels in Figs. 6 to 11. Channels are named in the plot titles. Linear regression for brightness temperature differences was performed over longitude and the best-fit line is drawn between ±20% of the longitude range of the data from each orbit. The first two rows of the regression plots represent the model comparison and the last row represents the comparison between the models and SSMIS measurements.

4 Summary, conclusions, and outlook

We have presented a comparative study showing how well the fast RTTOV agrees with reference model ARTS for the high-altitude channels 19–22 of SSMIS using globally distributed numerical weather prediction model profiles from Met Office. This study shows that the RTTOV Zeeman effect scheme for SSMIS implemented by Han et al. (2007) works well. The agreement between the forward simulations and the corresponding SSMIS measurements is generally good but there are some discrepancies; quantitative values of the comparison are summarized in Table 1.

We conclude, when comparing ARTS to RTTOV, that using a three-dimensional magnetic field in ARTS gives an increased standard deviation compared to using a two-dimensional magnetic field in ARTS for channels 19 and 20; this increase is from 0.3 to 1.8 K for channel 19 and from 0.27 to 1.7 K for channel 20. The brightness temperature
differences by a three-dimensional magnetic field for these channels are found to be up to \( \pm 7 \text{K} \) across the equator, whereas ARTS with a two-dimensional magnetic field is in the range \( \pm 1 \text{K} \) from RTTOV. Since we follow the numerical weather prediction profile top (and emulate the behavior of RTTOV above this top), we cannot be sure that these are the model differences for a proper atmosphere. Despite this limitation, our comparisons still suggest that the dimensionality of the magnetic field is important for the higher altitude channels. The natural top of the mesosphere variability is around 15 K, so potential modeling errors of up to 7 K is a lot; however, we have not yet tested how this translates to numerical weather prediction model errors at these altitudes. Today, the estimated numerical weather prediction model errors are about 10 K at these altitudes. These errors will be reduced by using RTTOV with two-dimensional magnetic fields and the information available in the higher altitude SSMIS channels, but we cannot estimate by how much – this must be tested using the present version of RTTOV as a reference operational setting. Still, it would be better to use a three-dimensional magnetic field in RTTOV than a two-dimensional magnetic field but a fast Zeeman scheme using a three-dimensional magnetic field is not yet available. It is difficult to update RTTOV for three-dimensional magnetic fields but it should be possible. The coefficients used in RTTOV are generated from a large set of calculations that fits the effective scalar line-by-line transmission to space (Eq. 2) to a predetermined set of predictors. The polarized transmission from a level to space depends on the polarized transmission across all levels closer to the sensor (through the Ts of Eq. 3). Therefore, using a three-dimensional magnetic field with the present set of predictors will not work, since changes at higher altitudes change the effective scalar transmission to space. We have not attempted to extend the present set of predictors to account for perturbations at higher altitudes and further study will be necessary on how to achieve this. Since the magnetic field is fairly slow changing (see Fig. 2 for an estimate), a level-by-level set of perturbations might be applied to transmissions on the right in Eq. (3), and predictors incorporated into RTTOV to simulate the effect of the perturbations on the left of Eq. (2). This would allow the user to perturb a fixed input field, as presently expected by RTTOV, into a field that varies along the radiation path.

Similar brightness temperature differences as for channels 19 and 20 between two- and three-dimensional magnetic fields are present for channel 21 but these differences are much smaller in magnitude. In regions where the magnetic field is strong (closer to the poles), the dimensionality of the magnetic field can give differences of about 0.5 K in local regions. The Zeeman effect is up to 8 K in these high magnetic field strength regions, so the Zeeman effect treatment in the models still agrees fairly well for a strong magnetic field. Near the equator, the differences over a swath of measurement are found to be about 1 K large due to the dimensionality of the magnetic field, whereas the Zeeman effect itself is only 1 to 2 K large. However, there are other effects than the Zeeman effect that are important in the comparisons of the models. The model difference at the equator is on average 3 K, and this is larger than the difference between using a three- or two-dimensional magnetic field. We cannot identify the reason for these 3 K model differences. In comparing models to measurements, the range of error is about \( \pm 7 \text{K} \) \( T_b \) for channel 21. The errors of Met Office profiles are expected to be large at higher altitudes, so we do not expect models and measurements to agree better than this for now.

Channel 22 is unaffected by the dimensionality of the magnetic field because it is mostly unaffected by the Zeeman effect; the channel experience at most only a few tenths of a Kelvin of the Zeeman effect. Other differences dominate model to model differences. As regard to channel 21, there is an unexplained brightness temperature difference across the equator. For channel 22 this difference averages to around \(-0.75 \text{K}\). Also, there seems to be a limit in the temperature range for RTTOV’s training data that lowers RTTOV accuracy at the highest atmospheric temperatures. This is seen above Antarctica, creating a model to model bias of about 1 K for regions with the highest atmospheric temperature in this study. Except for localized large differences between models and measurement, the modeled channel 22 shows a good agreement with the measurements. Since channel 22 measures at lower altitude than channel 21, the Met Office profiles are more accurate and this is reflected in the better agreement with SSMIS measurements.

Our results imply that RTTOV, with the new Zeeman scheme by Han et al. (2007), models the SSMIS data set with acceptable accuracy compared to sensor noise parameters of channels 21 and 22. This in turn shows that the concerns Kobayashi et al. (2009) raised on using RTTOV’s past Zeeman capabilities for data assimilation schemes are addressed in newer versions. We recommend that future iterations of numerical weather prediction software start using versions of RTTOV from version 10 and onwards for the assimilation of SSMIS channels 21 and 22. This would not improve much over using an older RTTOV version for channel 22, but it would greatly improve agreements for channel 21. If SSMIS channel 21 is modeled well by RTTOV it can be assimilated into the numerical weather prediction scheme and consequently help improve middle mesospheric temperatures. It is likely that model to model discrepancies for channel 21 can be reduced even more if the model top levels reached higher altitudes, since high-latitude weighting functions of channel 21 reach much higher altitudes than equatorial weighting functions; a level top at 0.01 Pa/100 km is also necessary for channels 19 and 20 to be modeled. The lack of a three-dimensional magnetic field in RTTOV is not ideal for channel 21 but neither is it a huge issue. Models and measurements differ by 7 K at the equator currently and three-dimensional magnetic field makes only about 1 K difference for this channel. An option to work around the dimensionality problem currently is to apply biases, similar to those we...
find between ARTS and RTTOV in this work, to correct the simulated measurements in the assimilation schemes. Especially regional biases have to be described for the inversions to apply these biases. Uncertainties in the atmospheric temperature field of the numerical weather prediction model levels at high altitude are nevertheless currently large and consideration of the higher altitude SSMIS channels can help mitigate these uncertainties.

As regards to an outlook, there is an ongoing effort to use ARTS for retrievals of atmospheric temperature profiles using all of the high-altitude SSMIS channels. The results of these efforts will be reported upon in future work.

Acknowledgements. This work was partly funded by EUMETSAT grant number NWP_VS13_02, with report number NWPSAF-MO- VS-049. The writing of this article mainly took place in Hamburg under a CliSAP stipend. The authors also want to acknowledge the communities that support, both by usage and development, the two radiative transfer simulators.

Edited by: D. Cimini

References


A method for remote sensing of weak planetary magnetic fields: Simulated application to Mars

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Bibliography:
A method for remote sensing of weak planetary magnetic fields: Simulated application to Mars

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1. Introduction

[1] We present a method for characterizing the magnetic anomalies from the crustal fields in the lower atmosphere of Mars that requires two perpendicular linear polarization measurements of the Zeeman effect. The maximum effect of the magnetic field on the signal is found at the Doppler broadening width at low pressures rather than at the magnetically induced line frequency shift, and the effect strongly increases with increasing magnetic field strength. Based on simulations of the Zeeman-affected spectral cross section of the 119 GHz O₂ line in a model Martian atmosphere at various magnetic field strengths, we conclude that it should be possible to probe the strength of the magnetic anomalies remotely with presently available technology. We discuss limitations of the method, how these results could be relevant to the interpretation of residuals in Herschel/HIFI observations of Mars, as well as the application to detection of exoplanetary magnetic fields. Citation: Larsson, R., Ramstad, J., Mendrok, S. A. Buehler, and Y. Kasai (2013), A method for remote sensing of weak planetary magnetic fields: Simulated application to Mars, Geophys. Res. Lett., 40, 5014–5018, doi:10.1002/grl.50964.

1. Introduction

[2] The fields of crustal magnetization on the Martian southern hemisphere are thought to be remnants of an ancient dynamo-driven planetwide magnetic dipole. This Martian dynamo likely ceased to function when the planet’s mantle solidified, decreasing the heat flux from the core. Orbital measurements by the magnetometer on Mars Global Surveyor, taken 100–400 km above the surface, have revealed the influence of the fields which predominate the southern hemisphere [Brain et al., 2003; Haider et al., 2011]. However, the influence of a varying solar wind flux and interplanetary magnetic field angle, with corresponding variations in the induced magnetosphere, as well the complexity of the fields, makes it difficult to accurately estimate the field intensities at the surface. According to Brain et al. [2003], the best fit of a power law function to the data implies a surface strength of ~15,800 nT over the strongest source but is dependent on assumed source depths. Furthermore, weaker fields may cover significant surface areas and hence atmospheric volumes. A detailed map of the near-surface crustal field may help constrain when and how the magnetic dipole ceased to function, in turn, maybe shed some light on the present topographical and magnetic dichotomy [Citron and Zhong, 2012]. At the time of writing, there has been no functioning lander with a magnetometer instrument on board that can do in situ measurements at the surface. Even if such an instrument was to be placed on a future lander, it would only be able to cover a single or a small range of positions on the surface.

[3] The presence and strength of a planet’s intrinsic magnetic field strongly affects its interaction with the solar wind, which in turn influences the rate of atmospheric escape [Haider et al., 2011; Lundin et al., 2011]. A prominent example is the planet-wide dipole field of Earth that shields the entire planet from the solar wind, except for the auroral oval where a polar outflow of ionospheric ions forms. The ionospheric ions partly escape the planet, but a large portion of the outflow is recycled in the plasmasphere and plasma sheet systems [Seki et al., 2001]. Analogous recycling in “mini-magnetospheres” formed by the Martian magnetic anomalies are thought by Lundin et al. [2011] to be the reason for fewer ions reaching the Martian magnetotail from the southern hemisphere compared to the northern hemisphere, which was also observed by Nilsson et al. [2011]. Outside the magnetized regions, the atmosphere is only protected by an induced magnetospheric boundary resulting from currents induced in response to the magnetic field frozen into the solar wind [e.g., Barabash et al., 2007].

[4] By preventing atmospheric escape, this shielding effect by an intrinsic magnetic field influences the long-term habitability of the planet. The terrestrial planets are generally thought to have featured similar atmospheric conditions at their formation; however, only Earth has retained an active hydrological cycle thought necessary for life [Hunten, 1993; Kasting, 1993]. With the ongoing discoveries of potentially habitable exoplanets [e.g., Selsis et al., 2007], it is thus crucial to remotely detect exoplanetary magnetic fields as such features seem to be closely linked to its potential for habitability.

[5] With Mars as proxy for weakly magnetized planets, we aim to show how spectroscopic observations of the Zeeman splitting of the 119 GHz O₂ line by planetary magnetic fields can perform this remote detection. Similar methods, but for stronger (~6 orders of magnitude) magnetic fields, are utilized in stellar physics to characterize the magnetic field of stars [e.g., Berdyugina and Solanki, 2002]. However, the authors are not aware of any previous works utilizing
2. Method

[4] We will here describe a method by which two polarized passive microwave spectrometers, with sufficiently high-frequency resolutions, can retrieve the magnetic field information from an atmosphere. Commonly known as the Zeeman effect, the physical phenomenon utilized is the splitting of certain lines in frequency as a function of the magnetic field. Only the most basic aspects of the theory of the Zeeman effect, the theory of line shapes, and polarized radiative transfer are discussed herein. We refer to previous work (R. Larsson et al., A treatment of the Zeeman effect using Stokes formalism and its implementation in the Atmospheric Radiative Transfer Simulator ARTS, accepted by Journal of Quantitative Spectroscopy and Radiative Transfer, 2013) for a more thorough description of the model and for derivation of all unreferenced quantities that follows in this work. The Zeeman effect on Earth atmospheric radiative transfer has been modeled for quite a while [Lenoir, 1967], but only recently have measurements become more regular as modern instruments are able to resolve the effect [Hartmann et al., 1996; Schwartz et al., 2006]. The method can be simplified to stating that the difference between two perpendicularly polarized signals after transfer through a planetary atmosphere may contain information about the planetary magnetic field.

2.1. The Zeeman Effect Signal

[5] The Zeeman effect can be described as a perturbation theory applied to transitions with a nonzero sum electron spin in an external magnetic field. Instead of an unperturbed line center for the transition, there are instead several lines associated with specific polarizations depending on the direction of the magnetic field. If the propagation direction of the radiation is perpendicular to the magnetic field, the Zeeman effect changes the linear polarization components. If the propagation direction of the radiation is parallel to the magnetic field, the Zeeman effect mixes the above extrema. Furthermore, in the general case, the polarization around the unperturbed line centers is rotated due to a difference in propagation speeds between the different polarization directions [Jeffries et al., 1989].

[4] In this work, we will focus on the O$_2$ transition associated with an unperturbed line center at 119 GHz. We choose this line as the basis of further discussion because it is one of the simplest lines available to present the theoretical basis of our method. The unperturbed line strength is divided between three perturbed lines. There is still a line at the unperturbed line center carrying the original line strength but for only one linear polarization. We will denote the polarization associated with this perturbed line as horizontal. The other two lines are displaced by approximately ±14 Hz/nT relative to the unperturbed line center. These are each associated with one type of circular polarization, and both are associated with the remaining linear polarization. The circular polarizations are from here on referenced as right circular and left circular, respectively. The linear polarization associated with these perturbed lines is referenced as vertical from here on. Note that an angular change of 180° for the magnetic field will switch which line carries what circular polarization but will not affect the linear polarization order at all. For other Zeeman-affected transitions, the energy perturbation scheme may be more complex, but it should be possible to translate all results herein with relative ease [Schadee, 1978; Berestetskii et al., 1980].

[4] The relative shift of the perturbed lines is very small on Mars for realistic magnetic field strengths. The pressure and Doppler broadening widths are usually much larger, though with a field of 10,000 nT, the Doppler broadening is on the same order of magnitude as the Zeeman shift for the 119 GHz line. This might create the impression that the Zeeman signal is often hidden from spectroscopic analysis. We intend to show, both through simulations and simplified analytical representation of the line cross section, that this is not necessarily the case. It should on the contrary be possible for instruments with frequency resolution on the order of the Doppler broadening width to detect the signal associated with the Zeeman effect. We furthermore suggest that the magnetic field is a necessary adjustable parameter for analysis of Mars O$_2$ signals by instruments with high-frequency resolution and that the strength of the southern magnetic anomalies can be inferred from the difference between the two perpendicularly linearly polarized components of such a signal.

2.2. The Polarized Line Shape

[10] We take a closer look at the line shape associated with any line center in an atmosphere in order to explain the results. The Faddeeva function describes the shape of the line as a function of pressure and temperature around a line center [e.g., Sampoorna et al., 2007]. The Faddeeva function is

\[ u(z) = e^{-z^2} \text{erfc}(-z), \tag{1} \]

where \( z = v' + ia \), and

\[ v' = v - v_0 - \frac{\Delta v_p}{\Delta \nu_D}, \quad a = \frac{\Delta v_p}{\Delta \nu_D}. \tag{2} \]

[11] In the equations above, \( \text{erfc}(-z) \) is the complex error function, \( v \) is the frequency variable, \( v_0 \) is the frequency of the unperturbed line center, \( \Delta \nu_D \) is the Zeeman frequency shift relative to the line center, \( \Delta v_p \) is the Doppler broadening width, and \( \Delta \nu_R \) is the pressure broadening width. The real part of the Faddeeva function is associated with attenuation and the imaginary part is associated with dispersion. A combination of the real and imaginary part can be used to describe line mixing in the theory of pressure broadening [see, e.g., Baranger, 1958; Fano, 1963]. We ignore line mixing by choosing the isolated 119 GHz line where we know the effect is negligible near the line center at low pressures (from, e.g., Makarov et al. [2011], the effect decreases linearly with pressure). Although the phase is important when considering propagation of the radiation through a medium with a complicated magnetic field, we will only discuss attenuation below since we think this is enough to demonstrate the method.

[12] A single line will have its signal strength distributed as described by equation (1). The Zeeman effect will cause
a change in the line shape by addition from each contributing polarized line center. Thus, a single linearly polarized sensor expects \(w(z)\), \((w_{x}\;+\;w_{y})/2\), or any mixing of these two to be the result of its measurements. Here \(w(z)\) represents the shape of the central line and \(w(z)\) the respective outer line shapes. The line strength is equally distributed between the perturbed components, i.e., the total cross section is 

\[
\sigma_{\text{z}} = \frac{1}{2} \sin^2(\theta) \cos 2\theta \left[ \frac{w(z) + w(\overline{z})}{2} \right],
\]

where \(\theta\) is the angle of propagation of the radiation and the magnetic field. The data from Hartogh et al. [2010] inherently represent total intensity by averaging two perpendicular linear polarizations. Our interpretation is that this approach leaves largely unconstrained conditions in analysis up to the modeler, when the Zeeman effect is significant. Essentially, the modelers may alter either the magnetic field or the atmosphere to produce similar effects in the final results and must use their best judgment to determine what is reasonable. For instance, a different temperature profile in the atmosphere, or a different vertical \(O_2\) distribution, may produce the same results in a model as the Zeeman effect would do. A better approach is to allow for the separation of the Zeeman effect from other atmospheric effects, e.g., by measuring the difference between the perpendicular linear polarizations, i.e., utilize the linearly polarized cross-section shape 

\[
\sigma_{\text{z}} = \frac{1}{2} \sin^2(\theta) \cos 2\theta \left[ \frac{w(z) + w(\overline{z})}{2} \right],
\]

where \(\eta\) is the anticlockwise angle between the axis of the vertical polarization component and the magnetic field projected on the plane defined by the propagation direction. Regardless of the geometry, a nonzero \(\sigma_{\text{z}}\) contains some magnetic contribution for a given atmospheric level. Combining this with the information from \(\sigma_{\text{z}}\), through \(\sigma_{\text{z}} = \sigma_{\text{z}} - \sigma_{\text{z}}\), provides the modelers with better constraints when estimating the atmospheric parameters. Note that a linear polarization measurement will only experience \(\sigma_{\text{z}} = \sigma_{\text{z}}\) or \(\sigma_{\text{z}} = \sigma_{\text{z}}\). Also note that the expected cross section for the total intensity when the Zeeman effect is ignored is \(w(z)\) for both linear polarization components, which are then centered at \(v_0\).

The expected cross-sectional residual from models ignoring the Zeeman effect is then \((1 + \cos^2 \theta) \sigma_{\text{z}}(\theta = 90, \eta = 0)\). This means that the Zeeman effect is seen even in polarization independent measurements and that only if the residual of \(\sigma_{\text{z}}\) is \(\sigma_{\text{z}}\) for magnetically affected measurements may we know the orientation. Otherwise, a nonzero \(\sigma_{\text{z}}\) means that \(\theta\) and \(\eta\) may be estimated from the residual above. This better constrains the problem of the magnetically dependent line shape, although it still leaves some interpretation up to the modeler. We will assume an idealized geometry for the strongest possible linearly polarized cross section, \(\theta = 90^\circ\) and \(\eta = 0^\circ\), for most of the discussion that follows. 

It is clear that the exponential of equation (1) contributes greatly to the drop-off rate of the shape function. With two closely adjacent, but oppositely polarizing lines, this can be used to approximate at which frequency one or the other polarization is dominant; the vertical polarization will dominate as the horizontal polarization decreases with increasing \(z^2\). We already know that the horizontal polarization signal will be stronger close to the unperturbed line center. Assuming the change in main polarization occurs at \(Re(z^2) \approx 1\), we can say that the vertical polarization extrema of equation (4) occurs at 

\[
v_{\text{max}} \approx v_0 \pm \sqrt{(\Delta v_0)^2 + (\Delta v_0)^2}.
\]

For weak magnetic fields and low pressures, these peaks are indeed found at \(v_{\text{max}} = \pm \Delta v_0\) from the line center, as can be predicted from Equation 5. An instrument capable of measuring the Zeeman effect on Mars must have a frequency resolution of the order of \(\Delta v_0\). Significantly better frequency resolution than \(\Delta v_0\) is not necessary to facilitate detection since the difference between horizontal and vertical polarization around \(\Delta v_0\) should be sufficient to determine the magnetic field. Instruments capable of this frequency resolution today include those presented by Hartogh et al., 2009 and Murtagh et al., 2002. If a copy of one of these instruments was placed in orbit around Mars, we think it would be able to map the magnetic field at middle to high altitudes, although such a copy of the Odin-SMR instrument must be altered to allow measurement of a secondary linear polarization. A somewhat similar instrument design for a Mars mission has been proposed by Kasai et al., 2012, though their work does not explicitly mention the goal of measuring \(O_2\) lines.

We find from Figure 1a that a signal-to-noise ratio of about 100 is required to detect and quantify a 1000 nT strong
detectable at the surface, though the peak of Mars for the 119 GHz O2 line. Figure (a) is of pressure and range of possible magnetic field strengths at between two perpendicular linear polarizations as a function Figure 1. reasonable integration times. probably not be mapped with the described line method for significantly reduced, however, so near-surface magnetic fields can center. The larger frequency perturbation is due to the differ-

maximum perturbation is at about 800 Pa, stronger fields (∼10,000 nT) may be detectable at the surface, though the peak of σ₀ will be shifted closer to 100 Δv₀. The signal strength will be signifi-
cantly reduced, however, so near-surface magnetic fields can probably not be mapped with the described line method for reasonable integration times.

Transitions of the type ΔJ = 0 and ΔN = ±2, which is the case for the 774 GHz line, will be more perturbed than trans-
sitions of the type ΔJ = ±1 and ΔN = 0, as is the case for the 119 GHz line. In this example, N is the quantum num-
ber associated with total angular momentum disregarding spin and J is the quantum number taking spin into account for the total angular momentum. The Zeeman effect signal should thus be more easy to detect at 774 GHz, compared to at 119 GHz. We simulated measurements for a simplified radiative transfer scenario in ARTS to emulate the results of Hartogh et al. [2010] for an ideal and constant magnetic field (see supporting information). This simplified scenario yields that a magnetic field strength of 10,000 nT should be able to explain most of the residual in Figure 4 (lower panel) of Hartogh et al. [2010]. However, the atmospheric profile and the magnetic fields in this approach were both assumed constant. The magnetic field should be stronger closer to the surface, where most of the O₂ signal originates. Most of the polarization difference around Δv₀, however, occurs at higher altitudes. Due to the logarithmically increasing sig-

netic field strength with increasing magnetic field strength, a single volume with a field strength of 20,000 nT should contribute about 10 times more to the signal than twice the volume with a field strength of 10,000 nT. This means that the contribu-
tion from a single strong source may be able to significantly change the shape of the overall signal.

[20] Let us now leave Mars and turn to the subject of exo-

planets. Detection of magnetization on exoplanets is still a field in its infancy. However, considering Mars as a proxy for weakly magnetized terrestrial planets outside the solar system, some remarks can be made from our analysis. Follow-

Figures 1a, it is easier to detect a weak magnetic field on an exoplanet with a cold lower atmosphere, compared to a warmer equivalent. This is because the relative strength increases logarithmically not only with increasing magnetic field but also with decreasing Doppler broadening.

[21] Current methods for detection of exoplanets are biased toward detection of big planets in close orbits around their parent stars, i.e., gas giants with relatively high equiva-

lent temperatures. However, the long-term operation of the Kepler telescope, in conjunction with technical improve-

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ments for radial-velocity follow-up as well as direct imag-

ings/measurements, should generate a host of suitable colder terrestrial candidates for remote detection of magnetic fields in the near future.

4. Conclusions

[22] It should be possible to isolate the signal generated by the Zeeman effect by measuring the difference between two perpendicularly polarized signals around O₂ lines on Mars. Two perpendicular linearly polarized sensors with frequency resolution on the order of Δv₀ around an unperturbed line center can be used to isolate the Zeeman effect from the remaining signal and allow quantification of the magnetic field. An added benefit of such an analysis would be better constraints on estimation of other atmospheric parameters. A cooled limb-sounding sensor should be able to map the mag-

netic field above 20 km on Mars for weaker magnetic fields. For stronger localized magnetic fields, this method should allow mapping at altitudes close to the surface.

[23] An average Martian magnetic field of 10,000 nT could explain significant parts of the residual associated with...
the measurements-analysis comparison by Hartogh et al. [2010]. However, it is impossible to quantify the effects of the magnetic anomalies without further analysis of the undisturbed spectral data, and even then it would be very difficult. Given the magnetic field model provided by Brain et al. [2003], it is difficult to estimate how large volumes of the Martian lower atmosphere carry 10,000 nT strong magnetic fields, though from our radiative transfer model, it should be clear that a few isolated stronger fields may contribute significantly more to the signal than their average geographical distribution implies.

[24] If a suitable exoplanet is found and the background noise can be kept sufficiently low, we suggest to attempt the method described in this paper in order to detect magnetization on the planet.

[25] Acknowledgements. The authors are thankful to Dave Brain for communications about the surface magnetic field on Mars. The authors are also thankful to Paul Hartogh for discussions about the measurements of Mars O2 by Herschel. Finally, the authors are grateful to the larger ARTS community for development and distribution of the model.

[26] The Editor thanks two anonymous reviewers for their assistance in evaluating this paper.

References


Martian magnetism with orbiting sub-millimeter sensor: Simulated retrieval system

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Martian magnetism with orbiting sub-millimeter sensor: Simulated retrieval system

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Abstract. A Mars-orbiting sub-millimeter sensor can be used to retrieve the magnetic field at low altitudes over large areas of the surface of Mars from measurements of circularly polarized radiation emitted by the 368 GHz ground-state molecular oxygen absorption line. We design a full retrieval system for one example orbit to show the expected accuracies on the magnetic field components that one realization of such a Mars satellite mission could achieve. We find that the two horizontal components of the magnetic field can be measured at about 200 nT accuracy, globally, with a vertical resolution of about 4 km from about 5 km up to 70 km in tangent altitude. The method and some of its potential pitfalls are described and discussed.

1 Introduction

In the past decades, there have been several proposals to fly a sub-millimeter sensor on a satellite mission to Mars. One such proposal is to fly the Far-InfraRed Experiment, presented by Kasai et al. (2012). In their work, Kasai et al. show that molecular oxygen, carbon monoxide, water (even heavy water), ozone, isotopologues of carbon dioxide, hydrogen peroxide, and various other hydrogen radicals all should have strong signals in the spectrum of Mars which they propose to observe. Additionally, wind speed parameters along the line of sight should have measurable readings. With this work we aim to develop the idea presented by Larsson et al. (2013) for remote measurement of magnetism by utilizing the Zeeman effect (Zeeman, 1897) on molecular oxygen in its ground state: $X(\Sigma_g^\pm)$. It is possible to combine this work with Kasai et al.’s idea into a single instrument that is capable of measuring and mapping both meteorological parameters and crustal magnetic structures, but this work will only focus on the magnetic aspects of flying such an instrument.

The Martian magnetic field is thought to be a remnant of a past global dipole that disappeared about 3.5 billion years ago (Acuña et al., 1998). All that remains of the past dipole is several magnetic sources in the crust, which were first measured in situ by the Magnetometer-Electron Reflectometer onboard the Mars Global Surveyor orbiter (Acuña et al., 1999) down to an altitude of 100 km. The strongest sources are located in the southern hemisphere, with strengths of up to 2000 nT at
100 km altitude. Estimations of the strongest magnetic field strength at the surface based on these measurements vary from just above 10,000 nT, up to almost 20,000 nT. The ongoing Mars Atmosphere and Volatile Evolution mission will provide further coverage of the magnetic field down to ~150 km altitude in normal mode, but during week-long campaigns its periapsis will be even lower at ~125 km altitude, improving the potential to map the crustal magnetism (Jakosky et al., 2015). There is to our knowledge one planned lander, InSight (http://insight.jpl.nasa.gov), which will carry a magnetometer to the equatorial surface of Mars.

The shape and distribution of the present field is informative for the crustal evolution of Mars (Nimmo and Tanaka, 2005). There are two main ideas about the magnetism's formation: either a large impact demagnetized the north leaving the south magnetized, or there was a southward migration of crustal material after the global dipole disappeared (see, e.g., Connerney et al., 2003; Citron and Zhong, 2012, for further discussions). Regardless of the reason, the strongest crustal field should be associated with the oldest intact crustal material since these regions are linked to the times when Mars still had an effective global dipole. Identifying the reasons why the northern hemisphere has a lower average elevation, and also a less magnetized crust, than the southern hemisphere is important for questions related to, e.g., how similar Mars and Earth were in their early years. The method we propose for measuring the crustal magnetic field is useful in this regard, as it allows the determination of the magnetic field strength at different altitudes in the atmosphere. This means that it would help in the creation of profiles of magnetic field data that in turn can be used to estimate the depths, nature and locations of the crustal field sources. Finding these sources characteristics accurately using satellite data is difficult — the available Martian magnetic field models differ in some regions by up to 2000 nT (cf. Cain et al., 2003; Morschauser et al., 2014) and the range of the strongest surface field is from just above 10,000 nT up to potentially 20,000 nT. The characteristics of the crustal field sources strongly limits the possible processes that led to the disappearance of the past dipole, to the north-south dichotomy and to the strong crustal magnetic sources.

2 Method

This work is based only on simulations. We perform limb simulations around the molecular oxygen absorption line at 368 GHz using a measurement scenario that achieves several measurements around the same latitude-longitude tangent profile during successive satellite revolutions. These simulated measurements are fed into a retrieval toolbox that estimates the errors of the magnetic field components in the tangent profile.

Section 2 is divided as follows. The first subsection summarizes the ideas behind the approach in generic terms. The second subsection goes over the basic aspects of the modeling theory. The last subsection describes the data required for the simulations and our practical design choices. Then Section 3 describes and discusses the results. Finally Section 4 summarize our conclusion.
2.1 Measurement idea

The magnetic field influences molecular oxygen through the Zeeman effect. The Zeeman effect changes the energy states of the molecule to split an otherwise singular absorption line into several closely separated lines as a linear function of the strength of the magnetic field. The direction of the magnetic field is important as emission and absorption are polarized by this splitting. The Martian crustal magnetic field is strong, but not strong enough to cleanly separate the split lines from the temperature and pressure broadening of the line shape. Measuring intensity peaks and valleys of the radiation on a frequency resolved grid to directly get the magnetic field strength by peak-to-peak frequency separation is not possible. Instead, the split lines act to broaden or shift the absorption profile by a few, up to some hundreds, of kHz. Such frequency broadening or shifting also happens from increased temperatures and from greater wind velocities.

So, an important question to ask is how can we distinguish the atmospheric effects from the magnetic effects on the absorption line? The most obvious way is to simply measure the polarization state of the radiation. Neither temperature nor wind polarizes the radiation so the level of polarization in the split/broadened spectra is from the magnetic field in clear-sky limb view. A full sampling of the polarization state of the radiation is thereby the best way to retrieve the magnetic field. However, it is more expensive and more difficult to build a sensor capable of measuring the different polarization components (so that the components then can be combined for the total polarization state of the radiation), than it is to build a sensor capable of measuring just one polarization component. Assuming we can only measure one polarization component, is it still possible to get distinct magnetic information? Our approach has been to set up an observational strategy that observes the same limb tangent profile from several directions, multiple times during a few satellite revolutions. Temperature broadens the absorption line shape the same regardless of observational direction through the limb. Wind shifts the frequency along just one axis. What remains of the signal after temperature and wind effects are accounted for is therefore the polarization state and frequency shift due to the Zeeman effect.

2.2 Theoretical considerations

We use the Atmospheric Radiative Transfer Simulator (ARTS; Buehler et al., 2005; Eriksson et al., 2011) to simulate measurements. The retrieval toolbox Q-package (Qpack; Eriksson et al., 2005) is used to determine magnetic field component error. Together, these code-bases set up our retrieval system.

The approach to radiative transfer taken by ARTS is to calculate the monochromatic pencil-beam polarized radiative transfer equation in Stokes formalism along the path of the radiation through a three-dimensional inhomogeneous atmosphere and magnetic field. Antenna size, sensor characteristics, and polychromatic signal averaging are considered (as described by Eriksson et al., 2006). The Zeeman effect module of ARTS (Larsson et al., 2014) is applied for these calculations to simulate the left circular polarization component as observed by the simulated sensor for 201 channels of 100 kHz Gaussian shape surrounding the central absorption line at 368 GHz. Circular polarization is noticeably more influenced by the magnetic field than linear polarization, and 10 MHz on both sides of the line capture most of the information given by the Zeeman effect. For circular polarization, the magnetic signal is strongest when the local magnetic field vector points directly at or is pointing directly away...
from the sensor (along the track of the measured radiation). So in limb viewing geometry radiative transfer, the horizontal magnetic field components are more important at the tangent point than the radial component. The ARTS simulations also give the Jacobian matrix for specified retrieval quantities (in our case the magnetic field components and, for testing, temperature, wind components, and the molecular oxygen volume mixing ratio).

We use a moderately non-linear error characterization method, as presented by Rodgers (2000), to estimate the errors associated with a simulated measurement on a retrieval quantity. This error characterization is from

$$x = x_a + S_a K^\top (KS_a K^\top + S_e)^{-1} (y - F(x) + K (x - x_a)),$$

where $x$ is the derived atmospheric variables and magnetic field, $x_a$ is the a priori atmospheric variables and magnetic input, at different retrieval grid points (pressure, latitude, longitude), $S_e$ is the covariance matrix of the a priori, $K$ is the Jacobian matrix, $S_e$ is the covariance matrix of the instrument error, $y$ is the simulated measurement vector (made up of several individual measurements), and $F(x)$ is the forward model simulations. With measurements $F(x) \neq y$, however with pure simulations the terms are identical. Therefore, the error itself is found from $F(x) = y - \epsilon$, where $\epsilon$ is the random noise of the observation — this 'noise' encompasses every error not accounted for by the simulated measurement especially defined instrumental errors. Thus the retrieval error of Equation 1 is $S_a K^\top (KS_a K^\top + S_e)^{-1} \epsilon$. We also estimate the smoothing of the calculations by the matrix $S_a K^\top (KS_a K^\top + S_e)^{-1} K$, which is called the averaging kernel. This matrix gives information on the measurement response of the system and the vertical resolution of the measurements. The method above gives a linear error estimate; even if a problem is inherently non-linear, the error is often still linear (Rodgers, 2000).

About the retrieval grid, as explained in the previous subsection, several measurements of radiation from the same tangent profile can be combined to find the magnetic field components. The observational geometry is important as the individual measurements will observe different parts of the atmosphere at higher altitudes but the same parts of the atmosphere at lower altitudes. We therefore use a retrieval grid that takes the three-dimensional inhomogeneous atmosphere and magnetic field into account by setting a 3-by-3 grid of latitudes and longitudes, with the central grid point at the latitude and longitude of the tangent profile. The latitude grid positions are separated by a change of 2 degrees, with the same horizontal distance separating the longitude grid positions. We use a vertical retrieval grid separation of 2 km from 0 km up to 100 km. So $x_a$ is a $3 \times 3 \times 51$ long vector of inputs per retrieval quantity.

For $S_a$, we assume that there is no correlation between the different retrieval quantities but that there is some in spatial distance. For the tests we performed of wind, temperature and volume mixing ratio retrievals, we use covariance matrices that works for Earth. For the magnetic field components, since the magnetic field is a mostly static variable, its covariance matrix should also be mostly static. However, in a Bayesian framework, the covariance matrix should describe the knowledge we have of the magnetic field at the time of measurement. As mentioned earlier, the strongest differences between models in Morschauser et al. (2014) was 2000 nT but many sources differ less. So different models give different results. For simplicity we set the uncertainty of the magnetic field at 1000 nT at all altitudes, and that the correlation in altitude is $e^{-1}$ after one order of magnitude pressure change. We also set a small correlation between horizontal grids of $e^{-1}$ after a horizontal distance equivalent to 1.5 degrees of latitude change.
2.3 Model inputs

2.3.1 Orbit and sensor considerations

A circular orbit at 330 km altitude with 97° inclination and ascending node at 0° is used in all simulations. This orbit was selected ad hoc, because it is able to cover Mars in a short time frame. We model a sensor with a 30 cm large antenna for a vertical resolution of about 5 km at the tangent points seen by an orbiter at 330 km altitude. The antenna size was chosen for these simulations, because it is reasonably small. We will only simulate left circular radiation and we assume 1500 K single sideband system noise temperature. This number is a rough extrapolation to lower frequencies from the expected system noise temperature of the Jupiter Icy Moons’ Sub-millimeter Wave Instrument’s 600 GHz band (see Sobis et al., 2011, 2014; Treuttel et al., 2016, for more details on the JUICE/SWI receiver). We enforce 2 seconds as the time of a measurement, dedicating one third to calibration efforts and the remaining ∼1.3 seconds as integration time.

The position of the tangent profiles tracks this orbit as a pseudo-orbit with the same orbital parameters but with an ascending node offset by half the longitude drift of a full satellite revolution. These tangent profiles can be observed in limb geometry four times within about two revolution, once per revolution before passing the tangent profile and once after passing the tangent profile. The tangent altitudes we select to observe of this tangent profile stretch from 6 km deep to 78 km high, with a 3 km separation for 25 tangent altitudes. So a total of 100 individual measurements are considered in the error characterization. We call the grouping of all individual measurements a measurement block. The error characterization of this work is from these measurement blocks. The results in the next sections track the tangent profile pseudo-orbit through 7 complete revolutions at a distance of 15 degrees of true anomaly between two retrieval profiles. This is enough revolutions and enough resolution to yield a global coverage for a global error characterization.

An example of observation geometry and orbit can be seen in Figure 1. As mentioned, we simulate 201 channels for the sensor. With 100 individual measurements in a measurement block, \( y \) is a 20100 long vector and \( K \) is a 20100 × (3 × 3 × 51 × \( n \)) large matrix, where \( n \) is the number of retrieval quantities (usually three for the magnetic field components) and the other numbers are from the retrieval grid. The position of all 100 of these individual measurements in the example of Figure 1 are shown in panel (a). Panel (b) of the same figure shows the grouping of individual measurements for one set of observations of the tangent profile. We call this smaller grouping a measurement cluster. A satellite moving towards a tangent profile will, by geometrical necessity, see the tangent altitude increase the closer it gets to the profile, and vice versa a satellite moving away will see the tangent altitude decrease the farther away it gets. Finally, panel (c) shows that there is a slight drift in tangent point positions between different measurements. We enforce both 2 seconds of measurement time, and we enforce constant tangent altitudes. It is thus expected that the tangent position will drift slightly; the greater circle of positions that can observe a tangent altitude does not strictly intersect the satellite orbit at discrete time intervals. The drift is accounted for in the calculations of \( K \) and \( y \).

The only spectroscopic effect included in our radiative transfer calculations is the contribution of the 368 GHz molecular oxygen absorption line. We select this absorption line, because the Zeeman effect line splitting frequency is linear in magnetic field strength. So the lower the frequency, the stronger the signal from the magnetic field becomes as Doppler broadening
Figure 1. Example of the geometry of a measurement block. Panel (a) shows the orbit of a satellite as thinner lines, satellite positions in the measurement block as larger circles, and the mean tangent position of the measurement block as a cross. This example retrieval point is above a location of moderate magnetism strength near the equator (750 nT at surface altitudes). Panel (b) zooms in to show the satellite positions at one of the clusters of satellite positions. The black stars show the discretely resolved orbit. Panel (c) zooms in to show the tangent positions. The original intent of the measurement block was to observe in the center of this block of individual measurements.

is also linear with absorption line frequency. The reason we are not simulating one of the 60 GHz band lines is because we consider the antenna diameter required to have a decent vertical resolution in limb view as too large to reasonably fly the sensor. Our line data is from a recently compiled planetary toolbox, which gives line pressure broadening as a function of atmospheric composition for mixtures of common planetary species\(^1\) by Mendrok and Eriksson (2014) who assume that the molecular oxygen pressure broadening by carbon dioxide is \(\sim 20 \text{ kHz/Pa at } 296 \text{ K for our absorption line. This is directly taken from the 118 GHz line value presented by Golubi\'atnikov et al. (2003). This spectroscopic toolbox allows for direct calculations\(^1\)Our atmospheric and spectroscopic data are available in Extensible Markup Language files designed for ARTS via www.radiativetransfer.org.}^{1}\)
in Mars’ carbon dioxide rich atmosphere. Note that collision-induced absorption between pairs of carbon dioxide molecules is also important for the total absorption in our frequency range. Using the model by Ho et al. (1971), we estimate that it can be as important as adding a 20 K baseline signal for a pencil beam tangential to the surface. This added absorption is not enough to make the atmosphere opaque. We can anyways ignore this effect because at 6 km altitude — our lowest tangent altitude — the collision-induced absorption is much weaker than at the surface. Still, we note this as a lacking feature to be added in the future.

To summarize orbit and sensor constraints, we present Figure 2 to give an overview of how a simulation of a measurement block looks like with the assumptions outlined above. Panel (a) contains peak brightness temperature measurements for 2 clusters (looking ahead and behind the tangent point) for one revolution, and again measurements for 2 clusters for another revolution, with each cluster having 25 measurements at tangent altitudes between 6 and 78 km. As expected, the main contribution to the signal strength is the tangent altitude (through which the column number densities are regulated). At 6 km measurement tangent altitude, the radiation signal has a peak brightness temperature of about 140 K, and at 78 km the same number is about 10 K. The sinusoidal pattern of measurements in each cluster comes from the resolution of the spectra: the peaks are at the line centers and the valleys are away from the line centers. Only a very small part of this signal is influenced by the magnetic field. This part of the signal is not clear from the brightness temperature in panels (a-b) but is instead shown in the Jacobian panel (c). We see that the magnetic signal is on the order of about 0.2 mK/nT as strongest per 2 km altitude level per 100 kHz spectrometer channel bin. The resolution of the antenna is indicated from the coverage of the circular central disk of the Jacobian panel. Again, the simulated full-width vertical resolution is around 5 km for a 30 cm antenna. The covariance matrix is shown for completeness in panel (d). The figure neither shows the full K nor the full $S_{\epsilon}$ matrices but is zoomed in on a single sub-matrix. Still, the figure presents the basic retrieval setup. The only missing entry required for the error characterization is $S_{\epsilon}$. This matrix is not shown because it is simply filled with a constant describing the noise of the sensor. This constant is the square root of the system noise equivalent temperature divided by the integration time times the spectrometer channel full-width — which turns out to be just below 0.1 K$^2$.

2.3.2 Atmosphere and magnetic field models

The molecular oxygen profile is assumed constant at a volume mixing ratio of 1400 parts per million volume, which follows the profile reported by Hartogh et al. (2010b). This profile was derived by observations of the HIFI instrument on Herschel as part of the Herschel Solar System Observations program (Hartogh et al., 2009) by using a temperature profile derived at the same day from carbon monoxide observations (Hartogh et al., 2010a). We use the northern spring (solar longitude $L_s = 0^\circ$) carbon dioxide volume mixing ratio, temperature profile, wind profile, and pressure profiles from the ARTS planetary toolbox by Mendrok and Eriksson (2014), who base it on the Laboratoire de Météorologie Dynamique’s Global Circulation Model [LMD GCM] by Forget et al. (1999). These atmospheric profiles only provide global averages during the season. We thus ignore most effects of time, presented errors are hence of average character. The a priori atmospheric profiles can be constrained by the measurements but we have not taken this into account in any of our simulations shown in this work, though we give an example of what adding the atmospheric components to the error characterization means for the errors of the magnetic components.
Figure 2. Example retrieval scenario. This is $y$, part of $K$, and part of $S_a$ from the example in Figure 1. Panel (a) is the simulated measurements $y$ of ARTS with individual clusters marked by their revolution number and looking direction. Each peak corresponds to an individual measurement — the horizontal axis gives the tangent altitudes. The bottom row zooms in on the marked region of $y$ to show an individual simulation at 48 km tangent altitude (panel b), a zoom on the transpose of the $K$ sub-matrix at the tangent point latitude-longitude grid point for one magnetic component (panel c), and its corresponding $S_a$ sub-matrix (panel d).

If the atmospheric parameters are not stable on the 2 hours of a revolution, then the evolution of the temperature and wind profiles must be accounted for in the retrieval setup. This is still possible without changing the theoretical formalism of the retrieval setup, if the problem remains moderately non-linear, but it complicates the preparation of the atmospheric data and the simulations. From a theoretical point of view, the error characteristics of the magnetic field will remain moderately non-linear even if temperature, wind, and volume mixing ratio is accounted for in the retrieval problem because there should be no correlation between the atmospheric parameters and the magnetic field.

The primary magnetic field in our altitude range is the crustal magnetic field (Brain et al., 2003). Our model magnetic field is from the spherical harmonics fit to a selection of Mars Global Surveyor crustal magnetic field vector data by Cain et al. (2003). The magnetic field in ARTS is an extraction of Cain et al.’s fit that has been gridded at a global resolution of 0.5 degrees latitude, 0.5 degrees longitude, and 5 km altitude from the surface up to 100 km altitude. The model by Cain et al. (2003) is based on a ninetieth order Legendre polynomial, so the spatial resolution is limited to ~30 km. Other models, such as Morschauser et al. (2014), differ from Cain et al.’s by about 2000 nT at most (see figure 9 of Morschauser et al., 2014), but are otherwise close. This 2000 nT is therefore an estimation of the accuracy of the magnetic field components with the present
data. Some authors (Brain et al., 2003) speculate that the strongest field strength at the surface is upwards to 20,000 nT. Cain et al. give the strongest field as 12,000 nT, so 8000 nT serves as an estimate of the potentially largest discrepancy today of the crustal magnetic field strength of Mars.

3 Results and discussions

The structure of this section is that we begin by presenting the results of running the measurement block of Figure 1. This example is used as a generic measurement block and noise levels are lower or higher depending on the geometry of observations. We then present an average for many observations spread out globally. There is a final summary at the end of this section showcasing where our results suggest that the suggested measurements would be useful given the expected noise levels of individual measurement blocks. Note that we define the magnetic field components as: $B_u$ is the east-west component of the magnetic field, $B_v$ is the north-south component, and $B_w$ is the radial component.

3.1 Example measurement

Figure 3 shows the results of running the retrieval system for the tangent profile of the measurement block in Figure 1 with the simulated measurements and Jacobian as in Figure 2. It shows that the measurement response is good (i.e., around unity) for the $B_u$ and $B_v$ components from the ground up to about 70 km. The $B_w$ component has a poorer response than the other two components, but the measurements are in this case sensitive to $B_w$ at altitudes around 40 km. The vertical resolution is about 4 km for $B_u$ and $B_v$ over the entire sensitive altitude range, which reflects the achievable resolution for the simulated antenna size and tangent profile altitude spacing. The vertical resolution is much worse for $B_w$ between 8 and 15 km. The observational error that $B_u$ and $B_v$ experience varies between around 150 nT to 200 nT in the sensitive altitude range. The observational error that $B_w$ experiences is much worse, but it settles close to 300 nT at sensitive altitudes. Note that the observation errors are low where the measurement response is low; without measurements there are no errors due to observations.

As for vertical structures, the main limitation at lower altitudes is that pressure broadening hides the magnetic signal, and the main limitations at higher altitudes is that there is very little molecular oxygen due to the lower pressure. The optimal magnetic signal is from around 40 km, which is why the noise at these altitudes is lower.

$B_w$ is more difficult to detect than the other two components because of the characteristics of the Zeeman effect. The multiple measurements from different azimuthal directions allow the angle between $B_u$ and $B_v$ to be tested almost directly, but $B_w$ acts only to broaden the absorption line in limb view. It is therefore difficult to measure it without more constraints. In fact, if we add retrievals of wind, temperature and molecular oxygen volume mixing ratio to the retrieval problem — thus reducing the constraints on the retrieval problem — the measurement response to $B_w$ is no longer good at any altitude. So we will ignore $B_w$ from here on since it is not measurable by the presented method. The horizontal magnetic components are not affected by the lessened constraints on the atmospheric parameters.
Figure 3. Retrieval information for Figure 1. The first row shows Qpack output following Equation 1. Panel (a) shows the response function per magnetic field component, panel (b) shows the vertical resolution per magnetic field component (zig-zag is from discrete number of vertical limb measurements at 3 km spacing), panel (c) shows the observation error per magnetic field component. The lower row (panels d-f) compares this observational error to a priori magnetic field components. The horizontal dashed line shows the highest tangent altitude.

3.2 Suggested operational setup

The average observation errors expected for our suggested operational setup scenario are presented in Figure 4. We simulate only 7 revolutions, or about half a Martian day, of measurements, since this gives a good coverage for the whole Martian globe with our ad hoc orbit.

We find that the global and profile average observation error for the $B_u$ component is 170 nT and that the same average observation error for the $B_v$ component is 200 nT. Near the equator, the two components have similar observation errors (almost identical to what is shown in Figure 3). Closer to the poles, $B_u$ has better observation errors, and $B_v$ has worse observation errors. The reason for this is the azimuthal angles of the observation geometry of a measurement block. With the select orbit and observational strategy, the tangent profiles are observed from the north-east/west and south-east/west azimuthal angles at the equator. Near the poles however, the azimuthal angles are almost aligned with the east-west direction. This indicates that it is possible to improve $B_v$ observation errors at polar latitudes to the same levels as $B_u$ by more observations from directly north or south of the tangent profiles. Similarly, it also indicates that it is possible to improve the equatorial observation errors for both horizontal components to the levels of $B_u$ at polar latitudes by focusing on east-west or north-south observation geometry depending on the component of interest.
Figure 4. Suggested operational setup scenario. Black lines represent the orbit through seven revolutions. Colored circles represent the estimated error. The maps show the estimations for errors per component averaged between 6 and 78 km.

3.3 Simple estimation of measurable area

We prepared Figure 5 to roughly show the areas over Mars surface where these measurements would be useful. This plot shows the magnetic field strength at 40 km altitude from Cain et al. (2003). It turns out that an area covering about 36% of Mars total area has magnetic field strengths above 200 nT. The areas with more than 1000 nT field strength cover about 4% of the surface. So our suggested measurements is estimated to roughly provide information on the Martian magnetic field over somewhere between 4 and 36% of the area of Mars.
4 Conclusions

We describe an idea that makes measurements of the Martian near-surface crustal magnetic field profiles possible using remote sensing techniques by combining several limb observations. We have performed radiative transfer simulations for radiation measurements in the atmosphere of Mars for one orbiting sensor. These radiative transfer simulations have been fed into a retrieval toolbox to find sensitivities to the magnetic field. Our work shows that limb observations of the sub-millimeter radiation of one absorption line of molecular oxygen can be used to measure two of the three components (the horizontal components) of the magnetic field with around 200 nT accuracy. The vertical resolution on such measurements will be about 4 km for a 30 cm antenna measuring the 368 GHz line from 330 km sensor altitude. The described measurements are sensitive to the magnetic field strength over about one-third of the Martian surface. We have made few assumptions on correlations in the retrieval system to let our method enhance measurement sensitivities rather than a priori sensitivities. With reasonable assumptions on the magnetic source fields or with different orbit/observation geometry, it should be possible to reduce the noise further. We suggest flying a sensor capable of measuring the molecular oxygen absorption line at 368 GHz on a satellite mission to Mars to make a detailed map of the Martian crustal magnetic field and thereby help find the depths, shapes and positions of the crustal field sources.
References


