Satellite based
Temperature Profile Determination
using Passive Microwave and
Radio Occultation Instruments

Berichte aus dem Institut für Umweltphysik Band 2
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Die vorliegende Arbeit ist die inhaltlich unveränderte Fassung einer Dissertation, die
im Jahr 2000 dem Fachbereich Physik/Elektrotechnik der Universität Bremen
Gutachter der Dissertation waren Prof. Dr. K. Künzi und Prof. Dr. G. Kirchengast.

Die Deutsche Bibliothek CIP Einheitsaufnahme
Engeln, Axel /von:
Satellite based temperature profile determination using
passive microwave and radio occultation instruments /
(Berichte aus dem Institut für Umweltphysik ; Bd. 2)
Zugl.: Bremen, Univ., Diss., 2000
ISBN 3-89722-453-4

Dissertation
zur Erlangung des Grades
Dr. rer. nat.
der Universität Bremen

vorgelegt von
Axel von Engeln

März 2000
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Abstract

This work investigates two different satellite-based methods to probe the temperature profile of the atmosphere. On the one hand, passive microwave emissions, on the other hand, radio occultation.

The actual characteristics of the passive microwave instrument Millimeter-Wave Atmospheric Sounder (MAS) were used for an investigation on the possibilities of these type of instruments. The MAS instrument operated onboard the Space Shuttle in the years 1992, 1993, and 1994. The characteristics of the radio occultation instrument were based on the GNSS Receiver for Atmospheric Sounding (GRAS); this instrument is currently developed by the European Space Agency.

The investigation of the different instrument was performed with the optimal estimation method, which uses a priori data for the inversion process. It offers a very easy way to characterize the error of the retrieved parameters. The influence of the temperature profile and the magnetic field of the Earth on the retrieval error of the temperature are determined.

Synthetic retrieval calculations showed that the MAS instrument allows the determination of the temperature profile between 20 and 90 km, with a minimum error of about 2 K in the stratosphere and errors up to 5 K in the mesosphere. The resolution varies between 4 km in the stratosphere and 10 km in the mesosphere.

The developed retrieval algorithm was used to derive stratospheric and mesospheric temperature profiles from actual observations of the MAS instrument onboard the Space Shuttle. A validation with different temperature measuring instruments onboard the Upper Atmosphere Research Satellite (UARS) was performed. Overall, agreement between the instruments was found. Additionally, a validation with ground-based Lidar data was performed.

Possible improvements for a future MAS, like the antenna size, the instrument noise, and the frequency resolution were investigated. Mainly the reduction in the noise of the instrument results in a direct improvement of the retrieval error at all altitude levels.

The GRAS instrument allows the determination of the temperature profile between about 0 and 40 km, above the signal-to-noise ratio is too low. The retrieval error is below 1 K for altitudes up to 30 km, when water vapor is either not present or perfectly known. Otherwise, the water vapor profile can be retrieved, leading to an increase of the temperature retrieval error at levels where water vapor is present. The water vapor profile can be determined up to 5 km for a dry atmosphere and up to 8 km for a moist atmosphere. The resolution for the temperature profile is 0.5 km throughout the troposphere and lower stratosphere and decreases to 1 km at the middle stratosphere. The water vapor profile resolution is 0.5 km.

The measurements of the two instruments have been combined using the optimal estimation method to retrieve one hybrid temperature profile, spanning an altitude interval from 0 to 90 km. The measurement errors entering the retrieval calculation were derived from the MAS and the GRAS instrument specifications. The actual MAS characteristics have been modified to represent a reasonable modern passive microwave receiver, e.g., better antenna, different system noise temperatures.

The obtained accuracy of the temperature profile depends on the chosen a priori constraint of the retrieval calculation. A very conservative estimate was assumed in this study, yielding a retrieval error of around 4 K in the mesosphere, and below 1 K for all altitudes up to 35 km.
Introduction

Mainly the incoming solar radiation is the generator of the temperature structure of the Earth’s atmosphere. About 30% of the solar energy flow are directly reflected into space and about 20% are absorbed at different altitudes in the atmosphere. The remaining 50% are penetrating through the atmosphere, being absorbed by the Earth’s surface. The surface heats up the atmospheric layers just above and the process of convection starts. The radiation balance of the Earth is kept by emitting at long wavelengths.

The resulting general temperature profile can be used to divide the atmosphere into four spheres, of which three are treated in this text. Namely, the troposphere, containing all the daily weather phenomena and extending up to altitudes of about 10 km, followed by the stratosphere, which stretches from about 10 km to about 50 km, and the mesosphere, which covers the altitude interval from about 50 km to roughly 90 km. The thermosphere, located above the mesosphere, is not considered in this text.

The different spheres are characterized by their vertical temperature gradient. Negative temperature gradients are found in the troposphere and mesosphere, whereas a positive gradient is found in the stratosphere. The regions with zero gradient are called tropopause (at about 10 km), stratosphere (at about 50 km), and mesopause (at about 90 km).\(^1\)

This description gives a rather general overview of the atmosphere. Focusing more on details, the temperature in the atmosphere varies with location and on different time intervals. Natural variations are caused by the solar input, volcanic activity, dynamics, and chemical composition. In addition, trends of the temperature development over periods of several decades have been observed, which are thought to be induced by anthropogenic activities.

---

1 The 'zero gradient' definition is in practice replaced by a more complicated definition that ensures unambiguity.

The following trends are attributed to anthropogenic influences:

The increase in greenhouse gas concentrations since preindustrial times have led to a positive radiative forcing of climate, tending to warm the surface and to produce other changes of climate (IPCC, 1996).

Lower to mid tropospheric measurements taken with radiosondes and with the Microwave Sounding Unit aboard the National Oceanic and Atmospheric Administration satellites show a less rapidly warming of the troposphere, which is attributed to natural causes (e.g., volcanic eruptions) and human activities (e.g., the cooling of the upper troposphere resulting from ozone depletion in the stratosphere) (National Academy of Sciences: Panel on reconciling Temperature Observations, 2000).

The stratosphere and the mesosphere show a cooling trend, mainly caused by the depletion of the ozone layer, see WMO (1998) and references therein.

Observation of the tropopause altitude shows an increase of the mean height by several hundreds of meters over the last decades, see WMO (1998) and references therein.

Thus, temperature information alone can give useful information about the state of the atmosphere and the influence of anthropogenic activities. The World Meteorological Organization regards the assessment of stratospheric temperature trends as a high priority in climate change research and treats it as an integral part of the ozone trends report in their Global Ozone Research and Monitoring Project-Reports. Besides information on trends and anthropogenic influence, temperature is an important parameter for weather forecasts, the understanding of chemical, dynamical processes, and the climate system as a whole. A priori knowledge of the temperature profile from numerical weather prediction model forecasts are accurate within 2 K for tropospheric altitudes whereas the error for stratospheric altitudes gradually increases to about 10 K at the stratosphere. Observations with higher accuracy are required to enhance our understanding of the climate system.

In this text, two different types of satellite borne temperature observations fulfilling these requirements are discussed, on the one hand the use of passive microwave emissions of the atmosphere, on the other hand the use of Global Navigation Satellite Systems (GNSS) signals by radio occultation.

Passive microwave instruments provide a good coverage of the temperature profile in the stratosphere and mesosphere, while radio occultation allows the determination throughout the troposphere, up to the middle stratosphere. Especially the radio occultation method is a promising tool for the detection of tropospheric and lower stratospheric temperature trends since it is based on a time measurement, which can be made with very high accuracy. Consequently, data from different satellites can be used without the need of intercalibration. Otherwise the detection of trends would be limited to data of one satellite, owing to a bias which might be present in the data. Radio occultation is overcoming this deficiency of other satellite borne observations.

Additionally, information about water vapor is available from radio occultation data. Water vapor is highly variable and plays a fundamental role in the transport of energy in the atmosphere, it has the greatest effect on the thermodynamics and dynamics of all constituents and dominates the global greenhouse effect. It is therefore highly desirable to obtain information about the water vapor amount in the atmosphere.

Radio occultation can not provide temperature information in the upper stratosphere and mesosphere, here passive instruments come into play. Passive microwave instruments allow temperature measurements up to altitudes of 90 km by using the emission lines of oxygen around 60 GHz.

Both instruments are not limited to day measurements, since they operate independent of solar emissions. This allows for example temperature determinations during polar nights, events especially important in the development of the ozone hole.

This text is separated into five parts covering the theory, and the different instruments: 'Theory', 'MAS', 'GRAS', 'MASGRAS', 'Overall Summary and Conclusions'.

The Theory part consists of three chapters and gives an introduction to the underlying theory of the propagation of electromagnetic waves in a medium like the atmosphere and the formalism of the retrieval (also called inverse) problem, which is encountered in remote sensing. Chapter 1 discusses the influence of the atmosphere on an electromagnetic wave, if absorption is negligible. This situation is encountered in the case of GNSS signals. The influence of the atmosphere is mainly a refractive one, owing to the changing density with altitude of the Earth's atmosphere. Chapter 2 outlines the situation for a passive microwave instrument, where absorption and emission processes determine the observed signal. The radiative transfer equation in its polarized and unpolarized version is derived from Maxwell's equations. Finally, Chapter 3 presents the mathematical process of the retrieval. The retrieval extracts the parameter of interest out of the quantity measured by the satellite, the problem is in general non-linear and underconstrained.

The second part, divided into six chapters, is dedicated to the Millimeter-Wave Atmospheric Sounder (MAS) instrument, a passive microwave instrument. An introduction to the MAS instrument is given in Chapter 4. Chapter 5 describes the polarized forward model for an atmosphere consisting of different layers. The actual setup of the retrieval is outlined in Chapter 6, while a retrieval analysis, based on measurement simulations, is presented in Chapter 7. Results of the temperature retrieval obtained from MAS data are given in Chapter 8, including a comparison with other satellite and ground based instruments. Alternative observation scenarios for a future MAS-like sounder are discussed in Chapter 9. Finally, a summary is given and a conclusion for this part is drawn.

The third part is dealing with the future radio occultation instrument GRAS (GNSS Receiver for Atmospheric Sounding), currently developed by the European Space Agency (ESA), and is divided into three chapters. Chapter 11 introduces the two positioning systems currently available, the American GPS and the Russian GLONASS. Chapter 12 establishes the concept of radio occultation, while Chapter 13 shows how to derive the atmospheric properties from the measurement. A summary, along with a conclusion of this part is given in Chapter 14.

The fourth part, separated into two chapters, assumes a theoretical installation of a passive microwave and a radio occultation instrument on the International Space Station. The passive microwave instrument is observing molecular oxygen lines around 60 GHz, while the radio occultation instrument is observing occultation events of GPS and GLONASS signals. The gain of a combination of the data of these two instruments is discussed,
allowing the derivation of the temperature profile from 0 km to 90 km altitude. Chapter 15 summarizes the necessary modifications of the retrieval algorithm to allow for data of different instruments, and describes the setup of the observation scenario. Finally, Chapter 16 discusses the temperature and water vapor retrieval results. A summary is presented and a conclusion is drawn in Chapter 17.

The final part consists of the ‘Overall Summary and Conclusions’.

Publications

The work described in this text has given rise to a number of publications:

1. The development of a retrieval algorithm for stratospheric and mesospheric temperatures from MAS data is described in:


2. An analysis of the impact of uncertainties in spectroscopic parameters on the retrieval error has been published in:

   as part of

3. A conference paper on the same subject has been published:

   Bühlner, S., A. v. Engeln, and K. Küni, Retrieval of atmospheric mixing ratio profiles from mm/sub-mm limb sounder data: Accuracy requirements on line broadening parameters, in *Atmospheric Spectroscopy Applications, Reims 96, workshop proceedings*, 1996.

4. The developed retrieval algorithm was used for an assessment of the impact of clouds on a planned sub-millimeter wavelength instrument called MASTER. This study was performed for the ESA. The results can be found in the final report:

as part of
Reburn, W. J., et al., Study on upper troposphere/lower stratosphere
CN, 1998.

5. The impact of instrumental parameters on the retrieval quality of an
instrument called SOPRANO was investigated in the following study.
SOPRANO is another ESA planned sub-millimeter wavelengths instru-
ment:
Bühler, S., et al., The retrieval of data from sub-millimeter limb sound-
ing, final report, *Tech. rep.*, ESTEC/Contract No 11979/97/NL/CN,
1998c.

6. The retrieval of stratospheric temperatures from MAS data has been
published in:
Wehr, T., S. Bühler, A. v. Engeln, K. Künzi, and J. Langen, Retrieval of
stratospheric temperatures from space borne microwave limb sounding

7. The retrieval of mesospheric temperatures from MAS data is published
in:
Engeln, A. v., S. Bühler, J. Langen, T. Wehr, and K. Künzi, Retrieval
of upper stratospheric and mesospheric temperature profiles from mill-
imeter-wave atmospheric sounder data, *J. Geophys. Res.*, 103, 31 735

8. A conference paper on the combination of passive microwave data with
radio occultation data is available at:
Engeln, A. v., S. Bühler, G. Kirchengast, and K. Künzi, Temperature
profile retrieval from surface to mesopause by combining gns radio
occultation and passive microwave limb sounder data, in *10th Confer-
ence on Satellite Meteorology and Oceanography*, pp. 240–243, AMS

9. A report on the same topic is published at:
Engeln, A. v., G. Kirchengast, and J. Ramsauer, Accuracy of tempera-
ture and water vapor profiles derived from MAS and GRAS data by op-
Inst. for Meteorol. and Geophys., University of Graz (IGAM/UG),
Austria, 1999.
Part I

Theory
1 Refraction in the Atmosphere

The GNSS satellites emit signals at radio frequencies, around 1.5 GHz, which are detected by receivers located on, for example, aircrafts, satellites, or cars. The signal is generally used to determine the position and velocity of an object, either on the Earth’s surface or above. The influence of the atmosphere on a signal at radio frequencies is mainly refractive. The refractive index is derived from Maxwell’s equations in this chapter. Furthermore, the relation between the refractive index and the atmospheric parameters temperature, pressure, and water vapor is deduced.

1.1 Maxwell’s Equations

These equations have been formulated by James Clerk Maxwell around 1865. To honor his achievement they are commonly referred to as Maxwell’s equations. They relate the electric field \( \vec{E} \), the magnetic field \( \vec{H} \), the electric displacement \( \vec{D} \), the magnetic induction \( \vec{B} \), the electric current density \( \vec{j} \), and the electric charge density \( \rho \) according to:

\[
\vec{\nabla} \cdot \vec{D} = \rho \tag{1.1}
\]

\[
\vec{\nabla} \times \vec{H} = \vec{J} + \frac{\partial \vec{D}}{\partial t} \tag{1.2}
\]

\[
\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \tag{1.3}
\]

\[
\vec{\nabla} \cdot \vec{B} = 0 \tag{1.4}
\]

where the derivative is with respect to time \( t \).

The relations between \( \vec{E} \) and \( \vec{D} \), and \( \vec{H} \) and \( \vec{B} \), known as the material equations, are:

\[
\vec{D} = \varepsilon_0 \vec{E} + \vec{P} \tag{1.5}
\]

\[
\vec{B} = \mu_0 \vec{H} + \vec{M} \tag{1.6}
\]

with the permittivity of vacuum \( \varepsilon_0 \), the permeability of vacuum \( \mu_0 \), the electric polarization \( \vec{P} \), and the magnetic polarization \( \vec{M} \).

The material equations are usually rewritten with the tensors of the permittivity \( \varepsilon \) and the permeability \( \mu \) as:

\[
\vec{D} = \varepsilon \vec{E} \tag{1.7}
\]

\[
\vec{B} = \mu \vec{H} \tag{1.8}
\]

This holds under the assumption that the induced polarizability \( \vec{P} \) (\( \vec{M} \)) will in general be a linear function of the field \( \vec{E} \) (\( \vec{H} \)):\(^1\)

\[
\vec{P} = \varepsilon_0 \chi_e \vec{E} \tag{1.9}
\]

\[
\vec{M} = \mu_0 \chi_m \vec{H} \tag{1.10}
\]

with the tensors of the electric susceptibility \( \chi_e \) and the magnetic susceptibility \( \chi_m \).

The tensors \( \chi_e \) and \( \chi_m \) will reduce to scalars in an isotropic medium, leading to:

\[
\vec{D} = \varepsilon_0 (1 + \chi_e) \vec{E} = \varepsilon_0 \varepsilon_e \vec{E} = \varepsilon \vec{E} \tag{1.11}
\]

\[
\vec{B} = \mu_0 (1 + \chi_m) \vec{H} = \mu_0 \mu_e \vec{H} = \mu \vec{H} \tag{1.12}
\]

introducing the relative permittivity \( \varepsilon_e \), the scalar permeativity \( \varepsilon \), the relative permeability \( \mu_e \), and the scalar permeability \( \mu \).

Equations (1.11) and (1.12) will, for free space, further reduce to:

\[
\vec{D} = \varepsilon_0 \vec{E} \tag{1.13}
\]

\[
\vec{B} = \mu_0 \vec{H} \tag{1.14}
\]

\(^1\) Which is valid for the field strengths encountered in the Earth’s atmosphere (Jackson, 1983)
1.2 Wave Equation

Equations (1.11) and (1.12) state that \( \mathbf{\tilde{B}} \) (\( \mathbf{\tilde{B}} \)) will be in direction of \( \mathbf{E} \) (\( \mathbf{\tilde{H}} \)). This does not generally hold for an anisotropic medium, where the physical properties of the medium are dependent on direction.

Conducting media allow additionally a transportation of charge expressed as a current. A simplified relation between the electric current density \( \mathbf{j} \) and the electric field strength \( \mathbf{E} \) is expressed by the differential form of Ohm’s law:

\[
\mathbf{j} = \sigma \mathbf{E} \tag{1.15}
\]

with the electric conductivity tensor \( \sigma \). The tensor \( \sigma \) is a material constant and will reduce to a scalar in an isotropic medium. Ohm’s law can be deduced from a kinetic gas model, where the Lorentz force is acting on a charged particle (Fliedbach, 1997). The material constant \( \sigma \) is dependent on the time between collisions of the moving particle, collisions can happen with lattice defects and phonons.

where Eq. (1.17) has been inserted after the order of differentiation with respect to time and space has been interchanged. In a similar manner, Eq. (1.17) will lead to:

\[
\Delta \mathbf{\tilde{H}} = \mu \epsilon \frac{\partial^2 \mathbf{\tilde{H}}}{\partial t^2} \tag{1.21}
\]

Equations (1.20) and (1.21) are standard wave equations, thus the solutions at a position \( \mathbf{r} \) have the general form of:

\[
\mathbf{E}(\mathbf{r}, t) = \mathbf{E}_0 \exp \left( i (\mathbf{k} \cdot \mathbf{r} - \omega t) \right) \tag{1.22}
\]

\[
\mathbf{H}(\mathbf{r}, t) = \mathbf{H}_0 \exp \left( i (\mathbf{k} \cdot \mathbf{r} - \omega t) \right) \tag{1.23}
\]

with the wave number vector \( \mathbf{k} \), pointing into the direction of wave propagation, and the angular frequency \( \omega \).

Inserting Eq. (1.22) into Eq. (1.20) yields:

\[
\mathbf{k}^2 \mathbf{E} = \mu \epsilon \omega^2 \mathbf{E} \tag{1.24}
\]

which can only be valid if the wave number vector \( \mathbf{k} \) fulfills:

\[
\mathbf{k}^2 = \frac{1}{\epsilon \mu} \epsilon^2 \omega^2 \tag{1.25}
\]

A general feature of wave equations like (1.20) and (1.21) for a non-absorbing media is that the factor \( \mu \epsilon \) is equal to the inverse of the square of the wave velocity \( c \):

\[
\frac{1}{c^2} = \mu \epsilon = \mu_0 \epsilon_0 \mu \epsilon \tag{1.26}
\]

Since electromagnetic waves travel with light speed \( c \) in vacuum, it follows:

\[
c = \frac{1}{\sqrt{\mu_0 \epsilon_0}} \tag{1.27}
\]

\[\text{2 Which is possible for a medium at rest (Hanel et al., 1992).}\]
1.3 Refractive Index

Equations (1.26) and (1.27) can be combined to yield:

\[ v = \frac{c}{\sqrt{\mu_0 \varepsilon_0}} \]  

(1.28)

stating that the actual velocity of the wave will be reduced by a factor \(1/\sqrt{\mu_0 \varepsilon_0}\) compared to the vacuum velocity of \(c\). The inverse of this factor is called the refractive index \(n\):

\[ n = \frac{c}{v} = \sqrt{\mu_0 \varepsilon_0} \]  

(1.29)

where Eq. (1.29) is called Maxwell’s relation. At radio frequencies, it is possible to rewrite Maxwell’s relation for waves traveling in the Earth’s atmosphere as:

\[ n = \frac{c}{v} = \sqrt{\varepsilon_r} \]  

(1.30)

since the relative permeability is 1.00000037 (Thayer, 1974).

This assumption does not hold for the frequency region around 60 GHz, where strong molecular absorption lines of oxygen are present.

1.4 Polarizability

The influence of the atmosphere on electromagnetic waves emitted by GNSS satellites can be understood with the refractive index as defined by Eq. (1.29), neglecting the effect of absorption. Passive microwave instruments, on the other hand, work with absorption and emission of radiation; these processes are dependent on the parameters of the atoms/molecules.

The connection between the macroscopic material constants \(\mu\) and \(\varepsilon\) and the microscopic polarizability \(\kappa\) of the atoms is given by the Clausius-Mossotti relation. Atoms exposed to a constant electric field \(\vec{E}\) always have an induced electric dipole moment \(\vec{p}\) and may have a permanent electric (or magnetic) dipole moment \(\vec{p}_p\).

The induced electric dipole moment of an atom is given by:

\[ \vec{p} = \kappa \vec{E} \]  

(1.31)

under the assumption that the time averaged charge distribution of the electrons is symmetric. The electrons follow the external electric field in a linear way for this case, which is valid as long as the external field strength is small compared to the internal one.

The charge distribution of molecules is in general not symmetric, so that the polarizability becomes a tensor \(\kappa\). Nevertheless, for gases, the molecules are randomly distributed and the total polarizability can be calculated as the sum of the mean polarizability (Born and Wolf, 1993):

\[ \kappa = \kappa_x + \kappa_y + \kappa_z \]  

(1.32)

in a coordinate system established by \(x, y, z\). For the electric polarization \(\vec{P}\) of an ensemble of \(n_m\) particles follows:

\[ \vec{P} = n_m \kappa \vec{E} \]  

(1.33)

The Clausius-Mossotti relation follows from Eq. (1.33) by considering that the total field \(\vec{E}\) is a sum of the external field and the internal field, generated by the other dipoles in the medium (Jackson, 1983):

\[ \frac{\varepsilon_r - 1}{\varepsilon_r + 2} = \frac{n_m \kappa}{3\varepsilon_0} \]  

(1.34)

So far the permanent dipole moment has been disregarded, if this is present the modified version of Eq. (1.34) reads (Greiner, 1986):

\[ \frac{\varepsilon_r - 1}{\varepsilon_r + 2} = \frac{n_m \kappa + \frac{\vec{P}_p^2}{3kT}}{3\varepsilon_0} \]  

(1.35)

with Boltzmann’s constant \(k\) and the temperature \(T\). This equation is known as Debye’s equation.
1.5 Dielectric Function

The relation between the relative permittivity and the polarizability derived in Section 1.4 is based on a constant electric field \( \vec{E} \). The relative permittivity as a function of frequency is given by the dielectric function.

The dielectric function can be derived from classical mechanics by the following considerations: An electromagnetic wave will lend to a displacement of a charge particle from its equilibrium state, the displacement will vary with the amplitude of the electromagnetic wave at the location of the particle. Focusing on atoms/molecules, the displacement of the nuclei is much smaller than that of the electrons and can therefore be ignored. If one assumes that the electron is bound to an equilibrium state by a simple restoring force and introduces a damping force that includes all processes which lead to a loss of energy, one can formulate the equation of motion for the electron as a simple, damped harmonic oscillator with a driving force given by \( \vec{E}(r, t) \). The solution of this equation will describe the radius vector of the bound electron under the influence of \( \vec{E}(r, t) \), from which the dipole moment can be calculated. Via Eq. (1.31) the polarizability follows and Eq. (1.34) will give the dielectric function for that electron (Born and Wolf, 1993). Atoms or molecules have a number of electrons with different damping and energy loss factors, introducing a number of different resonance frequencies of the harmonic oscillator. The derived dielectric function is in general complex and one generalizes the definition of the refractive index \( n_\text{x} \) such that:

\[
n_\text{x} = n_r + i n_i \tag{1.36}
\]

where the real part is given by Eq. (1.29) and the imaginary part describes the absorption. The absorption coefficient used in radiative transfer is defined as: \( \alpha = -2\pi n_i \).

The concept of a complex refractive index is generally used, but one uses quantum mechanics to calculate the accurate transition frequency of an atom/molecule instead of the classical approach described. The total absorption will be the sum of all individual lines, if one neglects line interference effects.

1.6 Refractivity

The velocity of light in the Earth’s atmosphere is very close to the vacuum velocity, it follows that the refractive index as defined by Eq. (1.29) is close to unity. Therefore, one introduces the refractivity \( N \), which is defined as:

\[
N \equiv (n - 1) \times 10^6 \tag{1.37}
\]

It is possible to derive on a theoretical basis quite accurate relations between \( N \) and the properties of the atmosphere, e.g., temperature \( T \), partial pressure of dry air \( p_\text{d} \), partial pressure of water vapor \( e \), the mean polarizability \( \kappa \) of the atmosphere, and the permanent dipole moment \( \vec{p}_\text{p} \) of water vapor. Dipole moments of other molecules can be neglected, only water vapor has to be considered, owing to the large abundance at low altitudes and the large permanent dipole moment.

More accurate and used in practice are experimental data for the calculation of \( N \) from atmospheric properties. Two different formulas are common, that of Smith and Weintraub (1953):

\[
N = k_1 \frac{p_\text{d}}{T} + k_2 \frac{e}{T} + k_3 \frac{e}{T^2} \tag{1.38}
\]

and the improved formula derived by Thayer (1974):

\[
N = k_1' \frac{p_\text{d}}{T} Z_\text{d}^{-1} + k_2' \frac{e}{T} Z_\text{w}^{-1} + k_3' \frac{e}{T^2} Z_\text{w}^{-1} \tag{1.39}
\]

where the constants are given as:

\[
k_1 = 77.60 \pm 0.01 \text{ K hPa}^{-1}
\]

\[
k_2 = 72 \pm 8 \text{ K hPa}^{-1}
\]

\[
k_3 = (3.75 \pm 0.03) \times 10^5 \text{ K}^2 \text{ hPa}^{-1}
\]

\[
k_1' = 77.60 \pm 0.014 \text{ K hPa}^{-1}
\]

\[
k_2' = 64.8 \pm 0.08 \text{ K hPa}^{-1}
\]

\[
k_3' = (3.776 \pm 0.04) \times 10^5 \text{ K}^2 \text{ hPa}^{-1}
\]
The factors $Z_d$ and $Z_w$ describe the non-ideal gas behavior and are known as compressibility factors for dry air and water vapor. They can be calculated according to Davis et al. (1985):

$$Z_d^{-1} = 1 + \rho_d \left( 57.97 \times 10^8 \left( 1 + \frac{0.52}{T} \right) - 9.4611 \times 10^{-4} \frac{T_c}{T^2} \right)$$

$$Z_w^{-1} = 1 + 1650 \frac{e}{T_c} \left( 1 - 0.01317 T_c + 1.75 \times 10^{-1} T_c^2 + 1.44 \times 10^{-9} T_c^3 \right)$$

with the temperature $T_c$ in °C.

Equation (1.38) can be rearranged by considering that the total pressure is given by $p = \rho_d + e$ and the introduction of a 'constant' $k_4 = k_3 + k_2 T - k_1 T$ to yield:

$$N = 77.6 \frac{p}{T} + 3.73 \times 10^5 \frac{e}{T^2}$$

$$= k_1 \frac{p}{T} + k_4 \frac{e}{T^2} \quad (1.40)$$

where $k_4$ has been calculated with a temperature of 273.15 K.

Five different atmospheres are chosen for an accuracy investigation of these approximations, spanning the range of possible observation scenarios: mid-latitude summer, mid-latitude winter, subarctic summer, subarctic winter, and tropical. The water vapor profiles are obtained from the FASCODE package (Anderson et al., 1986), temperature profiles are taken from an atmospheric model, the COSPAR International Reference Atmosphere (CIRA 86) (Fleming et al., 1990). The corresponding profiles are shown in Figure 1.1.

The approximation Eq. (1.40) is compared to the accurate formula (1.38) in Figure 1.2 (Left), deviations are within 0.02 % for the set of standard atmospheres. The Smith-Weintraub Equation (1.38) and the formula given by Thayer (1.39) have been compared in Figure 1.2 (Right), they agree within 0.1 %. Thus, the approximation given by Eq. (1.40) is very accurate and is therefore widely used in radio occultation data processing. Equation (1.40) is independent of wavelength which holds for the microwave region of the spectrum, the refractivity is wavelengths-dependent for frequencies above 300 GHz (Fischer, 1988).

---

3 Except for small effects around the absorption bands of oxygen (60 GHz and 119 GHz) and water vapor (22 GHz and 183 GHz).
Figure 1.2: Left: Comparison between the accurate Smith-Weintraub Equation (1.38) (SW) and the approximation given by Eq. (1.40) (SWa); Right: Comparison between the accurate Smith-Weintraub Equation (1.38) (SW) and Eq. (1.39) given by Thayer.
2 Radiative Transfer

Passive remote sensing instruments detect the radiation emitted from the atmosphere. The atmosphere is mainly emitting in the far infrared part of the spectrum, but the intensity in the microwave range is sufficient for satellite observation and has the advantage of being almost insensitive to aerosols and clouds. The detected intensity contains implicit information about the parameters of interest. The extraction of these parameters from the satellite measurement requires knowledge of the radiative transfer in the atmosphere. The radiative transfer equation describes the behavior of the electromagnetic wave while propagating through an absorbing and emitting medium. It is deduced from Maxwell’s equations in this chapter.

2.1 Wave Equation

The assumption of an isotropic atmosphere, as stated in Section 1.2, is not valid for frequencies where absorption lines of oxygen are present. The permanent magnetic dipole moment of oxygen will align with respect to the magnetic field of the Earth, thus breaking the isotropy. In contrast, isotropy is given for the permittivity, the approximation $\epsilon = \epsilon_0$ is valid.

In contradiction to Section 1.2 one starts with Eq. (1.17), since oxygen will interact with the magnetic component of the field. Acting with the same vector identity as given in Section 1.2 on Eq. (1.17) leads to:

$$\nabla (\nabla H) - \nabla^2 H = \nabla \times \varepsilon_0 \frac{\partial E}{\partial t}$$  (2.1)

After changing the order of differentiation and inserting Eq. (1.18) this yields:

$$\nabla (\nabla \cdot H) - \nabla^2 H = -\epsilon_0 \frac{\partial^2}{\partial t^2} \mu H$$

(2.2)

$$= -\epsilon_0 \mu_0 \frac{\partial^2}{\partial t^2} ((I + \chi_m)H)$$

(2.3)

by keeping in mind that the isotropy is not given for the magnetic part of the wave. The identity matrix is symbolized by $I$.

The spatial dependence of Eq. (2.2) is a function of $z$ only, if we assume a coordinate system in which the $z$ direction corresponds to the propagation direction. Performing the spatial derivatives will yield:

$$\frac{\partial^2}{\partial z^2} (H(z) - H(z) \vec{e}_z) + \epsilon_0 \mu_0 \frac{\partial^2}{\partial t^2} ((I + \chi_m)H(z)) = 0$$

(2.4)

with the unity vector in $z$ direction $\vec{e}_z$.

The $z$ component of the magnetic field is small, compared to the components in $x$ and $y$ direction, which follows from the following considerations:

The anisotropy of the atmosphere with respect to $\chi_m$ is only small, for the elements of that matrix the relation:

$$|\chi_m | \ll 1$$

(2.5)

holds (Lencor, 1967).

Electromagnetic waves are transverse, the $z$ components of the magnetic induction and the electric field are zero.

Using the $z$ component of Eq. (1.8) and inserting $B_z = 0$ yields:

$$H_z(z) = -\frac{\chi_m}{1 + \chi_m} H_x(z) - \frac{\chi_m}{1 + \chi_m} H_y(z)$$

(2.6)

Equation (2.6) states that the $z$ component of $\vec{H}$ is not equal to zero, caused by the slight anisotropy of the medium. But, compared to the other components, $H_z \ll H_x, H_y$ holds, and Eq. (2.4) simplifies to:

$$\frac{\partial^2}{\partial z^2} \tilde{H}(z) + \epsilon_0 \mu_0 \frac{\partial^2}{\partial t^2} ((I + \chi_m)\tilde{H}(z)) = 0$$

(2.7)
2.2 Coherency Matrix

The dimension of the matrix \((I + \chi_m)\) is generally \(3 \times 3\), but reduces to a 
\(2 \times 2\) matrix by disregarding the \(z\) component of the magnetic field.

Rearrangement of Eq. (2.7) and the introduction of a matrix \(G^2\) defined as:
\[
G^2 = -\varepsilon_0 \mu_0 (I + \chi_m)
\]

yields the wave equation:
\[
\frac{\partial^2}{\partial z^2}\bar{H}(z) - G^2 \frac{\partial^2}{\partial t^2}\bar{H}(z) = 0
\]

(2.9)

A general feature of wave equations is that the factor \(G\) is the inverse of the velocity of the wave. The solutions of this wave equation are:
\[
\bar{H}(z) = e^{\pm i(G\omega z - \omega t)} \bar{H}(0)
\]

(2.10)

for waves traveling in positive or negative \(z\) direction. The angular frequency is denoted by \(\omega\). The square root of \(G\), called the complex propagation matrix, is approximately given by (Lieber and Hufford, 1989):
\[
G = i \sqrt{\varepsilon_0 \mu_0} \left( I + \frac{1}{2} \chi_m \right)
\]

(2.11)

Errors are in the order of \(\chi_m^2\) (Lieber and Hufford, 1989).

2.3 Brightness Temperature

The specific intensity \(I_\nu\) for a frequency \(\nu\) of a radiation field is generally described by the brightness temperature in the microwave case. The brightness temperature \(T_B\) is defined as follows:
\[
T_B(\nu) \equiv \frac{\lambda^2}{2k} I_\nu
\]

(2.16)

where \(\lambda\) is the wavelength and \(k\) is Boltzmann’s constant. Historically, it is based on the Rayleigh-Jeans approximation to the Planck function. The Planck function \(B_\nu\) is given by:
\[
B_\nu(\nu, T) = \frac{2 \hbar \nu^3}{c^2} \frac{1}{e^{\hbar \nu/kT} - 1}
\]

(2.17)

where the Planck constant is denoted by \(h\). The Rayleigh-Jeans approximation \(B_{RJ}\) of the Planck function is given by:
\[
B_{RJ}(\nu, T) = \frac{2 \hbar \nu^3}{c^2} \frac{kT}{h\nu} = \frac{2kT}{\lambda^2}
\]

(2.18)

The brightness temperature \(T_B\) is equal to the physical temperature \(T\) of the medium in the Rayleigh-Jeans approximation.

The generalization of \(T_B\) to a matrix \(T_B\) is straightforward. The brightness temperature in a specific basis is given in the diagonal elements, the
off-diagonal elements give information about the cross correlation. The degree of polarization can be calculated by:

\[ P = \sqrt{1 - \frac{4|T_B|}{(Tr(T_B))^2}} \]  \hspace{1cm} (2.19)

where Tr denotes the trace of the matrix and the determinant of \( T_B \) is given by \( |T_B| \).

### 2.4 Radiative Transfer Equation

Lencir (1967) has shown that the real part of the coherency matrix has the same characteristics as the brightness temperature matrix \( T_B \) and Eq. (2.15) can be written as:

\[ T_B(z) = e^{G_{\omega z}} T_B(0) e^{G^1_{\omega z}} \]  \hspace{1cm} (2.20)

for an incident radiation \( T_B(0) \). Equation (2.20) does not incorporate the emission of the layer itself, and the complete radiative transfer equation for the polarized case is given by:

\[ T_B(z) = e^{G_{\omega z}} T_B(0) e^{G^1_{\omega z}} + T(I - e^{G_{\omega z}} e^{G^1_{\omega z}}) \]  \hspace{1cm} (2.21)

for one layer.

Lencir (1967) focused in his work on two cases, where the magnetic field direction and the observing direction are either perpendicular or aligned. These simplifications are possible for ground-based instruments by pointing the instrument accordingly, but they are unsuitable for satellite observations. The correct radiative transfer equation as given by Eq. (2.21) can be found in Rosenkranz and Staelin (1988).

The first term on the right hand side of Eq. (2.21) gives the effect of the layer on the incident radiation, the multiplication with the exponential of the matrix \( G \) leads in general to a change of the polarization and to absorption. The second part is the contribution from the layer itself, following the Rayleigh-Jeans approximation to Planck’s law. Strong absorption leads to a strong influence of the second term, while the incident radiation plays a minor role and the received signal gives information about the temperature of the layer. The signal is said to be saturated and the layer appears opaque. The first term is important for low absorption, the received signal gives no information about the layers temperature, the layer is said to be transparent.

The unpolarized version of the radiative transfer equation follows from Eq. (2.21) by considering that the brightness temperature matrices are diagonal for unpolarized calculation and commute with the matrices \( e^{-G_{\omega z}} \) and \( e^{-G^1_{\omega z}} \). Rearranging Eq. (2.21) yields:

\[ T_B(z) = T_B(0) e^{G_{\omega z}} e^{G^1_{\omega z}} + T(I - e^{G_{\omega z}} e^{G^1_{\omega z}}) \]  \hspace{1cm} (2.22)

\[ = T_B(0) e^{G_{\omega z} + G^1_{\omega z}} + T(I - e^{G_{\omega z} + G^1_{\omega z}}) \]  \hspace{1cm} (2.23)

The matrix \( G \) for an isotropic medium is defined as (see Eq. (1.12) and Eq. (2.11)):

\[ G = i \sqrt{\epsilon_0 \mu_0} \sqrt{\mu_e} \]  \hspace{1cm} (2.24)

\[ = i c^{-1} \sqrt{\mu_e} \]  \hspace{1cm} (2.25)

and it follows for Eq. (2.23):

\[ T_B(z) = T_B(0) e^{i k (n-n^*) z} + T(I - e^{i k (n-n^*) z}) \]  \hspace{1cm} (2.26)

\[ = T_B(0) e^{-2k n_1 z} + T(I - e^{-2k n_1 z}) \]  \hspace{1cm} (2.27)

with the wave number \( k = \omega / c \) and the complex part of the refractive index \( n_1 \) (see Eq. (1.29)).

Equation (2.26) gives the brightness temperature measured in the chosen basis. The received radiation is unpolarized and therefore independent of the basis, the scalar version of Eq. (2.26) gives the unpolarized radiative transfer equation:

\[ T_B = T_B(0) e^{-\alpha z} + T(1 - e^{-\alpha z}) \]  \hspace{1cm} (2.28)

with the absorption coefficient defined as:

\[ \alpha = -2k n_1 \]  \hspace{1cm} (2.29)
The two terms on the right hand side of Eq. (2.28) can be interpreted as the ones discussed in connection with Eq. (2.21), the difference being that the polarized case alters the phase and the intensity.
3 Inverse/Retrieval Model

The inverse/retrieval model calculates the variables of interest from the observed quantity, which is the observed brightness temperature in the case of the passive microwave limb sounder, or the refraction in the case of the radio occultation instrument. The variables of interest, e.g., the temperature profile and volume mixing ratios, are implicitly given in the observed quantity. The inverse model needs the forward model for the extraction of these variables. The forward model simulates the observed quantity for an observation scenario. Input variables to the forward model are the state of the atmosphere, defined by the temperature, pressure, and volume mixing ratio profiles. Additionally, the instrument characteristics have to be known.

The inverse model describes the unknown atmospheric parameters as a function of the measured quantity, calculated with the aid of the forward model.

3.1 Forward Models

For a passive microwave instrument, the forward model simulates the theoretical spectral power seen by the instrument by applying the radiative transfer equation for a number of atmospheric layers. The variables of interest are implicit in the radiative transfer equation and therefore in the received spectral power measured by the instrument. They are in general hidden in the absorption coefficient (complex propagation matrix) of the radiative transfer equation for volume mixing ratios. However, the temperature is explicitly given in the radiative transfer equation, and also implicitly in the absorption coefficient (complex propagation matrix).

For a radio occultation instrument, the forward model calculates the refraction caused by the varying density field of the Earth’s atmosphere. Temperature and water vapor information is implicitly given in the refraction.

3.2 Optimal Estimation Method (OEM)

The optimal estimation method reviewed by Rodgers (1976) is used for the inverse model. The forward model $F$ calculates the measurement vector\(^1\) $y$ from the unknown variables $x$ and the constant model parameters $b$:

\[ y = F(x, b) \]
\[ = Kx \] (3.1)

Eq. (3.2) follows under the assumption that the forward model can be linearized, $K$ denotes the weighting function matrix.

As mentioned above, the unknown variables are in general the atmospheric parameters of interest, profiles of volume mixing ratio for example, but can also be parameters of the instrument which change during the operation. Examples for $b$ are the known instrument parameters, or spectroscopic data.

The direct solution to Eq. (3.2) is given by:

\[ x = K^{-1}y \] (3.3)

Here, $K^{-1}$ denotes the pseudo inverse of the weighting function $K$.

The problem in mathematical terms can be expressed for two given spaces, the state space of the atmosphere and the measurement space, as following: The state vector $x$ describes the state of the atmosphere and $\mathbf{y}$ the measurement.

---

\(^1\) Note, that symbols with vector arrow have been used for vectors so far, following general notations for Maxwell’s equations. The notation here follows the one used by Rodgers (1976), which is common among the scientific community dealing with inverse problems in remote sensing.
the measurement vector \( \mathbf{y} \) represents the measurement quantity, here the received atmospheric signal. The matrix \( \mathbf{K} \) represents an operator which projects the state space into the measurement space.

Equation (3.3) does not work for remote sensing problems in general, since the problem encountered might be under-constrained. The OEM resolves this problem by the introduction of a second virtual measurement, which stabilizes the solution. This a priori information is usually taken from an atmospheric model and represents the knowledge of the state vector \( \mathbf{x} \) before the measurement was taken.

The solution of the OEM is not the exact state vector \( \mathbf{x} \), owing to errors of the instrument, but the most likely solution \( \hat{\mathbf{x}} \). The OEM for a linear problem is given by:

\[
\hat{\mathbf{x}} = (\mathbf{S}_0^{-1} + \mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K})^{-1} (\mathbf{S}_0^{-1} \mathbf{x}_0 + \mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{y})
\]  
(3.4)

where \( \mathbf{x}_0 \) is the a priori information, \( \mathbf{S}_y \) the covariance matrix of the measurement, \( \mathbf{S}_0 \) the a priori covariance matrix and \( \mathbf{K}^T \) the transpose of \( \mathbf{K} \).

One can see from Eq. (3.4) that \( \hat{\mathbf{x}} \) represents a weighted mean of \( \mathbf{x}_0 \) and the real state \( \mathbf{x} \) (given in measurement space by \( \mathbf{y} = \mathbf{K} \mathbf{x} \)). The weights are \( \mathbf{S}_0^{-1} \) and the projection of the measurement error into the state space: \( \mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K} \).

This is analogue to the scalar case: Two independent measurements \( x_1 \) and \( x_2 \) of a quantity \( x \) with variances \( \sigma_1 \) and \( \sigma_2 \) are combined to calculate \( \hat{x} \):

\[
\hat{x} = \left( \frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2} \right)^{-1} \left( \frac{x_1}{\sigma_1^2} + \frac{x_2}{\sigma_2^2} \right)
\]  
(3.5)

The retrieval of atmospheric parameters is in general a non-linear problem and an iterative approach using Newtonian iteration is necessary. Therefore the forward model is approximated by a Taylor series around the point \( \mathbf{x}_0 \):

\[
\mathbf{y} = F(\mathbf{x}_0) + \frac{\partial F}{\partial \mathbf{x}} \bigg|_{\mathbf{x}=\mathbf{x}_0} (\mathbf{x} - \mathbf{x}_0) = \mathbf{y}_0 + \mathbf{K}_0 (\mathbf{x} - \mathbf{x}_0)
\]  
(3.6)

where \( \frac{\partial F}{\partial \mathbf{x}} = \mathbf{K} \) is the Jacobian Matrix. The Taylor series is only calculated up to the first term, assuming that linearity is valid in the vicinity of \( \mathbf{x} \). The first iteration step starts from the a priori vector \( \mathbf{x}_0 = \hat{\mathbf{x}}_n \), calculating the next inversion step \( \mathbf{x}_{n+1} \) by:

\[
\mathbf{x}_{n+1} = \hat{\mathbf{x}}_n + \mathbf{D} (\mathbf{y} - \mathbf{y}_n - \mathbf{K}_n (\mathbf{x}_0 - \mathbf{x}_n))
\]  
(3.7)

where \( \mathbf{y}_n \) is the spectrum calculated with the forward operator by \( F(\hat{\mathbf{x}}_n, \mathbf{b}) \).

The contribution function \( \mathbf{D} \) is defined as:

\[
\mathbf{D} = (\mathbf{S}_0^{-1} + \mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K})^{-1} \mathbf{K}^T \mathbf{S}_y^{-1}
\]  
(3.8)

The Jacobian matrix \( \frac{\partial F}{\partial \mathbf{x}} = \mathbf{K} \) can be calculated analytically for a forward operator without correlation between the different levels of the retrieval, e.g., for volume mixing ratios. This analytical solution is not given for temperature retrieval when the temperature profile is assumed to be hydrostatic, since deviations of the temperature profile at a certain level for the calculation of \( \mathbf{K} \) will affect the pressure profile for all other altitudes.

The quality of the retrieval can be visualized with the aid of the averaging kernel matrix (AKM):

\[
\mathbf{A} = \left( \frac{\partial F}{\partial \mathbf{y}} \right) \cdot \left( \frac{\partial F}{\partial \mathbf{x}} \right) = \mathbf{D} \mathbf{K}
\]  
(3.9)

The retrieved state vector can be expressed as:

\[
\hat{\mathbf{x}} = \mathbf{A} \mathbf{x} + (\mathbf{I} - \mathbf{A}) \mathbf{x}_0
\]  
(3.10)

The AKM is a square matrix with the dimension of the retrieval parameters. A value close to 1 of the corresponding AKM diagonal element of a retrieval parameter indicates that the information comes from the measurement, a value close to 0 implies that the inversion parameter comes from the a priori information. The width of the averaging kernel matrix row gives the smoothing over an altitude range of the inversion parameter.

The error in the retrieval is represented by the statistical error covariance matrix \( \mathbf{S} \) of the last iteration:

\[
\mathbf{S} = \mathbf{S}_N + \mathbf{S}_M = (\mathbf{A} - \mathbf{I}) \mathbf{S}_0 (\mathbf{A} - \mathbf{I})^T + \mathbf{D} \mathbf{S}_y \mathbf{D}^T
\]  
(3.11)
where $S_N$ is the null-space error, $S_M$ the measurement error, and $I$ the identity matrix.

The first term in Eq. (3.11) represents the smoothing due to the limited altitude resolution of the retrieval and the second one the measurement noise that propagates into the retrieval. Equation (3.11) gives the error of the retrieval, assuming that other model parameters are perfectly known. Such parameters are for example the spectroscopic data, which are needed to calculate the absorption coefficients. The impact of different model parameters could be investigated by introducing these as retrieval parameters or by calculating a model parameter error $S_S$ that adds to Eq. (3.11):

$$S_S = D K_b S_b (D K_b)^T$$

where $S_b$ is the covariance matrix of the model parameters and $K_b$ is calculated in the same manner as $K$, by linearizing the forward model at some state $\vec{b}$:

$$K_b \equiv \frac{\partial F}{\partial b} \bigg|_{b_{-b}}$$

(3.13)

The correlation of different retrieval parameters can be extracted from the off-diagonal elements of the covariance matrix $S$ by:

$$C[i,j] = \frac{S[i,j]}{\sqrt{S[i,i] S[j,j]}}$$

(3.14)

Values of 1 of the correlation matrix $C$ correspond to full correlation, while 0 indicates no correlation, hence the diagonal elements are all 1 by definition.

### 3.3 Program Description

An inversion program applying the OEM was developed by Stefan Bühler, Tobias Wehr, and the author.

The simplified chart diagram of the inversion program is presented in Figure 3.1. The primary input parameters are the measurement spectrum $y$, the corresponding covariance matrix $S_y$, the a priori vector $\vec{x}_0$, and the covariance matrix $S_0$. The forward program calculates the synthetic spectrum $\tilde{y}$ by use of the a priori vector $\vec{x}_0$. The temporary matrices $R_y$ and $R_b$ will then be calculated, they are the inverse matrix of $S_y$ and $S_0$, respectively, and will not be altered during the calculation. The variable $n$ gives the iteration number and starts for the first iteration with $n = 0$. The major calculation time is spend in the forward program during the calculation of the Jacobian Matrix $K_n$.

Afterwards, the inversion program will perform the optimal estimation and calculate $\vec{x}_{n+1}$. The iteration loop will terminate when either the maximum number of iterations has been reached or the difference between the result of the former iteration $\vec{x}_n$ and the result of this iteration $\vec{x}_{n+1}$ are negligible.

The AKM matrix is calculated after the iteration loops terminates. The correct approach for the calculation of the AKM matrix $A$ and the error matrices $S_N$, $S_M$ is to take the final result $\vec{x}_{n+1}$ of the iteration and calculate the Jacobian Matrix $K$ and the sensitivity of the retrieval to the measurement $D = \partial I/\partial y$. In spite of that, it is possible to use the results of the $n$th iteration in the calculation if the iteration loop has converged and $\vec{x}_n \approx \vec{x}_{n-1}$ and $K_n \approx K_{n-1}$ holds.

The derivative $F'$ of the forward model $F$ with respect to the input parameter $x$ is calculated as:

$$F' = \frac{F(x + \Delta x) - F(x)}{\Delta x}$$

(3.15)

where $\Delta x$ should be small. $F'$ corresponds to one column of the matrix $K$ and has the dimension (number of frequencies) x (number of altitudes). The temperature profile has to be made hydrostatic for the retrieval, this is done by the hydrostatic equation. This step is only required for the retrieval of a temperature profile.
3.4 Retrieval Result Plots

The visualization of the retrieval results can be quite complicated, generally one is interested in the retrieved profile, the resolution of the profile, given by the AKM, the error of the obtained profile, and possible correlations with other retrieval parameters. The results presented here are generated with a visualization tool developed at the University of Bremen by Stefan Bihler, Joachim Urban, and the author. The tool allows the presentation of the essential information in a very compact format. Figure 3.2 is chosen as an example for the output, it shows the retrieval of a mid-latitude summer temperature profile from a synthetic measurement. The MAS instrument characteristics were used to generate the synthetic measurement. A thorough discussion on the MAS instrument is performed in the MAS part.

The title of the output gives the jobname of the calculation and the displayed species. The top left plot shows the a priori profile, the retrieved profile, and the true profile. The a priori profile is not identical to the true profile for this example, otherwise no true profile would have been indicated. The grey shaded area gives the a priori error of the profile. Horizontal bars indicate the statistical retrieval error, where the inner thicker part denotes the measurement error and the outer part the nullspace error, the total error is given by the vertical bars.

The top right plot gives information about the resolution of the performed retrieval, by showing the averaging kernel functions for the displayed species. For selected retrieval cases there are two numbers to the right of the retrieval level indicating the altitude and the full width at half maximum of the kernel function in kilometers. The solid black line represents the sum of all kernel functions.

The bottom plot to the left shows the error expressed by the square root of the ratio of the diagonal elements of $S$ to the diagonal elements of $S_0$. Additionally, the measurement error ratio (square root of the ratio between the diagonal elements of $S_M$ to the diagonal elements of $S_0$) and the null space error ratio (square root of the ratio between the diagonal elements of $S_N$ to the diagonal elements of $S_0$) can be included. Alternatively, the total error, corresponding to the 1σ error is given.

Figure 3.1: Flow chart of the retrieval program. The figure is discussed in Section 3.3.
The bottom right plot shows the correlations between the species displayed and other retrieval species or parameters. The information is obtained from the off-diagonal elements of $S$. The correlation matrix $C$ is derived from $S$ according to Eq. (3.14). Correlations do not introduce additional errors, they are a measure of the fraction of the statistical error that is correlated. A correlation with a species of almost unity, for example, indicates that the statistical error will be almost zero if that other species is not retrieved but perfectly known. The maximum and minimum correlation of the displayed species to another retrieval species/parameters at the altitude indicated is plotted. The minimum and maximum is found by searching all correlations, independent of the altitude of the other retrieval species/parameters. This results in almost symmetric correlations for species, since strong correlations at one altitude level are usually accompanied by strong anti-correlations at the adjacent retrieval levels. Scalar retrieval parameters, as displayed in this example, show only a single curve.

The text in the middle of each retrieval output gives information about additional parameters that are retrieved, and can include the error assumed on the measurement. The bottom of the page provides information about the program used for the output, the date of the plot generation, and the number of iterations calculated.

Figure 3.2: Synthetic temperature retrieval results for a mid-latitude summer scenario

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2 The actual meaning of the parameters displayed is discussed in the MAS part of this work.
Part II

MAS
4 MAS Instrument

The microwave emission of atmospheric trace gases is sensitive to temperature, the measurement of the temperature profile will therefore improve the accuracy of the trace gas profile measured in the same air volume. Moreover, information about the temperature distribution in the atmosphere is of direct interest to atmospheric physics and chemistry.

One method to measure temperature is based on the observation of molecular oxygen emission lines around 60 GHz, since molecular oxygen has a known volume mixing ratio over the considered altitude range (usually 0 km to 100 km) and a strong line spectrum.

This chapter describes the instrument characteristics of the MAS instrument, and gives an overview of the different scan scenarios.

4.1 MAS Instrument Characteristics

The MAS instrument was operated during the ATLAS1 missions 1-3 onboard of the Space Shuttle. Time and duration of the ATLAS missions are given in Table 4.1.

Table 4.1: ATLAS Missions

<table>
<thead>
<tr>
<th>ATLAS</th>
<th>ATLAS-1</th>
<th>ATLAS-2</th>
<th>ATLAS-3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Start time</td>
<td>March 24, 1992</td>
<td>April 8, 1993</td>
<td>November 3, 1994</td>
</tr>
<tr>
<td>Mission duration</td>
<td>9 days</td>
<td>9 days</td>
<td>11 days</td>
</tr>
<tr>
<td>Number of orbits</td>
<td>142</td>
<td>148</td>
<td>175</td>
</tr>
</tbody>
</table>

1 Atmospheric Laboratory for Applications and Science

Figure 4.1: Observation geometry for limb sounding

Main aims of the ATLAS missions were atmospheric science, solar science, space plasma physics and ultraviolet astronomy. The MAS instrument was part of the atmospheric science payload, studying the chemistry and physics of the upper atmosphere.

The MAS observes the limb perpendicular to the flight direction. The latitudinal coverage is either 70° N to 40° S or 70° S to 40° N, depending on the Space Shuttle orientation. The duration of one scan cycle corresponds to a ground distance of about 100 km. A detailed instrument description can be found in Croskey et al. (1992).

The schematic configuration of the limb sounding geometry is sketched in Figure 4.1, where rt denotes the tangent altitude.

The MAS is a passive microwave instrument, using heterodyne technique to measure the temperature profile, and VMR (Volume Mixing Ratio) profiles of ClO, O3, and H2O. It observes the 61.151 GHz oxygen line for the temperature measurement and the oxygen lines located at 62.968 GHz and 63.569 GHz for an accurate tangent altitude determination, since the altitude determination with the Shuttle navigation system is imprecise. The frequency resolution is given in Table 4.2, the coverage of the filter-channels is symmetric around the line center.

As a consequence of the heterodyne technique, the MAS observes not only at the center frequency of the individual oxygen lines, but as well at a second frequency interval. These two intervals are located symmetric to the local oscillator frequency (LOF). The LOF for the oxygen channels is 66.394 GHz. The two frequency intervals are referred to as upper and lower
sideband, where the MAS oxygen lines are all within the lower sideband. This kind of receiver is called a Double Sideband Receiver. A suppression of information coming from one band leads to a Single Sideband Receiver.

The tangent altitude information is extracted from the shape of the lines at 62.998 GHz and 63.569 GHz, therefore the high resolution of the temperature line is not necessary. These lines can be used for temperature measurements as well, however, the 61.151 GHz line allows a better determination in the mesosphere.

The Oz VMR profiles are obtained from the line at 184.377 GHz, H2O from the line at 183.310 GHz and ClO by using the line at 204.352 GHz. Retrievals of these profiles were already performed by Hartmann et al. (1996), where a combination of model and meteorological data was used for the temperature profile.

4.2 MAS Observation Scenarios

The MAS scans the atmosphere in different modes, depending on the species and the altitude of interest. The scan scenario consists of four phases, the first phase is the downscan from altitudes of about 130 km to altitudes of 10 km. The second phase is a hot calibration of the receiver with a body of a known temperature at the lowest tangent point. This is achieved by a mirror, placed in the ray path. The third phase is the upscan from about 10 km to 130 km, followed by the fourth phase, a cold calibration with the cosmic background radiation. The movement of the antenna (velocity that was used to perform the vertical scan) of the up and down scan was varied according to the main focus of the observation.

<table>
<thead>
<tr>
<th>Line</th>
<th>Bandwidth [MHz]</th>
<th>Number of Filter-channels</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>[GHz]</td>
<td>40 MHz</td>
</tr>
<tr>
<td>61.151</td>
<td>400</td>
<td>10</td>
</tr>
<tr>
<td>62.998</td>
<td>400</td>
<td>10</td>
</tr>
<tr>
<td>63.569</td>
<td>400</td>
<td>10</td>
</tr>
</tbody>
</table>

Figure 4.2: Positions of MAS 'IMPS' mode tangent points for the ATLAS1 mission

In total, there are three major scan modes, the 'IMPS' mode is focusing on stratospheric observations, and the scan between 130 km and altitudes of about 70 km is performed with high velocity, in order to increase the integration time in the stratosphere. The positions of the 'IMPS' measurements for the ATLAS1 mission are presented in Figure 4.2.

The second mode is the 'POIN' mode, where a pointing to a certain altitude is performed. The 'POIN' mode has been used to observe the weak ClO line, no scan information is available for this observation scenario. The measurement positions for the ATLAS1 mission are shown in Figure 4.3.

The third major mode is 'SCAN', where the scan between 130 km and 10 km is performed with a uniform velocity. This mode is suited best for the detection of mesospheric temperatures. The available 'SCAN' mode measurements for the ATLAS1 mission are presented in Figure 4.4.
MAS tangent points, Mode: POIN, year: 1992

Figure 4.3: Positions of MAS ‘POIN’ mode tangent points for the ATLAS 1 mission

MAS tangent points, Mode: SCAN, year: 1992

Figure 4.4: Positions of MAS ‘SCAN’ mode tangent points for the ATLAS 1 mission
5 Forward Model

Data simulation is performed by use of the forward model, as introduced in Chapter 3. The model $F$ contains all the known information about the atmospheric composition such as species, spectroscopic parameters, volume mixing ratios and the temperature/pressure profile. Using this information, the forward program will perform the radiative transfer (see Chapter 2) for a number of atmospheric layers and calculate the theoretical received signal, depending on frequency and altitude. It applies the instrument characteristics like antenna pattern, sideband and filter-channel convolution. The output of $F$ is used in the inverse model to find the true profiles of the species of interest in an iterative process.

Generally it is possible to use the unpolarized form of the radiative transfer equation in the calculations, nevertheless this approximation is not valid for oxygen molecules since oxygen interacts with the magnetic field of the Earth via a magnetic dipole moment, making the radiative transfer polarized. This leads to Zeeman-Splitting of the oxygen lines. The modeling of this effect requires a polarized radiative transfer calculation through the atmosphere. The forward model has to be extended by additional features such as the Earth's magnetic field. The magnetic field depends on the geographic location, thus the location of the instrument and the observation direction has to be taken into account. It is feasible to use an unpolarized approximation below 50 km, by omitting information from the line center. This is possible since most of the information can be acquired from the lineshape which is at these altitudes dominated by pressure broadening. Temperature retrieval from MAS data, where this approximation was applied, can be found in Wehr et al. (1998).

This chapter introduces first the spectroscopy necessary to model the molecular oxygen lines around 60 GHz. A suitable form of the radiative transfer for a number of layers is derived next. Afterwards, the different instrument effects on the observed brightness temperature are explained, followed by the effects introduced by the magnetic field.

5.1 Spectroscopy

Most of the molecule lines encountered in the microwave frequency region are caused by molecular rotation and the interaction of the electric part of the electromagnetic wave with the electric dipole moment of the molecule. The specific parameters like center frequency, intensity, quantum numbers of each line are given in a spectroscopic catalog, from which the unpolarized absorption coefficient, as given by Eq. (2.29), can be calculated.

The process responsible for the molecular oxygen lines around 60 GHz is not a pure rotational one. The line spectrum of molecular oxygen is the result of spin flip transitions at different rotational levels. The spin $S$ results from two unpaired electrons leading to $S = 1$ for the O$_2$ molecule. The orbital angular momentum is zero and the spin angular momentum is coupled to the rotational angular momentum through a weak magnetic field arising from the molecular rotation. This coupling can be approximated by a Hund's case (b) (Gordy and Cook, 1970), and the vector addition of $S$ and the rotational quantum number $N$ leads to a total of 3 levels of the total angular momentum $J$ per rotational level. Two different transitions are permitted: from the $J = N$ to the $J = N + 1$ level (designated as $N+$ lines) and between the $J = N$ and the $J = N - 1$ level (designated as $N-$ lines). Only odd $N$ values are allowed owing to symmetry requirements. Applying a magnetic field will split up a $J$ level into $(2J + 1)$ sublevels.

The oxygen spectrum around 60 GHz is presented in Figure 5.1, where the strongest oxygen lines at a tangent altitude of 100 km are visible. The MAS measures the 9+, 15+, and 17+ lines. The different intensities reflect the Boltzmann distribution.

The sublevels are classified according to their magnetic quantum num-

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1 The transition between level $J = N + 1$ to $J = N - 1$ are forbidden and transitions between levels with different $N$ quantum numbers are found at sub-millimeter wavelengths (see Section 9.1).
5.2 Integrated Radiative Transfer Equation

The unpolarized and polarized form of the radiative transfer equation derived in Chapter 2 are valid for a one layer scenario. The radiative transfer through the atmosphere is performed by separating the atmosphere into small, homogeneous layers, with a layer size of around 1 km. The received signal is a sum of emissions from each layer, partially absorbed by subsequent layers. Assuming that the atmosphere is divided in $n$ atmospheric layers, it follows:

$$T_B = \sum_{i=1}^{n} (P_i P_i' - P_{i-1} P_{i-1}') T_i$$

With the definitions:

$$P_n \equiv I$$
$$P_{i-1} \equiv P_i E_i$$
$$E_i \equiv e^{-G_i z_i}$$

with thickness $z_i$ of layer $i$.

The emitted radiation is elliptically polarized, the polarization and intensity of the lines depend on the angle between the direction of the magnetic field and the propagation direction $\Phi$. A angle of $\Phi = 0^\circ$ (observing parallel to the field) will reveal the $\sigma^+$ and $\sigma^-$ lines, both circular polarized. Perpendicular observation ($\Phi = 90^\circ$) will reveal all three lines linear polarized, the emitted linear component of the electric field of the $\sigma$ lines is oriented along the magnetic field and the one of the $\pi$ lines is perpendicular to it. All other angles lead to a superimposition of the $\sigma$ and $\pi$ lines resulting in elliptical polarization.

The complex propagation tensor $G$ can be calculated according to:

$$G(v) = \frac{i}{c} \left( I + \sum_{\Delta M=-1}^{1} P_{\Delta M} \sum_{M_J} A_{M_J,\Delta M} \delta(v) \right)$$

with the identity matrix $I$, the magnetic quantum number of the upper energy level $M_J$, the polarization $P$ as a function of the magnetic quantum number transition, and the complex refractivity of a certain Zeeman transition $A$.

\footnote{Which is the $J = N$ level for both the $N^+$ and the $N^-$ transition (Croom, 1978).}
The matrix $P$ in a linear basis can be found in Lencir (1968). A linear basis proves to be convenient for the MAS, since the MAS observes a linear component of the emitted radiation.

The complex index of refraction $A$ is given by:

$$A_{M_J, \Delta M}(\nu) = S_{M_J, \Delta M} F_{M_J, \Delta M}(\nu, \nu_{\text{rel}})$$

(5.6)

in which $S$ stands for the line strength of the unsplit line and $\xi_{M_J, \Delta M}$ for the relative intensity of the considered Zeeman line, depending on $M_J$ and $\Delta M$. $F_{M_J, \Delta M}$ is the lineshape factor, where the use of the approximation by Hui et al. (1978) to the Voigt function is recommended, since the Lorentz approximation of the lineshape does not apply to mesospheric emissions (Rosenkranz and Staelin, 1988). $\nu$ and $\nu_{\text{rel}}$ are the frequencies where the calculation is performed and the center frequency of the Zeeman component respectively. $\nu_{\text{rel}}$ depends on the strength of the magnetic field and is located within a few MHz around the center of the unsplit line, when applying Earth’s magnetic field values. Formulas to calculate $\nu_{\text{rel}}$ and $\xi$ can be found in Rosenkranz (1993), expressions to calculate $S$ are available in Liebe and Hufford (1989).

The frequency shift $\Delta \nu$ of the $\sigma^\pm$ lines can be calculated according to Rosenkranz (1993):

$$\Delta \nu = 0.028026 \frac{\text{MHz}}{\text{\mu T}} B \frac{M(N - 1) \pm N}{N(N + 1)}$$

(5.7)

where $B$ is the magnetic strength in [\mu T]. Applying Equation (5.7) to the 9+ line and a maximum magnetic field strength of 60 [\mu T] yields a maximum frequency shift from the unsplit line center of $\pm 1.66$ MHz. Thus the high resolution filter-channels of the MAS sufficiently cover the magnetically split line.

The frequency difference $\Delta \nu_{\text{eff}}$ between two Zeeman lines of the same $\Delta M_J$ is for the 9+ line:

$$\Delta \nu_{\text{eff}} = 0.028026 \frac{\text{MHz}}{\text{\mu T}} B \frac{N - 1}{N(N + 1)}$$

(5.8)

Applying a typical magnetic field strength of 50 [\mu T] yields a spacing of 125 kHz for the Zeeman lines. The width of the narrow MAS filter-channels is 200 kHz, hence it is not possible to resolve single lines.

The positions and normalized intensities of the 57 Zeeman lines of the 9+ line are presented in Figure 5.2. The strong $\sigma$ lines to the left and right of the line center will lead to a very sharp cut of the detected emissions at high altitudes.

Since the observed signal depends on the magnetic field, it is necessary to take the variation of the magnetic field along the observation path into account. The calculation of the $G$ matrix is done in vertical steps of 1 km along the integration path. Calculating the magnetic field for each of these integration points would slow down the program considerably. It is justified to use a linear interpolation scheme since the magnetic field strength and angle variations with the geographic positions are generally smooth (Barradough, 1986), except close to the magnetic poles.

The magnetic parameters are calculated by the International Geomagnetic Reference Field (IGRF) model (Barradough, 1986). They are calculated at the tangent point location and in addition, at the geographic locations where the integration path reaches an altitude of 120 km. The
atmospheric signal from altitudes above 120 km is negligible. In total, the field is calculated at three different locations along one integration path. One MAS scan through the atmosphere is simulated by the calculation of the magnetic field at tangent altitudes from 0 km to 120 km in vertical steps of 1 km, so that there are in total 363 magnetic field parameters calculated for one scan. Linear interpolation is used for all points lying in between; the maximum angle between these reference points occurs at a tangent altitude of 0 km and is 11° great circle distance.

The calculation of the absorption coefficients in the unpolarized case is done only once, since they do not depend on the geographic location, thus it is possible to separate the absorption coefficient calculation from the radiative transfer calculation in the forward model.

This separation is not possible for the polarized forward model, approximating the magnetic field with the values at the tangent point and calculation of the polarized absorption coefficients only once leads to errors of more than 10% in the received brightness temperatures. These errors are caused by the variation of the magnetic field along the integration path, which can exceed 1%. Therefore the polarized absorption coefficients for the line of interest are calculated during the integration along the path. All other lines, including other oxygen lines, can be calculated unpolarized and will add equal quantities to the diagonal elements of the $G$ matrix. In order to optimize the program, only brightness temperatures for frequencies up to ±27 MHz around the line center are calculated polarized, since the polarization decreases with the distance from the line center. All other frequencies are calculated unpolarized. This approximation leads to errors < 1% in the calculated brightness temperatures. A reduction of this error is possible by an implementation that considers a magnetically broadened line.

The MAS observes a linear component of the emitted electric field, where the orientation is along the scan direction (elevation). Therefore the received spectrum does not only depend on the magnetic field parameters but also on the angle $\Theta$ between the projected magnetic field in the plane perpendicular to the integration path and the scan direction in this plane since the coordinate system for the emitted ellipse is established by this projection. The angle $\Theta$ is calculated from the magnetic field parameters at 120 km, where the atmospheric signal emerges because the linear polarization basis follows the magnetic field along the integration path.

### 5.2.1 Instrumental Effects

Instrument effects are, strictly speaking, not part of the radiation transfer through the atmosphere, because the emitted atmospheric signal is independent of the observing instrument. In spite of that, for data evaluation, it is necessary to consider the influence of the instrument upon the received signal. Three instrument effect can be distinguished:

- Antenna pattern convolution
- Sideband convolution
- Filter-channel convolution

These are the three general instrument effects that must be considered. Moreover there could be other effects introduced by the instrument, such as a baseline.

#### Antenna Pattern Convolution

The atmospheric signal is detected by the antenna. The vertical and horizontal resolution of the instrument is limited by the antenna pattern. An antenna that is sensitive to radiation coming from a very small volume of the atmosphere would be ideal, but in reality the resolution is finite. The first limit to the spatial resolution is within the radiation transfer through the atmosphere, where the received signal is the sum of contributions coming from different locations along the integration path (see Figure 4.1). The second limit is residing in the antenna pattern.

The MAS antenna pattern for the oxygen lines is presented in Figure 5.3. Antenna patterns are usually determined in azimuth and elevation, but it is possible to integrate the influence of the azimut and use a 1-dimensional pattern. The correct approach is a convolution of the 2-dimensional pattern with the atmosphere, but it is reasonable to assume that the atmosphere is homogeneous in horizontal direction.
The MAS instrument is primarily sensitive towards radiation where the electric field vector vibrates in the plane defined by the scan direction and the propagation path. The received signal would be independent of the orientation of this plane for unpolarized radiation, this does not hold for polarized emissions (see Section 5.2.3). The sensitivity toward the radiation where the electric field vector vibrates in the plane defined by the azimuth (horizontal) direction and the propagation path is about 1% of the sensitivity in vertical (scan) direction.

The effect of the antenna pattern is visualized in Figure 5.4, where the difference between two forward calculations is plotted, one with an ideal antenna, the other one with the MAS oxygen antenna pattern.

The difference at 0 km is very small, but moving at a fixed frequency from lower to higher tangent altitudes shows the occurrence of an oscillation. The brightness temperature calculated with an ideal antenna pattern are higher than the one calculated with the MAS antenna at lower altitudes. This picture reverses with increasing altitude. The occurrence of the oscillation depends on frequency, it appears at lower altitudes further away from the line center. The oscillations occur approximately at the altitude where the brightness temperature at a certain frequency is saturated, meaning signals from lower altitudes have no influence upon the received signal.

**Sideband Convolution**

The received brightness temperature is a weighted mean of the signal band $S$ and the image band $I$. The sideband efficiency $s_\nu$ gives the brightness temperature $T_{B,\nu}$ at a given frequency $\nu$ as following:

$$T_{B,\nu} = s_\nu T_\nu^S + (1 - s_\nu) T_\nu^I$$  \hspace{1cm} (5.9)
This is the principle of the heterodyne receiver, which converts the signal down to a frequency that can be amplified. This frequency is approximately 5.2 GHz for the MAS 9+ line, therefore the sideband efficiency will be calculated at this frequency. Typically two sideband values are retrieved per line and linear interpolation is used for all frequencies in between.

The sensitivity of the MAS towards the sideband efficiency is high, therefore pre-mission laboratory measurements are not sufficient and \( s_p \) is introduced in the retrieval.

The MAS is receiving information in the signal band around 61.151 GHz and in the image band at 71.637 GHz. The major signal in the image band comes from the wings of the oxygen lines at 60 GHz and 118 GHz and from the water vapor continuum emissions since there are no strong atmospheric lines around 71.637 GHz. The image band gives information about the temperature profile at altitudes below 25 km, since the signal band saturates at about 25 km (see Figure 5.4).

**Filter-Channel Convolution**

The filter-channels of an instrument are sensitive to emissions over a certain frequency range, the sensitivity is described by the filter-channel curve. The received brightness temperature for a certain filter-channel is derived by a convolution of the spectrum over the channel width of the filter.

Typical examples of normalized filter-channel curves for some of the inner channels of the MAS are presented in Figure 5.5.

**5.2.2 Instrumental Resolution**

The effect of the instrumental resolution is visualized in Figure 5.6. The top plot shows the model calculation for the emitted linear component of the brightness temperatures which is observed by the MAS, no instrument characteristics have been applied. The brightness temperatures, after the instrument characteristics (antenna pattern, sideband, and filter-channel convolution) have been applied, are shown in the bottom plot. All calculations are performed with a mid-latitude summer scenario.

The dip in the center of the line at a tangent altitude of 70 km results from the signal at altitudes of about 80 km, where the line saturates. The measured brightness temperature is equal to the physical temperature of the atmosphere for this case, when no instrument characteristics are applied. The brightness temperature is lower because of the lower temperature at 80 km. The dip disappears at an altitude of 80 km and the influence of the magnetic field dominates the line shape. The fine structure within ±2 MHz around line center results from the individual \( \sigma \) and \( \pi \) lines.

The finite resolution of the MAS instrument allows only the detection of the general form of the emitted brightness temperatures (Figure 5.6, bottom plot), no individual \( \sigma \) or \( \pi \) lines can be resolved. The general form will be either concave (\( \sigma \) lines are more pronounced), convex (\( \pi \) lines are more pronounced) or flat (emerging radiation is unpolarized). The received
brightness temperature can vary from one filter-channel to the adjacent one by more than 60 K when $\sigma$ lines are observed.

The three instrument effects are visible in Figure 5.6:

The antenna pattern leads to higher brightness temperatures in the wings of the line due to contributions from lower tangent altitudes.

The sideband leads to a decrease of the detected intensity.

The filter-channel resolution smooths over a frequency interval.

Figure 5.7 shows the hypothetical unpolarized case, where the magnetic field is zero and Zeeman splitting does not occur. The top plot shows the brightness temperature with no instrument characteristics applied, the bottom plot the brightness temperature after the application of the instrument characteristics.

The brightness temperatures show a smaller half width at half maximum since no Zeeman splitting is considered. The half width of the line decreases with altitude, due to a decreasing influence of the pressure broadening. The half width for altitudes $> 90$ km is constant, the influence of the pressure broadening is negligible and only the Doppler broadening determines the lineshape.

The high resolution plot at the top shows identical temperatures at the line center for tangent altitudes up to 100 km. This implies, that the line saturates at altitudes around 100 km, which is above the mesopause. Figure 1.1 shows the used atmospheric mid-latitude summer temperature profile, the mesopause can be found at 90 km. The unpolarized brightness temperatures saturate at a higher saturation point in comparison to the polarized calculation, since all oxygen molecules absorb and emit at the center frequency.

The high resolution line at a tangent altitude of 70 km in Figure 5.7 can be interpreted as following: Far away from the line center no saturation occurs, the lineshape is visible and the brightness temperatures increase towards the line center. The brightness temperatures saturate at about 200 K, $\approx 0.8$ MHz beside the line center. This corresponds to an altitude of about 75 km (see Figure 1.1). Moving further towards the center reveals decreasing brightness temperatures, since the saturation point in the atm-
5.2 Integrated Radiative Transfer Equation

mosphere moves further up, until it reaches the mesopause. The picture reverses here, the atmospheric temperatures are increasing with altitude, leading to increasing brightness temperatures.

The unpolarized MAS brightness temperatures in the bottom plot are not able to follow the very fine features around the line center of the 70 km high resolution brightness temperatures because of the limited filter-channel resolution. In addition, a decrease of the received signal with increasing altitude is observed, because the line is smaller than the filter-channel width.

The broadening of the line due to the magnetic fields is negligible below 50 km and it is possible to perform unpolarized retrievals by avoiding the use of the channels close to the line center. The polarized and unpolarized brightness temperatures for the total band of the MAS are compared in Figure 5.8, where the tangent altitudes cover the range from 40 km to 80 km. The emitted brightness temperatures for altitudes up to 50 km contain sufficient information in the outer channels, but the line is too narrow above. Most of the information about temperatures above 50 km comes from channels around the line center and these ones are highly affected by the Zeeman splitting.

An increase of the possible temperature retrieval range for unpolarized calculations can be obtained by the introduction of a different lineshape. The influence of the magnetic field could be described as an additional broadening parameter beside the pressure and Doppler broadening. This approximation is not appropriate above altitudes of about 80 km, because the signal is dominated by polarized emissions. The upper limit for this approximation varies with magnetic field, magnetic field strengths of 30 μT will for example allow unpolarized calculations up to 85 km, strengths of 50 μT only up to 80 km.
5.2.3 Magnetic Effects

The degree of polarization $P$ can be calculated as:

$$ P = \sqrt{1 - \frac{4|T_B|}{(\text{Tr}(T_B))^2}} $$

(5.10)

where $\text{det} T_B$ denotes the determinant of $T_B$ and $\text{Tr}$ stands for the trace. The degree of polarization changes with frequency and altitude, higher tangent points lead in general to higher degrees of polarization.

The polarization for different magnetic field strengths and angles is shown in Figure 5.9, the observation configuration is the same as in Figure 5.6, with either the magnetic strength or angle set constant. The upper plot shows the dependence of $P$ on the magnetic field strength $B$. The polarization for the case of $B = 0 \mu$T is zero and the emitted radiation is unpolarized. The $\sigma$ lines move further away from line center with increasing $B$ and the $\pi$ lines in the center become visible. The overlapping of $\sigma$ and $\pi$ lines at line center leads to low polarization. The $\sigma$ lines possess higher polarization because the influence of the $\pi$ lines decreases with distance from line center while the $\sigma$ line intensities increase. The situation for different angles $\Phi$ is presented in the bottom plot, the magnetic field is calculated according to the model and is about $58 \mu$T. An angle of $0^\circ$ reveals only the $\sigma$ lines, increasing the angle leads to observation of the $\pi$ lines around line center and a decrease of the $\sigma$ line polarization due to superimposition of the $\pi$ and $\sigma$ lines.

The MAS receives only a linear polarized component of the spectrum, hence the information in the spectrum does not only depend on the magnetic field parameters but also on the orientation of the observed linear component with respect to the magnetic field.

The dependence of the received brightness temperature on the magnetic field strength is shown in Figure 5.10 top, where the simulated MAS brightness temperatures are calculated for a tangent altitude of 80 km. The magnetic field is set constant, the angle $\Phi$ varies and is calculated with the magnetic model. An increasing magnetic field leads to a broadening of the observed line. The $0 \mu$T calculation has the highest brightness temperature in the center. The received signal consists of information coming from al-

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Figure 5.8: Unpolarized and polarized MAS brightness temperatures for tangent altitudes 40 km to 80 km. Note that the frequency scale is different from the previous figures.
Polarization at different Magnetic Strengths

Figure 5.9: The degree of polarization at a tangent altitude of 50 km for different magnetic field strengths and angle, the observation configuration is identical to the one used in Figure 5.6, with either the magnetic strength or angle set constant.

Polarization at different Magnetic Angles

titudes above and below the nominal tangent point due to the integration path and the antenna beam width. The signal for all four constellations is not saturated for an observation at 80 km tangent altitude, thus the observe temperatures correspond to the signal emerging at 80 km. The signal of the 0 μT calculation is stronger, owing to the stronger emissions along the integration path, because all O₂ molecules are emitting at the center frequency. A lower tangent point will split up the three calculations with B ≠ 0, since they all saturate at lightly different altitudes, the 20 μT calculation shows the lowest temperatures, caused by the saturation at higher altitudes. The brightness temperatures at line center will vary slightly with the tangent point, even if the line is saturated, caused by the varying integration path for different tangent altitudes. A higher tangent point results in the strongest signal observed in the 20 μT calculation, the emissions are concentrated around the line center. The line of the 0 μT calculation is too small at these altitudes, the signal is decreasing.

It follows that the information in the spectrum at altitudes above 70 km is strongly dependent on the magnetic field strength. A strong magnetic field will lead to a signal in more filter-channels, thus improving the statistics of the measurement. The magnetic strength will furthermore influence the corresponding altitude from where the received signal in the center emerges.

The influence of the angles Φ and Θ on the received brightness temperature can be seen in Figure 5.10 (middle and bottom), where the angle between the magnetic field and the integration path is set constant and the resulting brightness temperatures are shown. Two cases have been investigated: the Θ = 0° case where the projected observed linear component is oriented along the magnetic field lines and the Θ = 90° case where the component is perpendicular to the field. The magnetic field strength is calculated according to the IGRF magnetic model and is about 57 μT at the tangent point.

Both cases are identical for the 0° calculation, where the σ lines are circular polarized, and the measured intensity in any linear polarization basis is identical. With an increasing angle the σ lines are elliptically polarized, and at an angle of 90° linear, oriented along the magnetic field lines. The high polarization of the σ lines and the alignment of these lines along the magnetic field lead to an increase of the observed brightness temperature.
and to a doubling of the measured brightness temperature at ±1.5 MHz from line center in the Θ = 0° case. The polarization of the signal in the center is low since the contribution to the polarization at the line center comes mainly from the π lines (see Figure 5.9). The signal in the center is not saturated, and the increase of Φ leads to a higher intensity for all tangent altitudes above the saturation point. A lower tangent point would lead to identical brightness temperature at line center for all angles because the line saturates just below 80 km and the polarization is low.

The line width in the Θ = 90° case for Φ > 0° is smaller than that in the Θ = 0° case because the influence of the σ lines is weaker. The plateau in the center widens with angle owing to the increasing influence of the π lines. The observed brightness temperature in the center is decreasing with angle since the influence of the π lines leads to higher absorption, and thus the line saturates at higher altitudes. The influence of the angle is visible at all tangent points below 80 km, where the 0° calculation has the highest brightness temperature since it saturates at the lowest altitudes.

Figure 5.10: Brightness temperatures at 80 km tangent altitude for different magnetic field strengths and angle, observation configuration as in Figure 5.6, with either the magnetic strength or angle set constant. Two cases are investigated for the angle variation: (1) Θ = 0° the projected observed linear component is oriented along the magnetic field lines (2) Θ = 90° the component is perpendicular to the field.
6 Retrieval Setup

The retrieval simulations require a number of parameters to be specified. The most important ones are a priori profiles, a priori errors, measurement errors, and the retrieval grid. These parameters are outlined in the following sections.

6.1 Measurement Error

The noise characteristic of passive microwave instruments is described by the radiometer formula:

$$\Delta T = \frac{\beta T_{\text{sys}}}{\sqrt{Wt}}$$

(6.1)

introducing the channel width $W$, the integration time of the measurement $t$, the system noise temperature $T_{\text{sys}}$, and an instrument specific factor $\beta$. The factor $\beta$ is equal to 1 for the MAS, $T_{\text{sys}}$ is equal to 1500 K for the 9+ line, and 900 K for the two other lines. The integration time is 0.04 s. The resulting measurement error, or noise per channel, $\Delta T$ for the three different channel widths is given in Table 6.1.

<table>
<thead>
<tr>
<th>Filter-channel width [MHz]</th>
<th>$\Delta T$ [K]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>9+</td>
</tr>
<tr>
<td>40.0</td>
<td>1.2</td>
</tr>
<tr>
<td>2.0</td>
<td>5.3</td>
</tr>
<tr>
<td>0.2</td>
<td>16.8</td>
</tr>
</tbody>
</table>

Table 6.1: MAS filter-channel and corresponding measurement errors

The step width has been chosen by a trade-off between resolution and precision. The major limitation in the vertical resolution is the MAS antenna beam width (see Section 5.2.1), limiting the attainable resolution to 4–5 km. The full width at half maximum (FWHM) of the MAS antenna, defined as the full width of the antenna pattern at the point where the response has decreased by a factor 2, is $\approx 0.4^\circ$. This corresponds to $\approx 12$ km at the tangent point, hence, it is possible to retrieve temperatures on a finer grid than the given FWHM of the antenna, due to additional information coming from the pressure broadening of the line.

The a priori error has been set to 10 K for all altitudes, the corresponding a priori temperature profile has been taken from the CIRA 86 atmospheric model (Fleming et al., 1988). No correlations between the different temperature retrieval levels are assumed, these would introduce off-diagonal elements not equal to zero in the $S_0$ matrix.

The a priori pressure profile is generated from the temperature profile via the hydrostatic equation (Roedel, 1992):

$$\rho = \rho_0 \cdot \exp \left( -\frac{Mg}{RT} z \right)$$

(6.2)

where $\rho$ is the pressure at altitude $z$, $\rho_0$ the ground pressure, $M$ is the molecular weight, $R$ the universal gas constant, $T$ the temperature and
6.3 Instrument Parameter Retrieval Setup

A number of uncertain instrument parameters have been introduced to the retrieval, because the retrieval is highly sensitive to uncertainties in these parameters.

**Sideband Efficiency:** The received brightness temperature is a weighted mean of the signal band $S$ and the image band $I$ according to Equation (5.9). The sideband efficiency is assumed to behave linearly within the band, and two parameters at the borders of each band have been retrieved. The a priori value is set to 0.5 for an ideal double sideband receiver, the a priori error to 0.1.

**Tangent Altitude Offset:** The determination of the tangent point altitude with the Shuttle navigation system is not accurate enough for temperature retrievals. A change of 1 km in the tangent altitude can lead to changes of up to 20% in the simulated brightness temperatures. A correction to the tangent altitude calculated from the Shuttle data was performed by Berg (1995), using the 2 oxygen lines at 62.998 GHz and 63.569 GHz. This correction is used as the a priori value for a more accurate retrieval of the tangent point position by a tangent altitude offset.

The a priori error of this retrieval parameter is set to 1 km.

**Forward Model Scaling Factor:** The forward model scaling factor scales the brightness temperatures generated by the forward model at all levels and frequencies and can compensate inaccuracies in the antenna characteristic. This factor was retrieved in the unpolarized temperature retrievals performed by Wehr et al. (1998) but has proven to be redundant in the polarized calculations, owing to the filters that are applied to the spectrum (see Section 6.4).

**Magnetic Model Scaling Factor:** The width of the received lineshape for altitudes > 80 km reflects the strength of the magnetic field (see Figure 5.10 top). Hence, it is possible to introduce a magnetic scaling factor in the inversion. A scaling factor of one indicates that the line width calculated with the magnetic parameters of the IGRF model are correct. Yet, data evaluation exhibited discrepancies between the reproduced spectra and the MAS spectra, where the magnetic field strength from the IGRF model is up to 10% different from the actual field. The source of this error is not clear yet, possible sources are wrong magnetic field data from the IGRF model or problems in the instrument, e.g., frequency stability of local oscillators. The a priori value is set to 1.0, the a priori error to 0.1.

It is not possible to retrieve the angle between the magnetic field and the observation direction, because the angle influences mainly the polarization of the received radiation and the sensitivity of the MAS with respect to polarization is not high enough (see Figure 5.10 middle and bottom).

$g$ the gravitational constant. Equation (6.2) assumes that the temperature profile is independent of $z$ which is not true for the atmosphere. The altitude dependence of $T$ is considered by the introduction of small altitude steps $z$ so that the temperature is constant within that slab.
6.4 MAS Data Filters

First temperature retrieval results from MAS data revealed problems at low altitudes. Generally, the retrieved temperature profiles are too low at the tropopause altitude. The hydrostatic equation introduces correlations between all levels, low tropopause temperature can therefore influence all retrieved temperatures. The low tropopause temperature effect is removed from the MAS data by a filter, that truncated all measurements to an altitude range from 30 km to 110 km. Two positive side-effect of this filter have been observed:

1. The minimization of horizontal smoothing. The signal in the center of the line comes mainly from altitudes around 80 km, independent of the tangent altitude (see Figure 5.6). This gives a good statistic even though the signal is weak. But it leads to horizontal smoothing of the received signal, because it is detected at different geographic locations, as a result of the limb scanning technique observing perpendicular to the flight direction.

2. The impact of an error in the tangent altitude offset onto the retrieved profile is smaller.

A second filter is introduced to reduce the sensitivity towards continuum emissions. Continuum emissions have almost no frequency dependence in a band and are resulting from the overlap of distant strong lines. These emissions have been filtered out by the calculation of a mean of the 2 outermost left and right filter-channels of the band at each tangent altitude. This value is subtracted from all brightness temperatures at that tangent altitude, in the MAS measurement and in the forward model.

Positive side-effect is the reduction of the sensitivity towards the sideband efficiency. Data evaluation of MAS spectra showed that the retrieved sideband efficiency is constant for all performed inversions and behaves almost like an ideal double sideband receiver ($s_\nu = 0.5$). A mean of the retrieved sideband efficiency is calculated, and all retrievals are performed with this setting. The retrieval of a sideband efficiency is no longer needed.
7 Synthetic Retrievals

A sensitivity study is performed before retrieving temperature profiles from MAS measurements, in order to evaluate the influence of different parameters on the quality of the retrieval of temperature profiles from the 9+ line. Investigated parameters are for example the magnetic field strength and the angle between magnetic field and observation direction.

7.1 Setup

The synthetic spectrum is generated by the forward program, which is used in the inversion calculation as well. The MAS instrument characteristics have been applied. The magnetic field calculation is performed for the location used in Figure 5.6. The synthetic measurement represents one MAS scan cycle and consists of 111 spectra for an altitude range from 0 km to 110 km in 1 km steps. Each spectrum gives the brightness temperatures for the 50 filter-channels of the 61.151 GHz line, thus, the measurement vector \( \mathbf{y} \) entering the retrieval has a dimension of 5550. No MAS data filter is applied (see Section 6.4). The applied a priori errors for the retrieval are defined in Section 6.2.

7.2 Synthetic Retrieval Results

Figure 7.1 summarizes the result of one temperature inversion. An a priori not equals true scenario is chosen to test the robustness of the retrieval algorithm. The a priori temperature profile is a mid-latitude winter one, while the true corresponds to a mid-latitude summer scenario. Additional parameters retrieved are sideband efficiency, tangent altitude offset, magnetic model scaling factor. The a priori sideband efficiency has been initialized with an a priori value of 0.6, the true value is 0.5. The a priori tangent altitude offset is set to 1 km, while the true value is 0 km. The a priori magnetic model scaling factor is set to 1.1, the true value is 1.0. The pressure initialization at 36 km is performed with a 10% higher value, compared to the correct one.

The retrieval algorithm converges to the true profile after about three iterations. Deviations between the true and the retrieved profile are within the errors, except at tropospheric regions where the retrieved profile is not able to follow the true profile, owing to the lower resolution. The deviations below 20 km leave an impact on the sideband efficiency parameter, 0.51 instead of 0.5 is retrieved. These retrieval deviations could be removed by a higher retrieval resolution in the troposphere, but the focus of the MAS instrument is on stratospheric and mesospheric temperature retrieval. Here, the true profile is well captured.

The values of the additional retrieval parameters converge after two iterations. The sideband efficiency and the magnetic model scaling factor are retrieved with very low errors. The tangent altitude offset is about 600 m above the correct value of 0.0 km, caused by the wrong pressure initialization. The retrieval error is around 0.02 km. The error introduced by refraction is around 20 m in the middle of the stratosphere, see Figure 12.6 right, hence it is justified to ignore the error introduced by refraction for the detection of stratospheric temperature profiles.

The averaging kernel elements show that a meaningful retrieval of temperature is possible between 0 km and 90 km, with varying resolution. The averaging kernel elements below 20 km are very broad, tropospheric temperature retrieval with a resolution of 10 km is rather poor, other instruments are better suited for this task. The kernel at 24 km is smaller than the one at the retrieval levels above and below, caused by the saturation of the signal band. Kernels below 24 km obtain information out of the image band.

The error ratio indicates, that stratospheric retrieval is possible with an retrieval error between 2 K and 3 K, mesospheric retrieval errors are around 5 K. The peak at around 24 km results from the saturation of the
signal band and from the smoothing introduced by the profile representation. The information below 24 km comes entirely from the image band, the major error results from the measurement error, the smoothing error is slightly lower. The mesospheric temperature retrieval error increases above 65 km because the information in the line shape is decreasing and the main information is found in the inner channels which saturate at about 80 km. This, and the decreasing vertical smoothing is the reason for the dip at 80 km. The signal is too weak above 90 km, all the information comes from the a priori and the error ratio is close to one.

The error correlations of the two sideband retrieval parameters are very similar, they show oscillating correlations with altitude. Strongest correlations are found at the altitude where the image band provides temperature information, around 10 km. The same oscillating behavior is found for the tangent altitude offset retrieval, indicating that higher temperatures at one level have a similar effect as lower temperatures at the adjacent levels. This is a result of the hydrostatic equation, which introduces correlations between different temperature levels. The magnetic model scaling factor is only weakly correlated with the temperature retrieval. A weak correlation is still present because temperature changes the Doppler broadening of the line, and the pressure broadening via the hydrostatic equation, resulting in a different line width.

The influence of the discussed MAS data filters on the retrieval error is presented in Figure 7.2. The continuum subtraction has a high impact on the retrieval error at low altitudes, since filter-channels at the edges of the band provide temperature information from strongly broadened lines. The error is slightly below the ‘No filter’ calculation at altitudes around 30 km, caused by noise introduced by the continuum subtraction. The restriction of the measurement to tangent altitudes above 30 km has an impact on the retrieval error at all retrieval levels. No information is available at altitudes below 10 km, high error ratios are found up to altitudes of 25 km. The finite width of the antenna pattern gathers information at altitudes below 30 km. The information gathered by the antenna pattern is zero at 10 km, thus 20 km are covered by the antenna. This correspond to an angle of 0.61° and to an antenna response of –17 dB, as given by the MAS antenna pattern in Figure 5.3. The retrieval errors at levels above 30 km are affected on the
one hand by the antenna pattern, on the other hand by the disregarding of the inner filter-channels. The antenna pattern influence is present at stratospheric altitudes, while the inner filter-channels, which saturate in the mesosphere, degrade the accuracy at mesospheric altitudes.

### 7.3 A Priori Effects

It has already been mentioned that the a priori error determines the weight of the measurement. Very low a priori errors lead to more weight on the a priori profile. It is possible to ignore the measurement completely, thus retrieving the a priori profile. A misleading side effect is that the error of the measurement is very low in this case.

The retrieval results of a mid-latitude summer scenario with a 2K a priori error are presented in Figure 7.3, the calculation is otherwise identical to the one presented in Figure 7.1. The retrieval is unable to capture the temperature profile around 80 km to 90 km, owing to the low a priori error. The averaging kernels are smaller at all altitudes, compared to the realistic retrieval calculation with a 10K a priori error. They show higher values of the FWHM of the kernel function and are hardly developed at altitudes above 60 km. The total error of the retrieval is below 2K for all altitudes. The correlations are similar to the 10K a priori error calculation, the major differences occur at altitudes above 60 km.

### 7.4 Magnetic Effects

The influence of the strength of the magnetic field and the angle between observation direction and the magnetic field has been investigated here. The altitude information in the spectrum depends partly on the magnetic strength, since the width of the plateau in the middle of the line (see Figure 5.6) reflects the strength of the magnetic field.

In Figure 7.4 left, the error profiles according to Equation (3.11) have
Figure 7.3: Synthetic temperature retrieval results for a mid-latitude summer scenario with an a priori error of 2 K. Please refer to Section 3.4 for a general description of the individual plots.

Figure 7.4: Error ratios for different magnetic field strengths and angle, the observation configuration is identical to the one used in Figure 5.6, with either the magnetic strength or angle set constant. Left: variation of the magnetic field strength, middle and right: variation of the angle, the two cases are the ones described in Figure 5.10.

been plotted for 4 different magnetic field strengths. The maximum error is the a priori error of 10 K. All O₂ molecules absorb at the center frequency and the inner channels saturate at an altitudes of about 100 km for the unpolarized calculation \( B = 0 \mu T \). The line is very small and the statistical information is low, but the error profile exhibits lower errors above 100 km in comparison to the other calculations. All the information for altitudes below 90 km is obtained from the lineshape and consequently the error is large for altitudes of 70 km to 90 km. A magnetic field \( > 0 \mu T \) leads to more information in the range from 80 km to 90 km, because more filter-channels receive a signal. The 20 \( \mu T \) calculation possesses the lowest error at 90 km, all the inner channels are saturated around this altitude. An increase of
7.5 Temperature Effects

The error of the retrieval is affected by the temperature profile as well. Generally, the temperature profile varies with latitude, as shown in the different scenarios in Figure 1.1. Different latitudes correspond to different magnetic field strengths, yielding different errors of the retrieval, as discussed in Section 7.4. The magnetic field dependence has been removed from the spectrum by calculating all 5 scenarios at the same position, where this position is the one given in Figure 5.6.

Figure 7.5 shows the error ratios of the five scenarios. The structure of the error ratios for different temperature profiles can be understood with the pressure broadening mechanism, which varies inversely with temperature (Gordy and Cook, 1970). The magnitude of the temperature profile is dominating the error of the retrieval at altitudes above 80 km, lower temperatures correspond to lower error ratios. Even though a higher temperature of the air parcel being sampled leads to higher detected brightness temperature (see Eq. (2.21)), thus improving the signal-to-noise ratio, the dominating effect here is the pressure broadening. Lower temperatures correspond to stronger pressure broadening, providing more information. Altitudes between 35 km and 50 km show very similar error ratios, independent of the actual temperature of the sampled air parcel. The information provided by pressure broadening is sufficient and independent of the actual temperature. The best performance is achieved with a subar-
tic winter scenario between 15 km and 30 km. This scenario has no pronounced tropopause and very cold temperatures between 20 km and 30 km (see Figure 1.1), leading to a sensitivity in the signalband channels of the instrument, while these are opaque for the other scenarios, resulting in the peak of the error ratios around 25 km.
8 MAS Results and Comparison with other Instruments

The mission duration of the MAS was very short, about 2 weeks/year and coinciding measurements in time and space are difficult to obtain. One satellite candidate for a validation is the Upper Atmosphere Research Satellite (UARS). Five instruments onboard the UARS satellite provide temperature measurements, three of them have been chosen to validate the MAS temperatures. A set of MAS data has been compared to results of the limb-viewing instruments Microwave Limb Sounder (MLS), Cryogenic Limb Array Etalon Spectrometer (CLAES), and Improved Stratospheric and Mesospheric Sounder (ISAMS).

In addition, a validation of single profiles with ground based measurements is performed by use of temperature profiles obtained at various Lidar stations.

8.1 Comparison with Satellite Instruments

A MAS data set taken on March 28, 1992 over Saudi Arabia and Iran was used for the comparison with the UARS data. The tangent point moved from 7° latitude, 32° longitude to 32° latitude, 56° longitude.

Two UARS tangent point tracks close to the MAS tangent point track were chosen for the comparison. One track moves from 7° latitude, 44° longitude to 32° latitude, 80° longitude, east of the MAS measurement; the other one is in the west of the MAS profile locations, moving from 7° latitude, 20° longitude to 30° latitude, 48° longitude. Both tracks were obtained on UARS day 198, corresponding to March 27, 1992.

The profile locations are presented in Figure 8.1, which also visualizes the different scan scenarios of the instruments. The Universal Time (UT) of the scenarios is indicated. Note that the comparisons include a local time difference of ≈ 6 hours, which will introduce some diurnal temperature variability of 2K at most (Andrews et al., 1987).

8.1.1 MAS Instrument

Figure 8.2 shows the MAS temperature deviations from the CIRA 86 model. The deviations are with respect to the CIRA 86 profile for March, latitude 20°. Five MAS temperature profiles have been smoothed horizontally with a boxcar average to get a resolution similar to that of the UARS instruments. The left ordinate shows the data on the original altitude grid, the right ordinate shows the averaged pressures.

Two areas can be identified in Figure 8.2: an area of smooth variations below 60 km (stratosphere and lower mesosphere) and a highly variable area above 60 km (mesosphere). The stratosphere extends up to ≈ 50 km; the mesosphere extends to 90 km.
8.1.2 MLS Instrument

The MLS is an instrument using a similar technique as the MAS. A combination of the 15+ and 17+ line is used for the temperature determination. An instrument description can be found in Barath et al. (1993). The Zeeman splitting is included in the calculations, but the MLS has no high resolution filter-channels, which limits the available information to an upper altitude of \( \approx 55 \text{ km} \). The temperatures for altitudes below 22 hPa is linearly interpolated from the National Center for Environmental Prediction (NCEP) data, above 0.22 hPa the profile relaxes to the climatology. The MLS data retrieval is performed on a pressure grid. The error of a single profile is 1.5 K at 10 hPa and increases to 3 K at 0.46 hPa (Fishbein et al., 1996).

The deviations of the MLS temperature measurements from the CIRA 86 model for the month of March, latitude 20°, can be found in Figures 8.3 and 8.4, where the MLS data are shown on the original pressure grid (left ordinate) and projected onto an altitude grid using the hydrostatic equation (right ordinate).

The stratospheric MLS temperatures are all below the CIRA 86 model; differences are up to 8 K. The differences increase toward higher latitudes. The layer of enhanced temperature, visible in the MAS data, is not present in the MLS data. Lower mesospheric temperatures are above the CIRA 86 model at lower latitudes and agree at higher latitudes.
8.1 Comparison with Satellite Instruments

8.1.3 CLAES Instrument

The CLAES instrument measures infrared thermal atmospheric emissions. It obtains temperature profiles by using features of the CO₂ spectrum in the spectral channel at 789-793 cm⁻¹. The principal reference to the CLAES instrument is that of Roche et al. (1993).

The temperature deviations from the CIRA 86 model for the month of March, latitude 20°, are presented in Figures 8.5 and 8.6. The variations are not as smooth as those in the MLS data, but similar features as in the MLS measurements are observed. The temperatures in the stratosphere are generally lower than those in the CIRA 86 model; lower mesospheric temperatures are above those in the CIRA 86 model.

8.1.4 ISAMS Instrument

The ISAMS instrument is an infrared radiometer which uses a combination of interference filters and pressure modulators to select the spectral emissions from the molecules of interest. Emissions from the CO₂ 15 μm vibration-rotation band are used to establish the temperature profiles. The temperature retrieval program uses a combination of sequential and optimal estimation techniques as described by Rodgers (1976). For a detailed instrument description refer to Taylor et al. (1993).

The temperature deviations from the CIRA 86 model for the month of March, latitude 20°, are presented in Figures 8.7 and 8.8. ISAMS detected lower temperatures than those in the CIRA 86 model throughout the stratosphere. The lower mesosphere has higher temperatures in the CIRA 86 model, while temperatures in the middle mesosphere are below CIRA 86 with deviations of up to 16 K.
Figure 8.5: Deviations of the CLAES temperatures from the CIRA86 temperatures, obtained on March 27, 1992 (UARS day 198), for the profile locations presented in Figure 8.1 (east of MAS). The tick marks at the top show the latitude positions of the CLAES profiles.

Figure 8.6: Same as Figure 8.5 but for profile locations west of MAS.

Figure 8.7: Deviations of the ISAMS temperatures from the CIRA86 temperatures, obtained on March 27, 1992 (UARS day 198), for the profile locations presented in Figure 8.1 (east of MAS). The tick marks at the top show the latitude positions of the ISAMS profiles.

Figure 8.8: Same as Figure 8.7 but for profile locations west of MAS.
8.2 Comparison with Lidar Instruments

The Lidar data was obtained at the following sites:

- CRESTech (Lidar Laboratory, Center for Research in Earth and Space Technology) (Carswell et al., 1991), Location: North York, Ontario 43.08° N 79.5° W
- IFA-CNR (Istituto di Fisica dell’Atmosfera) (Gobbi et al., 1995), Location: Frascati 41.8° N 12.7° E
- OHPE (Observatoire de Haute-Provence) (Chapin and Hauchecorne, 1984), Location: 43.93° N 5.7° E
- JPL (Jet Propulsion Laboratory) (McDermid et al., 1990; Leblanc et al., 1998), Location: Table Mountain Facility (TMF), 34.4° N 117.7° W

Only Lidar data with a temperature error below 10 K entered the comparison. The error of the temperature profile obtained at the Lidar sites is < 1 K for altitudes below 50 km, except for the profiles obtained at CRESTech, where the error is < 4 K.

A map with the MAS tangent point track and the position of the Lidar site has been added for illustration to the temperature profile comparison. The information of one scan cycle is obtained by a scan of the tangent point from about 130 km down to about 10 km and back up to 130 km. The up and down subscans have different geographic locations and they are merged in the retrieval to one measurement scan. The averaged horizontal position of a measurement tangent point track is a mean of the up and down track, assuming that both subscans cover the same altitude range. Consequently, the MAS tangent point track follows the positions of one of the subscans for cases where only one subscan was covering the altitude interval. This effect causes the slightly distorted tangent point track in Figures 8.9 and 8.12 because the upper atmosphere interval was only covered by the upscans.

The comparison with the CRESTech profile is performed with a MAS temperature profile obtained on March 29, 1992. The mean tangent point position is at 43.9° N and 81.8° W. The CRESTech profile was obtained 4 days later. Figure 8.9 summarizes the results. Moreover, the temperature profile for the MAS location obtained from the NCEP database is added. The MAS data show a lower and warmer stratosphere than observed by the Lidar at CRESTech. The warmer stratosphere is confirmed by the NCEP data, but the location is 8 km higher. The results at altitudes below 40 km and in between 50 km and 60 km are in good agreement. The cooling of the stratopause within the following days is confirmed by the NCEP data. In addition, the profile confirms that the temperature gradient below 40 km is constant during these days.

For the comparison with the IFA-CNR results a MAS measurement obtained on March 28, 1992 is used, the mean tangent point position is 40.8° N and 11.4° E. The nearest IFA-CNR profile in time was taken on March 19, 1992. The comparison is presented in Figure 8.10. The MAS measurement exhibits some oscillations around the NCEP profile below 40 km, the IFA-CNR profile shows higher temperatures in this region. The altitude of the stratopause is 45 km at approximately 270 K in all 3 datasets. The stratopause of the IFA-CNR data shows much more structure, since the...
Lidar has a higher resolution. Both data sets show a stratopause extending over 10 km and similar temperature gradients above 50 km.

The comparison with the temperature profile obtained at OHP is performed with a MAS measurement taken on March 28, 1992. The mean MAS tangent point position is at 9.25° E and 43.60° N. The OHP profile was taken on March 24, 1992. Both measurements show very good agreement in the upper stratosphere and in the mesosphere (see Figure 8.11). The NCEP data has been added to the plot, where this data show lower temperatures at the stratopause. The slightly higher temperatures of the MAS data can be explained by the vertical smoothing, the MAS profile is not able to follow the NCEP measurement exactly at the stratopause owing to the different resolution. The middle stratosphere agrees very well with the MAS data, while the OHP data detects lower temperatures. A temperature inversion is present in the mesosphere of the MAS data at about 80 km. The presence of these inversion layers above OHP has already been reported in Hauchecorne et al. (1987), where amplitude and altitude of the inversion agrees with the reported observations. These inversion layers are only short time scale features over a few days, which explains the absence of an inversion layer in the OHP data four days earlier. The vertical extension of temperature inversion layers is usually < 10 km and cannot be reproduced accurately by the MAS data.

The closest profile in time and space measured at the TMF is shown in Figure 8.12 and was taken on March 19, 1992. The MAS measurement was taken on March 27, 1992, where the mean tangent point was located at 118.32° W and 35.75° N. The NCEP data shows a distinguished stratopause at 48 km, while this is not present in the other two datasets. The TMF
stratopause shows much more structure and the MAS results determine a stratopause with almost constant temperatures over a vertical interval of 15 km. MAS and TMF show very similar temperature distribution in the mesosphere.

A general feature is striking in the Lidar comparison for all MAS data, the lower temperatures at 90 km, compared to the a priori profile. As mentioned above, the a priori profile is the corresponding CIRA 86 profile for the month and latitude of the MAS measurement. The a priori profile for the month March was taken, since all MAS measurements were performed at the end of March. The seasonal variation of the mesopause temperature at northern mid-latitudes corresponds to a cooling of \( \approx 5 \text{ K/month} \) for the period of February to May. This indicates that an a priori profile of the month April would have been more appropriate.
9 Future MAS Instruments

The MAS instrument was built in the 80’s and flew at the beginning of the 90’s. The technical possibilities have advanced significantly since the first assembly of the MAS instrument. This chapter discusses some of the possible improvements that can be applied to a future MAS-like sounder. It is assumed within this discussion that this improved MAS is placed on a Low Earth Orbit (LEO) satellite at an altitude of 820 km, with an advanced antenna, and sideband suppression.

These new instrument characteristics are taken from a study for future sub-millimeter limb sounder, performed for the European Space Agency (ESA) by Reburn et al. (1998) and Böhler et al. (1998). The antenna pattern of the first study is taken, it is given for a frequency of 200 GHz. The FWHM of an antenna varies with frequency, higher frequencies lead to smaller FWHM. The MASTER antenna is scaled down to the MAS frequency, according to a rule of thumb given in Eq. 1.33 of Janssen (1993):

\[
\text{FWHM} = \frac{1.5\lambda}{D_a}
\]

(9.1)

where \(D_a\) is the diameter of the antenna, and \(\lambda\) the wavelength at the reference frequency. The newly generated antenna pattern has a FWHM about 3 times larger at 60 GHz compared to the original MASTER antenna at 200 GHz. The FWHM of the antenna at 60 GHz is \(\approx 0.18^\circ\), corresponding to 10 km at the tangent point for an orbiter altitude of 820 km.

The suppression of the image band doubles the observed brightness temperatures at altitudes above 30 km in comparison to the original MAS observation, since the image band of the 9+ line contains no information at these altitudes and the signal is close to zero. The error of the retrieval is decreased in the stratosphere, owing to the better signal-to-noise ratio, while no information for tropospheric temperatures is available, which is provided by the image band.

The actual integration time of the measurement is left at 0.04 s, which is a high resolution measurement. The ESA proposed sensors use an integration time of 0.3 s, reflecting the higher orbit, thus the signal-to-noise ratio would be further improved by this integration time. The nominal case for the presented calculations is the MAS system noise temperature of 1500 K.

The resolution of the retrieval grid is improved to meet the new characteristics of the instrument, the new resolution along with the a priori error is given in Table 9.1.

Table 9.1: Temperature retrieval resolution and corresponding a priori errors for an advanced MAS instrument

<table>
<thead>
<tr>
<th>Range [km]</th>
<th>Resolution [km]</th>
<th>A priori error [K]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 (\leq x \leq 20)</td>
<td>5.0</td>
<td>10.0</td>
</tr>
<tr>
<td>20 (\leq x \leq 60)</td>
<td>4.0</td>
<td>10.0</td>
</tr>
<tr>
<td>60 (\leq x \leq 90)</td>
<td>5.0</td>
<td>10.0</td>
</tr>
<tr>
<td>90 (\leq x \leq 100)</td>
<td>10.0</td>
<td>10.0</td>
</tr>
</tbody>
</table>

9.1 Alternative Line Selection

The MAS instrument is observing the 9+ line at 61.151 GHz, this is the strongest oxygen line of the 60 GHz line cluster. Additionally, the lines located at 62.998 GHz and 63.569 GHz are detected, they are mainly used for the determination of the tangent altitude offset, but provide temperature information as well.

Detection of mesospheric temperature requires strong lines, since the signal-to-noise ratio determines the error of the retrieval. The brightness temperature observed at a tangent altitude of 100 km for all oxygen lines between 0 GHz and 3000 GHz are shown in Figure 9.1, no instrumental effects are included. The cluster of lines around 60 GHz and the single line at 118 GHz are caused by spin flip transitions at different rotational levels, the rotational quantum number \(N\) is constant. The rotational quantum number changes by 2 for lines at higher frequencies and the spin orientation
with respect to $N$ in a manner that the selection rule $|\Delta J| \leq 1$ is fulfilled, leading to the triplets visible in Figure 9.1. The decreasing brightness temperatures are mainly a consequence of the increasing Doppler broadening with frequency, thus the absorption at a specific frequency decreases and the line in no longer opaque at the center frequency. The equally spaced triplets on the frequency grid belong to the spectra of pure rotational transitions.

The lines around 60 GHz are the strongest within the oxygen lines spectra, as can be seen in Figure 9.1, providing the better signal-to-noise ratio. Lines at higher frequencies, on the other hand, provide a higher resolution, as given in Eq. (9.1), but the signal-to-noise ratio is lower, owing to the intensity of these lines and the higher system noise temperature at higher frequencies (Reburn et al., 1998; Bühler et al., 1998). Consequently, the focus here is on the oxygen lines around 60 GHz.

The retrieval error of different oxygen line observations around 60 GHz is investigated by moving the observation frequency to the line center. The actual strength of the individual lines can be seen in Figure 5.1, the obtained error ratios for a mid-latitude summer scenario are presented in Figure 9.2.

The 9+ line has the lowest retrieval error for the upper stratosphere, and at the mesopause. Saturation at line center happens at about 75 km for the weaker 21+ line and at 65 km for the 25+ line, resulting in a slightly better error ratio at these altitudes, compared to the 9+ line. The saturation point moves up in the atmosphere with the strength of the line.

Weaker lines show better retrieval error at low altitudes, owing to a lower altitude where the band saturates. A wider band width would also improve the retrieval of temperatures at lower altitudes, since information of the pressure broadening for higher pressures is not covered with the MAS band width of 400 MHz (see Section 9.4).

The suppression of the image band doubles the observed brightness temperatures at altitudes above 30 km, as mentioned earlier on, and the accuracy of the temperature retrieval is enhanced. A similar enhancement in stratospheric temperature accuracy including sideband convolution can be obtained by moving the local oscillator frequency in-between the 7+ and 9+ line, thus doubling the observed brightness temperatures, since
both lines are almost equally strong. A retrieval calculation where a combination of the 7+ and 9+ line is observed is included in Figure 9.2, the obtained retrieval error is close to the one of the 9+ line without sideband convolution.

9.2 Noise Temperature Improvements

The system noise temperature $T_{sys}$ of the MAS for the 9+ line is 1500 K, the integration time 0.04 s.

Figure 9.2: Error ratios for the observation of different oxygen lines, the improved MAS corresponds to the 9+ calculation.

Figure 9.3: Error ratios at different $T_{sys}$, the improved MAS corresponds to the 1500 K calculation.

The signal-to-noise ratio of a receiver can either be improved by an increase of the integration time, or by a decrease of $T_{sys}$, as given in Eq. (6.1). The integration time enters the calculation of the noise with a one over square root factor, an increase in the integration time by a factor of 9 has the same effect as a decrease of $T_{sys}$ by a factor of 3. The drawback of a longer integration time is the increased smearing of the measurement along the track, while improvements of $T_{sys}$ result in a direct reduction of the noise per channel. The influence of $T_{sys}$ on the retrieval error has been investigated in Figure 9.3, where a mid-latitude summer scenario is chosen. A reduction in $T_{sys}$ results in a direct accuracy gain at all altitudes.
9.3 Antenna Improvements

An instrument at a higher orbit will have a poorer resolution with an unchanged antenna, since the FWHM corresponds to a wider interval covered at the tangent point. The effect of different antenna patterns on the error of the retrieval is visualized in Figure 9.4. All retrievals are performed with a mid-latitude summer scenario.

The employment of a smaller FWHM improves the temperature retrieval throughout the troposphere up to the mesosphere. The retrieval error of a calculation with the original MAS antenna has been compared to these results, this antenna yields a slightly worse error ratio than the 2.0 FWHM scenario. The MAS antenna was employed on the Space Shuttle, which has a typical orbiter altitude of about 300 km. Taking this into account improves the retrieval error to almost that of the 1.1 FWHM calculation. Although, the resolutions at the tangent point are very similar, 10 km for the nominal antenna and 12 km for the original MAS antenna, the MAS antenna shows a slightly worse retrieval error. This conduct can be understood by the actual shape of the antenna pattern, the MAS antenna has no well developed beam center, equal sensitivity is obtained over an interval of $\approx 0.07^\circ$.

9.4 Filter-Channel Improvements

The total bandwidth of the MAS instrument is 400 MHz, centered around the line of interest. The filter-channel coverage of the MAS can be found in Table 4.2. Future instruments will cover a wider range of frequencies and observe different lines within one band. The total bandwidth proposed for future satellite instruments covers several GHz, with a resolution of 3 MHz, as for example discussed with the SORPANO instrument in Bühler et al. (1998). The possible retrieval errors of a 10 GHz band centered at 60 GHz is shown in Figure 9.5. The impact of the filter-channel width has been investigated. The retrieval error is unaffected by the filter-channel width for altitudes below 25 km. The 3 MHz resolution is very similar to

Figure 9.4: Influence of different antennas on the error ratio of the temperature retrieval, the FWHM of the antenna is varied with the factor indicated in the legend, a factor of 1.0 corresponds to the improved MAS.
caused by pressure and Doppler broadening are only covered by the 2 MHz filter-channels, as can be seen in Figure 5.6.

The impact of a 9 MHz wide high resolution band covering the line center has been investigated. The original MAS has a high resolution band of 4 MHz. Additionally, the width of the filter-channels covering this 9 MHz band is varied, different channel width of 0.05 MHz, 0.1 MHz, 0.2 MHz, and 0.3 MHz are assumed. The retrieval error can be found in Figure 9.6. Furthermore, the impact of the total bandwidth is varied between the different calculations, since the total bandwidth determines the retrieval error at low altitude. Total bandwidths of 200 MHz, 400 MHz, 600 MHz, and 800 MHz are calculated. The improved MAS with a total bandwidth of 400 MHz, a high resolution bandwidth of 4 MHz, covered with 0.2 MHz filter-channels, has been included for comparison.

The retrieval error at low altitudes is improved by the widening of the band from 400 MHz to 600 MHz. Coverage of 800 MHz around the line center does not further improve the error. The improved MAS calculation deviates from the ‘400, 0.20 MHz’ one at about 25 km, the filter-channel width of 3 MHz compared to 4 MHz of the improved MAS improves the retrieval error. This is not visible in the calculation covering a band of 10 GHz, there, enough information is provided by several lines simultaneously observed. The 200 MHz calculation provides no temperature information below 25 km. The retrieval error at mesospheric altitudes is hardly improved by finer filter-channels, the improved MAS shows the lowest error, since the two 2 MHz wide filter-channels, covering additionally the line center, improve the statistics (see Table 4.2). Very high resolution filter-channels are necessary to improve the error at mesospheric altitudes, in order to cover individual Zeeman lines. As mentioned earlier, the spacing between two Zeeman lines is around 125 kHz, thus, 50 kHz filter-channels are not sufficient.

Figure 9.5: Error ratios for a band covering the frequency range of 55 GHz to 65 GHz with different filter-channel resolutions.
Figure 9.6: Error ratios for filter-channel combinations. The first number gives the total width of the band covered with 3 MHz filter-channels; the second number gives the width of the high resolution filter-channels that are used to cover 9 MHz around the line center.
10 Part Summary and Conclusion

Synthetic retrievals were performed to verify the inversion method and to investigate the temperature information that can be gained from observation of the 9+ line at 61.151 GHz. The OEM showed good results for synthetic retrievals, the true profile was found in less than 5 iteration steps. Simultaneously, instrument parameters were retrieved, which showed convergence within 2 iterative steps. The OEM was proven to be a well suited method to retrieve MAS temperature profiles in the stratosphere and mesosphere.

The performed calculations show the potential of retrieving temperature up to 90 km with an altitude resolution between 4 km and 10 km when applying the MAS instrument characteristics. Accurate knowledge of the magnetic field and the positions of the tangent point and the instrument is necessary, because the strength of the magnetic field determines the saturation altitude of the inner channels. This saturation point can vary by more than 10 km for channels around the line center and by up to 5 km for the center channels for different magnetic field strengths. The observation configuration can influence the error of the obtained profile in the mesosphere by 1.5 K, the influence of the magnetic strength can be as high as 2.0 K.

The error is < 6 K at mesospheric altitudes. Considering that the amplitude of mesospheric temperature inversions layers can exceed 20 K, it follows that the MAS can detect such layers.

The developed software was afterwards used for the retrieval of MAS temperature profiles. The retrieved profiles were compared to different Lidar sites, to data from the UARS satellite, and to NCEP data.

Two UARS limb-viewing tracks close in time and space of the instruments MLS, ISAMS, and CLAES were used for a comparison with MAS results. Temperature profiles derived from the MAS oxygen line located at 61.151 GHz were compared. Deviation from the CIRA 86 model for the month of March, latitude 20°, were investigated.

All three UARS instruments show lower temperatures throughout the stratosphere, with deviations from the CIRA 86 model of up to 12 K. The MAS shows lower temperatures in the stratosphere as well, with an exception near 40 km and at 30 km. Near 40 km the MAS detects a layer of enhanced temperature, not present in the UARS data. The results at 30 km are less reliable owing to the truncation of the measurement at 30 km. Otherwise, the MAS data agree with the UARS data in the stratosphere.

Lower mesospheric temperatures between altitudes of 50 km and 60 km are above the CIRA 86 model with differences of up to 12 K in the CLAES and ISAMS data and up to 8 K in the MAS one. The middle mesosphere is only sampled by one UARS instrument. ISAMS detects lower temperatures than those of the CIRA 86 model, deviations are up to 16 K. The MAS detects lower temperatures of up to 24 K. The major differences in the MAS data occur at an altitude of 70 km, where the bottoms of temperature inversion layers have been observed by the HALOE instrument on UARS. Otherwise, mesospheric temperatures are highly variable with latitude.

Overall, a general agreement between the MAS temperature profiles and the temperatures derived from UARS data is found. Stratospheric temperatures are generally below those of the CIRA 86 model; lower mesospheric temperatures are above those of CIRA 86. The upper mesosphere is colder than the CIRA 86 model in the ISAMS and MAS data.

The major problems for a comparison with Lidar data are the rather limited measurement times of the MAS, about 2 weeks/year, and consequently the difficulty of finding data sets that coincide in time and space. This problem was overcome by including data from NCEP analysis, to verify the development of the temperature profile with time. The comparison with the ground based Lidar data showed good agreement in the stratosphere, but the stratosopause temperatures do not agree that well. This is mainly due to the different resolution of the instruments and the different times of the measurements.

Concentrating on the development of future passive microwave limb sounder instruments, possible improvements of an MAS-like instrument have...
been discussed. Assuming that this future instrument is located on a satellite with an orbit altitude of 820 km, the impact of different instrument parameters has been addressed. Investigated parameters are the line selection, the antenna pattern, $T_{sys}$, and the filter-channel and band width.

The MAS oxygen line at 61.150 GHz proves to be the best choice for the detection of mesospheric temperatures using microwave emissions, since it is the strongest line available within the frequency region from 0 GHz to 3000 GHz and the detector technology provides instrument with low noise values.

A strong signal-to-noise ratio is required for mesospheric temperature sounding, hence improvements of $T_{sys}$ show a direct gain in the retrieval error for all retrieval levels. The suppression of the image band increases the signal-to-noise ratio too, but information about temperatures below 20 km is lost.

The impact of the antenna pattern has been investigated by varying the beam width of the antenna. Only substantial reductions of the beam width result in an improvement in the retrieval error. Variations of 10% are not significant.

An improvement in the retrieval error is possible by a different band width of 600 MHz around line center, and the usage of finer filter-channels for the coverage of the pressure broadening in the line wings. The MAS high resolution filter-channels prove to be sufficient, only a substantial decrease in the width would lead to an improvement in the error of mesospheric temperature retrieval.

The gain of a 10 GHz band centered around 60 GHz leads to an improvement of the stratospheric and mesospheric retrieval errors, but other methods as the decrease of $T_{sys}$ are more effective.

The optimal choice for a MAS like future instrument is the combination of a strong line in one of the sidebands and a weak line in the other. Mesospheric temperatures are obtained by the strong line, stratospheric from both lines, and tropospheric from the weak line. The band width should be enlarged to cover 600 MHz, preferably covered with 6 MHz filter-channels. The high resolution filter-channels of the MAS have proven to be sufficient for mesospheric temperatures. $T_{sys}$ should be as low as possible, since it results in a direct improvement of the retrieval error at all altitudes.
Part III

GRAS
11 GPS and GLONASS

The radio occultation method is based on the detection of signals from
the American Global Positioning System (GPS) or the Russian Global
Navigation Satellite System (GLONASS). These two systems are nowadays
combined under the name Global Navigation Satellite System (GNSS).
GNSS signals are used for accurate position determination on the Earth.
This chapter gives an overview of the principles of the GNSS position
determination. The overview description is mainly extracted from the book
by Hofmann-Wellenhof et al. (1994) and the Internet page given by Dana
(1999) for the GPS, while information about GLONASS comes mainly from
their homepage GLONASS (2000).

11.1 Principle of GNSS
Position Determination

GNSS is a radio-based navigation system, giving three-dimensional coverage
at all locations on the Earth 24 hours a day in all weather conditions.
The principle of the location determination is based on satellite ranging
by the calculation of the distances between the receiver and the position
of four or more satellites. The location of the receiver on Earth can be
calculated by determining the distance from each of the satellites to
the receiver, assuming the satellite positions are known. The GNSS principle
determines the actual position by ‘triangulation’.

A GNSS receiver determines the distance between a GNSS satellite and
the receiver by measuring the time it takes a radio signal (the GNSS sig-
nal) to travel from the satellite to the receiver. Radio waves travel in the
atmosphere approximately at the speed of light in vacuum, the significance
of the change of the speed of light in a medium will become clear later in
this text. The distance from the satellite to the receiver can be determined
if the time it takes for the signal to travel from the satellite to the receiver
is known. This requires the knowledge of the exact time when the signal
was transmitted and the exact time when it was received.

In order to perform this task, the satellites and the receivers use very ac-
curate clocks which are synchronized to generate the same code at ‘exactly’
the same time. The code received from the satellite is compared with the
code generated by the receiver. The time difference can be determined by
comparing the codes. Since clocks can never be totally synchronized, four
satellite signals are needed to determine the three distances and the correct
travel time of the signal for normal navigation. Consequently, the naviga-
tion system has been designed to assure that there are always four satellites
within the field of view. More satellites are needed when no a priori in-
formation about the position is available. Generally, it is assumed that the
position is on the Earth surface, or at a certain altitude above.

11.2 Global Positioning System

The build up of a complete GPS constellation started in 1978 with the
launch of the first four satellites. There were seven operational satellites
which provided about 5 hours of navigation coverage daily for testing by
the year 1985. The system was formally declared as having met the require-
ment of ‘Full Operation Capability’ in 1995, with a total of 24 operational
satellites.

Each GPS satellite is powered by solar cells. The satellites have a period
of 12 hours and are placed in a roughly circular orbit at about 20200 km alti-
tude, moving with a velocity of about 2700 m/s. The GPS system provides
specially coded satellite signals that can be processed in a GPS receiver,
allowing the receiver to compute position, velocity and time. Generally,
one can divide a satellite navigation system into three segments:
Space Segment: consists of the GPS satellites. These satellites are emit-
ting radio signals, carrying information to allow for the determination of
the position. The nominal GPS operational constellation has 24 satellites (21 active and 3 spare ones). Often there are more than 24 operational satellites as new ones are launched to replace older satellites. The satellites are placed in six orbital planes, with nominal four satellites in each plane. The orbital planes are equally spaced, 60° apart, and inclined at about 55° with respect to the equatorial plane. This constellation assures the user a visibility of four to eight satellites above 15° elevation from any point on the Earth.

**Ground Segment**: consists of a system of tracking stations. The Master Control facility is at Schriever Air Force Base in Colorado while four more so-called Monitor Stations are located around the globe. These monitor stations receive signals from the satellites which are incorporated into orbital models for each satellite. The models compute precise orbital data, called ephemeris, and satellite clock corrections for each satellite, which are uploaded to the satellite by the Master Control station. A subset of this data is then send by the satellite to GPS receivers via radio signals.

**User Segment**: consists of the GPS receivers and the user community. A GPS receiver is able to convert signals of the satellites into position, velocity, and time estimates. These receivers are used for navigation, positioning, and nowadays more and more for atmospheric research.

**Navigation**: is the primary function of GPS. Navigation receivers are made for aircraft, ships, ground vehicles, and for hand-carrying by persons.

**Positioning**: very accurate position determination is possible by using GPS receivers at reference locations providing corrections and relative positioning data for remote receivers. This technique is called Differential GPS (DGPS). Land survey, geodetic control, and plate tectonic studies are examples. Less precise positioning is possible by using GPS data alone. Even other satellites are equipped with GPS receivers for accurate position determination.

**Atmospheric Research**: GPS signals can be used to determine the electron density of the ionosphere, and to provide information about the temperature and the water vapor content in the atmosphere.

### 11.2.1 GPS Satellite Signals

The satellites utilize two microwave carrier signals to transmit data to the receiver. The L1 frequency at 1575.42 MHz carries the navigation message and the Standard Positioning Service (SPS) code signals. The L2 frequency at 1227.60 MHz is used to measure the ionospheric delay by Precise Positioning Service (PPS) equipped receivers. Three binary codes modulate the L1 and/or L2 carrier phase.

**C/A Code (Coarse Acquisition)**: modulates the L1 carrier phase. The C/A code consists of a repeating 1 MHz Pseudo Random Noise (PRN) code. Only the L1 carrier signal is modulated with this noise-like code, spreading the spectrum over a 1 MHz bandwidth. The C/A code repeats every 1023 bits (one millisecond). Each satellite has a different C/A code, which allows the identification of a GPS satellites by their PRN number, a unique identifier for each PRN code. The C/A code is the basis for the civil SPS.

**P-Code (Precise)**: modulates the L1 and L2 carrier phases. The P-Code consists of a very long (seven days) 10 MHz PRN code. The P-Code is encrypted into the Y-Code during the Anti-Spoofing (AS) mode of operation. This encrypted Y-Code requires a classified AS Module and is only for use by authorized users with cryptographic keys (e.g. military). The P (Y)-Code is the basis for the PPS.

**Navigation message**: modulates the L1-C/A code signal. This message is a 50 Hz signal consisting of data bits that describe the orbits of the GPS satellite, corrections to the satellite reference clock, and other relevant system parameters (see Section 11.2.2).

### 11.2.2 GPS Navigation Message

The GPS navigation message consists of time-tagged data bits marking the satellite transmission time of each subframe. A data bit frame consists of 1500 bits divided into five 300 bit subframes. The data bit frame is transmitted every thirty seconds.

The structure of the five GPS subframes is given in Table 11.1. Subframe
one is used to sent clock corrections of the transmitting satellite, while sub-frame two and three are used for precise orbital data sets of this satellite. Subframes four and five convey different system data, being successively transmitted. An entire set of twenty-five frames (125 subframes) makes up the complete navigation message that is sent each 12.5 minutes. The complete system data contains for example information about the approximate orbits of all satellites over an extended period of time (almanac), a complete ionospheric correction model, and other system parameters and flags that characterize details of the system. The almanac allows the calculation of all satellite positions for periods up to months, while the ephemeris data is only valid for short sections of the satellite orbits. The ionospheric model is used in the receiver to correct the influence of the ionosphere on the position determination.

Table 11.1: Data bit frame structure of the GPS navigation message

<table>
<thead>
<tr>
<th>Subframe</th>
<th>Content</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Clock corrections</td>
</tr>
<tr>
<td>2</td>
<td>Orbital Data 1</td>
</tr>
<tr>
<td>3</td>
<td>Orbital Data 2</td>
</tr>
<tr>
<td>4</td>
<td>Ionospheric Model, etc.</td>
</tr>
<tr>
<td>5</td>
<td>Almanac data for all satellites</td>
</tr>
</tbody>
</table>

11.2.3 GPS Position Determination

Generally, the GPS system allows two different ways of position determination:

**PPS:** only available to authorized users with cryptographic equipment and keys, e.g., American and allied military. The obtained accuracy is given by Enge and Misra (1999) as:

- 21 meter horizontal accuracy
- 28 meter vertical accuracy

**SPS:** available to civilian users worldwide. The accuracy is intentionally degraded by the Department of Defense by the use of Selective Availability (SA). SA degrades the accuracy of the SPS signals by a time varying bias. A different bias is used for each satellite and the calculated position is a function of the combined SA bias of each satellite used in the determination of the position. The SA is a low frequency bias of a few hours and the determined position cannot be effectively averaged over periods shorter than a few hours. The obtained accuracy is (Enge and Misra, 1999):

- 100 meter horizontal accuracy
- 156 meter vertical accuracy

The accuracy can be increased significantly by the use of DGPS techniques. The idea behind DGPS is to correct bias errors at one position with measured bias errors at a known position. A reference receiver, or base station, computes corrections for each satellite signal and transmits the corrections for example by radio waves to other receivers. Within the vicinity of the base station (100km), the accuracy for DGPS is generally below 1m and can go down to 1cm in horizontal and 2cm in vertical direction for an integration time of about 1 minute.

11.3 Global Navigation Satellite System

GLONASS is the Russian counterpart to the United States GPS and both systems share the same principles in the data transmission and positioning methods.

In 1982 the first GLONASS satellites were set into orbit. Although the initial plan was to complete the system by 1991, the deployment of the full constellation of satellites has only been achieved in 1996. The different segments are:

**Space Segment:** GLONASS, as GPS, is formed by 24 satellites located in three orbital planes inclined at about 65° to the Earth's orbital plane, with a roughly circular orbit at an altitude of 19100km and a period of about 11 hours and 15 minutes. Each satellite is identified by its
11.3 Global Navigation Satellite System

slot number, which defines the orbital plane and the location within the plane. The three orbital planes are separated by 120°, and the satellites within the same orbit plane by 45°. With the breakdown of the Russian empire and the financial problems the constellation has degraded to 9 active satellites (February, 2000).

**Ground Segment:** Ground Control Center and time standards in Moscow, plus 4 more Monitor Stations entirely located in former Soviet Union territory.

**User Segment:** see Section 11.2

### 11.3.1 GLONASS Satellite Signals

While GPS uses only 2 different frequencies for the transmission of the GPS data, GLONASS uses different frequencies for the identification of the satellite. All satellites transmit simultaneously in two frequency bands to allow the user to correct for ionospheric delays on the transmitted signals. Each satellite has allocated a particular frequency within the band, determined by the frequency channel number of the satellite. Nevertheless, two satellites in the same orbit, occupying antipodal locations, transmit in exactly the same frequency, with a few exceptions.

The actual carrier frequency can be derived from the channel number \( k \) by applying the following expressions:

\[
L1: f_1(k) = 1602 MHz + k \frac{9}{16} MHz
\]

\[
L2: f_2(k) = 1246 MHz + k \frac{7}{16} MHz
\]

Superimposed onto the carrier frequency, the satellites modulate their navigation message.

Users of GLONASS are not subject to the GPS constraint of encryption; its operators have adopted a policy of providing unrestricted accessibility so that both civilians and the military have access to the highest accuracy.

### 11.3.2 GLONASS Navigation Message

The carrier frequencies L1 and L2 are modulated with the following binary signals:

- **C/A Code:** 0.511 MHz pseudo random ranging code modulated on L1 and L2
- **P-Code:** 5.11 MHz high accuracy code, modulated on L1 and L2

Navigation message transmitted at 50 bits per second on L1 and L2.

100Hz auxiliary meander sequence modulated on L1 and L2.

The GLONASS navigation message is transmitted as repeating superframes. A superframe consists of five frames, and a frame consists of 15 strings. The superframe has a duration of 2.5 minutes, the frame 30 seconds, and the string 2 seconds.

Table 11.2 shows the frame structure of the GLONASS system, it includes immediate and non-immediate data. The immediate data relate to the satellite that transmits the given navigation signal. The non-immediate data (almanac) relate to all satellites in the GLONASS constellation. Within each frame the total content of immediate data for a given satellite and a part of non-immediate data are transmitted. The data contained in strings 1-4 relate to the transmitting satellite (immediate data), it is not updated in one superframe. The strings 5-15 of each frame contain non-immediate data (almanac) for the 24 satellites. The frames 1-4 contain almanac for 20 satellites (5 satellites per frame). The fifth frame contains the remaining data for 4 satellites.

Table 11.2: Frame structure of the GLONASS navigation message

<table>
<thead>
<tr>
<th>String</th>
<th>Content</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Immediate Data 1</td>
</tr>
<tr>
<td>2</td>
<td>Immediate Data 2</td>
</tr>
<tr>
<td>3</td>
<td>Immediate Data 3</td>
</tr>
<tr>
<td>4</td>
<td>Immediate Data 4</td>
</tr>
<tr>
<td>5</td>
<td>Almanac</td>
</tr>
<tr>
<td>...</td>
<td>Almanac</td>
</tr>
<tr>
<td>15</td>
<td>Almanac</td>
</tr>
</tbody>
</table>
11.3.3 GLONASS Position Determination

The GLONASS system has two types of navigation signals:
- standard precision navigation signal with an accuracy of:
  - 65 meter horizontal accuracy
  - 70 meter vertical accuracy
- high precision navigation signal, where the accuracy is similar to the PPS of the GPS constellation. The higher precision is obtained by a different clock rate and is, other than for the GPS, also available to the civilian user.
12 Radio Occultation Method

The radio occultation method can be used to probe the atmosphere of a planet by using signals at radio frequencies. The source of the radio signal is generally a GNSS satellite, since the intensity of other natural sources is usually too low. The radio signal allows the determination of atmospheric parameters such as density, temperature, pressure, water vapor, and electron density. The principle of radio occultation and how it can provide information about the state of the atmosphere is described in this chapter.

12.1 Historic Overview

The radio occultation method was first applied to investigate the atmospheres of Mars and Venus by Fjeldbo and Eshleman (1965); Phinney and Anderson (1968); Fjeldbo et al. (1971) and in later years also for the outer planets and their satellites, e.g., Lindal et al. (1983, 1985). The communication links or other radio signals to and from the flyby spacecraft can be used to probe the atmosphere. The situation for a radio wave transmitter located on the spacecraft, and receiving stations on the Earth is illustrated in Figure 12.1.

The electromagnetic waves (EMW) emitted by the satellite propagate through the atmosphere of the planet of interest in a limb sounding geometry. The changing refractivity along the path leads to a so-called bending of the rays, caused by the combined effects of the ionosphere and the neutral atmosphere. Consequently, a signal emitted by the satellite and detected by a receiver on Earth will carry information about the ionosphere and the neutral atmosphere. Profiles of temperature, pressure, density, and water vapor of the neutral atmosphere can be derived from the bending of the

12.2 Radio Occultation of the Earth’s Atmosphere

Whereas the missions to other planets yield valuable information on the atmospheric conditions of this planet, this information is not sufficient for the Earth’s atmosphere. A flyby of a spacecraft will only provide very
limited coverage of the planets atmosphere. The Earth’s atmosphere has been studied extensively within the last few years and point measurements were conducted with balloons, rockets, and airplanes. Only global information will provide the information needed for accurate environmental and weather prediction.

Using the radio occultation method for the Earth’s atmosphere was first proposed in the 1960s by Fischbach (1965) and Lasigian et al. (1969). However, a global coverage would require multiple orbiting transmitters and receivers, leading to unacceptable costs. The situation changed with the installation of the GNSS constellation in the 1980s.

The principle of the radio occultation is shown in Figure 12.2. The GNSS transmitter emits an EMW which is detected by the receiver on a LEO satellite. One LEO satellite, using only the GPS signals, would be able to detect about 250 setting events and 250 rising events per day (Kursinski et al., 1997), a fully installed GLONASS system would double the number of soundings.

The frequencies of the EMW for the GPS/GLONASS system fall into the radio frequency region. The EMW will interact with the medium inbetween the transmitter and the receiver, where two major interactions can be distinguished for the Earth’s atmosphere:

Refraction due to the ionosphere
Refraction due to the neutral atmosphere
Consequently, a GPS/GLONASS signal emitted by the transmitter and detected by the receiver will carry information about the ionosphere and the neutral atmosphere.

The detected quantity is the bending of the ray,\(^1\) mainly caused by the changing refractivity field of the Earth. The calculation of the total bending for the Earth’s atmosphere is described in Section 12.2.1.

The ionospheric influence on the bending is removed by the method described in Section 12.2.3 if the interest is focused on the neutral atmosphere.

The determination of atmospheric parameters from radio occultation is very similar to the problem encountered in seismic studies, where one wants to determine the varying density of the Earth’s body along the propagation path of a seismic wave. The determination of atmospheric parameters is described in details in Section 12.3.

A first prototype of concept mission for radio occultation was the GPS Meteorology (GPS/MET) experiment, led by the University Corporation for Atmospheric Research (UCAR) in Boulder, U.S.A. (Ware et al., 1996). The instrument was launched in April, 1995 onboard the small research satellite MicroLab-1. The mission continued until March, 1997, measuring up to 150 GPS settings per day during dedicated periods. The possible 250 setting events per day were not reached, owing to gaps in the ground network tracking and memory limitation onboard the satellite. In total, about 70,000 occultation events were collected, several thousand have been compared with correlative data sets and a statistical agreement within 1 K root mean square of averages for an altitude range of 1 km to 40 km was found (Rocken et al., 1997).

### 12.2.1 Bending Angle

The bending angle \(\alpha\) is defined in Figure 12.2. An EMW emitted by a GNSS satellite and received by a LEO satellite will encounter a varying density and hence varying refractivity field along the path, introducing a bending and a retardation. The ray passing through the atmosphere will follow Fermat’s principle of least time globally and Snell’s law locally in the geometric optics approximation (Born and Wolf, 1993).

The angle \(\alpha\) can be expressed as a function of the impact parameter \(\alpha\) or the radius to the tangent point \(r_t\), as given in Figure 12.2. The impact parameter is defined as the distance between the Earth’s center and the perpendicular to the asymptotic ray path. The radius to the tangent point is defined as the point along the path were the distance to the Earth’s surface is minimized.

The situation given in Figure 12.2 holds only for local spherical symmetry. Deviations from local spherical symmetry are introduced by the atmosphere and the elliptical shape of the Earth. The elliptical shape of the Earth can be compensated for by the introduction of a different Earth’s

---

\(^1\) In practice, the bending angle is derived from the phase path delay, as discussed in Section 12.2.2.
center and a radius of curvature, depending on longitude and latitude. This radius is a fit to the actual shape of the Earth at the occultation event, it is larger than the Earth’s radius at the poles and smaller than the Earth’s radius at the equator. The influence of a non-spherical atmosphere cannot be corrected that easily and will in general introduce errors in the retrieved atmospheric profiles.

The mathematical treatment is as follows: Fermat’s principle of least time along a given path $S$ with a varying refractive index $n$ can be expressed as:

$$\int_S n(s) \, ds = \text{minimum} \quad (12.1)$$

Snell’s law is written as:

$$n \sin \beta = \text{const} \quad (12.2)$$

with $\beta$ being the angle between the ray path and the gradient of the refractive index. The ray path in the atmosphere is lying in a plane under spherical symmetry (Gorbunov and Sokolovskiy, 1993) and the scenario shown in Figure 12.3 follows, where a constant refractive index within a concentric shell is assumed. Applying Snell’s law (Eq. (12.2)) at point $P$ yields:

$$\frac{\sin \gamma}{\sin \beta_2} = \frac{c_1}{c_2} = \frac{n_2}{n_1} = \frac{r_2}{r_1} \quad (12.3)$$

with the speed of light $c_1$ and $c_2$ in concentric shell 1 and 2. From geometry it follows for $\sin \gamma$:

$$\sin \gamma = \frac{r_1}{r_2} \sin (\pi - \beta_1) = \frac{r_1}{r_2} \sin \beta_1 \quad (12.4)$$

Combining Eq. (12.3) and (12.4) yields:

$$n_1 r_1 \sin \beta_1 = n_2 r_2 \sin \beta_2 \quad (12.5)$$

The introduction of more layers, so that $n$ becomes a continuous function of the radius $r$, yields a relation to the impact parameter $a$:

$$n(r) r \sin \beta = \text{const} = a \quad (12.6)$$

since Eq. (12.5) must hold for all layers. This equation is also known as Bouguer’s rule (Born and Wolf, 1993). Equation (12.6) reduces to:

$$a_0 = n(r_1) r_1 \quad (12.7)$$

at the tangent point $r_1$ where $\sin \beta = 1$. The relation between the angle $\beta$ and the bending angle $\alpha$ is:

$$\alpha = \phi + \beta - \frac{\pi}{2} \quad (12.8)$$
as can be seen in Figure 12.4. The differential form of Eq. (12.8) follows as:

$$d\alpha = d\phi + d\beta \tag{12.9}$$

The differential $d\beta$ can be derived from Eq. (12.6):

$$d\beta = -\frac{a (n + r \frac{dn}{dr})}{nr\sqrt{(nr)^2 - a^2}} dr$$

$$= -\frac{a (n + r \frac{dn}{dr})}{nr\sqrt{(nr)^2 - a^2}} dr \tag{12.10}$$

while the differential $d\phi$ is given by:

$$d\phi = \frac{\tan \beta dr}{r} \tag{12.11}$$

which can be seen in Figure 12.4. Expressing the angle $\beta$ in terms of the impact parameter $a$, given by Eq. (12.6), the differential $d\phi$ can be expressed as:

$$d\phi = -\frac{a dr}{r \sqrt{(nr)^2 - a^2}} \tag{12.12}$$

Inserting the Equations (12.10) and (12.12) into Eq. (12.9) yields:

$$d\alpha = -\frac{a}{\sqrt{(nr)^2 - a^2}} \frac{dn}{dr} dr = -\frac{a}{\sqrt{(nr)^2 - a^2}} d\ln(n) dr \tag{12.13}$$

By integrating along the whole path we get an expression for the total bending angle $\alpha$:

$$\alpha(a) = 2a \int_{r=\infty}^{r=r_f} \frac{d\ln(n)}{\sqrt{(nr)^2 - a^2}} dr \tag{12.14}$$

where the integration is only performed down to the tangent point, since we assumed a symmetric atmosphere.

Equation (12.14) is an Abelian integral, that addresses the forward calculation of $\alpha(a)$ from a given $n(r)$. The integral can be inverted to calculate the refractive index as a function of tangent altitude (Fjelkbo et al., 1971):

$$n(r_f) = \exp\left(\frac{1}{\alpha} \int_{r=\infty}^{r=r_f} \frac{\alpha(a)}{\sqrt{a^2 - a'^2}} da\right) \tag{12.15}$$

where the impact parameter $a_t$ corresponds to a tangent altitude $r_t$ as given in Eq. (12.7).

Equation (12.15) allows a direct determination of the refractive index, from which the atmospheric parameters can be derived (see Section 12.3). The $\alpha(a)$ are not a continuous function of $a$, the measurement is usually performed with a sampling rate between 10 Hz and 50 Hz. Theoretically, the resolution of $n$ could be as high as the sampling rate, but in practice the resolution is limited by Fresnel diffraction (see Section 12.4).

Despite the possibility to invert Eq. (12.15) directly, this text concentrates on inversion using the OME, owing to the rigorous error treatment which is possible with that method and the straightforward combination of measurements of different instruments (see Section 15.1).
12.2 Radio Occultation of the Earth’s Atmosphere

Figure 12.5: Radio occultation geometry in a spherically symmetric medium. The
tangent point is indicated by TP.

12.2.2 Derivation of the Bending Angle
from Doppler Shift Measurements

The relative motion of the GNSS and LEO satellite will provide a scan of the
atmosphere, this scan is in general neither vertical nor coplanar. The
actual bending angles as a function of $a$ or $r_1$ of an occultation event are
derived from the Doppler shift measurements, since the frequency of the
EMW is precisely known.

The scenario is visualized in Figure 12.5, where ionospheric effects on
the bending are disregarded and local spherical symmetry is assumed. The
radius of the LEO satellite is $r_L$, the one of the GNSS satellite $r_G$. The
velocities of the two satellites are $\vec{v}_L$ and $\vec{v}_G$ respectively. An idealized
ray leaves the GNSS satellite at an angle $\phi_G$ and is received by the LEO
satellite at an angle $\phi_L$.

The LEO satellite has in general an orbit altitude of 600 km to 1000 km,
while the GNSS satellites are at about 20 000 km. Occultation events will
be setting ones for an antenna observing opposite flight direction and rising
ones for flight direction observation.

The impact parameter $a$ can be calculated according to:

$$a = r_L \sin \phi_L = r_G \sin \phi_G$$  \hspace{2cm} (12.16)

The atmospheric bending angle $\alpha$ is given by:

$$\alpha = \phi_L + \phi_G + \gamma - \pi$$  \hspace{2cm} (12.17)

The Doppler shift $f_D$ of the carrier frequency $f$ measured at the receiver
can be then calculated as follows:

$$f_D = \frac{\phi_G}{c} \sin \phi_G - \frac{\phi_L}{c} \sin \phi_L$$

$$+ \frac{c^2}{c^2} \cos \phi_G + \frac{c^2}{c^2} \cos \phi_L + \text{Rel}(\phi_G, \phi_L, \phi_G, \phi_L, c)$$  \hspace{2cm} (12.18)

where the superscripts $r$ and $\theta$ denote radial and tangential velocities of the
satellites, respectively, in the plane defined by the ray path and the
center of the Earth. The last term takes relativistic effects to the Doppler
shift into account (Vorob’ev and Krasil’nikova, 1994).

Using Eq. (12.16) and Eq. (12.18), the angles $\phi_G$ and $\phi_L$ can be calcu-
lated, since the satellite positions and velocities are precisely known. The
last step is the calculation of the angle $\gamma$ by the use of Eq. (12.17), since
the angle $\gamma$ is known from the satellite positions.

The bending angles vary roughly exponentially with altitude, as a result of the first term in Eq. (1.40). Typical bending angles are shown in Figure
12.6, left, along with the difference between a tangent altitude following
from a straight line calculation and one including refraction. The bending
angles vary over more than four orders of magnitude, the detection of such
a quantity is technically difficult, therefore one measures the excess phase
path instead, which is defined as the difference between the actual ray path
and the straight line path $\Delta L$:

$$\Delta L_1 = \int_{GNSS}^{LEO} n(s_1) ds_1 - S_0 = r_1 \lambda_1$$  \hspace{2cm} (12.19)

$$\Delta L_2 = \int_{GNSS}^{LEO} n(s_2) ds_2 - S_0 = r_2 \lambda_2$$  \hspace{2cm} (12.20)

where $S_0$ is the straight line from the GNSS satellite to the LEO, $\lambda_1$ and $\lambda_2$the wavelengths of the GNSS signal, and $r_1$ and $r_2$ represent real numbers.
Note that:

the actual paths of $L_1$ and $L_2$ will in general be different, owing to the
dispersive influence of the ionosphere.

the wavelengths $\lambda_1$ and $\lambda_2$ are not the wavelength corresponding to
the actual frequencies of the GNSS satellite, owing to the Doppler shift.
the Doppler shift encountered in the detection of passive microwave emissions of the atmosphere is a few kHz for frequencies around 60 GHz, the Doppler shift for radio occultation is generally above 10 kHz.

Technically, a phase lock is performed: the receiver on the LEO satellite calculates which GNSS satellite is within the field of view from the on-board information about the satellite orbits. The Doppler shift is calculated for this constellation and the receiver is searching for the GNSS signal. Once the signal is found, an on-board oscillator generates a reference signal in line with the received one. Both signals are compared with sampling rates between 10 Hz and 50 Hz, the received signal will start to differ from the on-board one, owing to the movement of the satellites and the influence of the atmosphere. The atmospheric difference is called phase path delay or excess phase path, depending whether the difference in time or distance is calculated. Setting events are technically easier to track, the phase lock can be performed close to the surface. It is expected that rising events will in general be tracked frequently from about 5 km upwards.

12.2.3 Ionospheric Correction

The ionosphere is a dispersive medium, meaning the refractive index is a function of frequency. It can be calculated according to Klobuchar (1996):

\[ n^2 = 1 - \frac{X}{1 - i Z} = \frac{X}{1 - i Z} \pm \left( \frac{Y_L^2}{X^2} + Y_T^2 \right)^{1/2} \tag{12.21} \]

where

\[ X = \frac{e^2}{4 \pi^2 \varepsilon_0 m} \cdot N_e \cdot \frac{1}{\nu^2} \tag{12.22} \]

\[ Y_L = \frac{\mu_0 e}{2 \pi m} \cdot \frac{\vec{F}}{\cos \theta} \tag{12.23} \]

\[ Y_T = \frac{\mu_0 e}{2 \pi m} \cdot \frac{\vec{F}}{\sin \theta} \tag{12.24} \]

\[ Z = \frac{v}{2 \pi \nu} \tag{12.25} \]
with the electron density $N_e$, the electron charge $e$, the electron mass $m$, the collision frequency $v$, the frequency of the incoming signal $\nu$, the geomagnetic field $H$, and the angle between $H$ and the propagation direction $\theta$. Equation (12.21) can be approximated for the microwave range by:

$$n = 1 - \frac{40.3}{\nu^2} N_e$$

(12.26)

which yields for the refractivity $N$:

$$N = \frac{40.3 \times 10^6}{\nu^2} N_e$$

(12.27)

with $N_e$ given in [e/m$^3$] and $\nu$ in [Hz].

The refractivity of the ionosphere, as expressed in Eq. (12.27), adds to the total refractivity of the neutral atmosphere, as given by Eq. (1.40). Consequently, $N$ and $n$ are frequency dependent and the measured bending angles $\alpha$ will contain information about the total electron content along the path. This is, on one hand, valuable data on the highly variable ionosphere,\footnote{Total electron contents between $10^{16}$ and $10^{19}$ electrons/m$^2$ have been measured (Klobuchar, 1996).} but introduces errors for the sounding of the neutral atmosphere. A correction of the bending angles with the two frequencies $\nu_1$ and $\nu_2$ of the GNSS satellite is (Vorob’ev and Krasil’nikova, 1994):

$$\alpha(a) = \frac{\nu_1^2 \alpha_1(a) + \nu_2^2 \alpha_2(a)}{\nu_1^2 - \nu_2^2}$$

(12.28)

Equation (12.28) corresponds to a first order approximation of the refractive index as given in Eq. (12.21), higher orders will leave a residuum in the measured bending angles.

An additional complication is the fact, that the two rays do not generally travel along the same path, owing to the frequency dependent refractive index. Consequently, they will pass different altitude levels, and one has to assure that rays with corresponding impact parameter are used in Eq. (12.28). This is usually achieved by interpolation of the $\alpha$ angles and selection of the corresponding $a$. Applying this first order approximation allows to obtain the temperature profile with an error below 1K for altitudes up to 50–60 km, under normal ionospheric conditions (Ladretier and Kirchengast, 1996). Practically, additional error sources (e.g., upper boundary assumption) limit the 1K accuracy of temperature profiles to below 40 km.

### 12.2.4 Attenuation of GNSS Signals

The radiation transfer equation, as described in Section 5.2, can be applied straightforwardly to the absorption of GNSS signals by the atmosphere. The polarized version of the radiation transfer equation is not necessary, and Eq. (2.28) can be used. Only the first term on the right hand side of Eq. (2.28) must be considered for a signal incident on the atmosphere, contributions by the second term do exist in radio occultation as well, but they are not measured. Performing the integration through the atmosphere, and calculating the ratio between the incident intensity and the measured one, yields the picture given in Figure 12.7.

The top left plot shows the ratios for the L1 frequency of the GPS signal, the top right one the corresponding results for the L2 frequency. The absorption of oxygen has been removed in the bottom plots, they show that the absorption is caused by the wings of the oxygen lines around 60 GHz, the absorption of water vapor is negligible. Consequently, the absorption is stronger for cold atmospheres, since the pressure broadening varies inversely with the temperature $T$ (Gordy and Cook, 1970).

Other sources for attenuation are extinction by particle scattering and defocusing by sharp refractive gradients. Kursinski et al. (1997) showed that the extinction of the signal by suspension of water droplets or ice particles in the atmosphere is negligible. Defocusing is caused by rapidly changing horizontal refractivity structures, near parallel rays entering the atmosphere are bend differently, the rays diverge (multi-path effects). The signal intensity at the receiver is reduced, or the signal is completely lost for large refractivity gradients (Kursinski et al., 1997).
12.3 Derivation of Atmospheric Parameters from Bending Angles

Once the bending angles of the neutral atmosphere are known, information about the atmospheric parameters density $\rho$, pressure $p$, temperature $T$, and water vapor volume mixing ratio can be directly derived via the refractive index $n$ or the refractivity $N$.

12.3.1 Density

The dry air density $\rho_d$ as a function of altitude $z$ can be calculated by neglecting the moist term in Eq. (1.40). The ideal gas law states:

$$\rho_d = \frac{p_m d}{T R} \tag{12.29}$$

with the universal gas constant $R$ and the molar mass of dry air $m_d$.

Equation (12.29) in combination with Eq. (1.40) yields:

$$\rho_d(z) = \frac{m_d}{k_1 R} N(z) = \text{const} \cdot N(z) \tag{12.30}$$

where the constant value is given by: $4.488 \times 10^{-3} \text{ kg/m}^3$.

Thus, it is possible to generate the density profile directly from the measurements of the bending angles. The density values above about 60 km altitude, where no measurements are available, are taken from models.

12.3.2 Pressure

The pressure profile can be obtained from the density profile by applying the hydrostatic equation, which states that the gravitational force $F$ acting on an air parcel must be balanced:

$$dF = -\rho g(z, \varphi) \, dx \, dy \, dz \tag{12.31}$$

and by considering that a force divided by an area is the pressure $p$:

$$dp = -\rho g(z, \varphi) \, dz \tag{12.32}$$

where $g(z, \varphi)$ is the altitude dependent acceleration of gravity, which can be calculated for a position at an altitude $z$ and latitude $\varphi$ as (Roedel, 1992):

$$g(z, \varphi) = 9.806 (1 - 0.0026 \cos 2\varphi) (1 - 3.1 \times 10^{-7} z) \tag{12.33}$$
The pressure profile is obtained by integrating Eq. (12.32), generally one starts at the top of the atmosphere and performs the integration downwards, since initial pressure errors decrease exponentially with the scale height of the atmosphere:

\[ p(z) = \int_0^\infty g(z', \varphi) \rho(z') \, dz' \]  
(12.34)

### 12.3.3 Temperature

With the calculated pressure profile the temperature profile is obtained directly from the ideal gas law, as given by Eq. (12.29):

\[ T(z) = \frac{p(z)}{\rho_d(z)} \frac{m_d}{R} \]  
(12.35)

### 12.3.4 Water Vapor

Significant amounts of water vapor will introduce an ambiguity in the obtained profiles of \( \rho \), \( p \), and \( T \), especially in warmer regions of the troposphere.

If an independent temperature information is accessible, the partial water vapor pressure follows directly from Eq. (1.40):

\[ e(z) = \frac{N(z)T^2(z) - k_1p(z)Z(z)}{k_1} \]  
(12.36)

This equation can be used to determine the sensitivity of the water vapor profile retrieval towards temperature uncertainties, under the assumption that no a priori information on temperature is available. Using standard error propagation, with errors of the respective parameter denoted with \( \sigma \), yields:

\[ \sigma_e = \frac{1}{k_1} \sqrt{(2NT - k_1p)^2 \sigma_T^2 + T^2 \sigma_N^2 + k_1^2 T^2 \sigma_p^2} \]  
(12.37)

One can calculate the relation between errors in temperature and errors in water vapor by assuming a best case where all errors map directly through to an error in temperature and the profiles of \( N \) and \( p \) are, relatively seen, free of errors:

\[ \sigma_e = \frac{1}{k_1} (2NT - k_1p) \sigma_T \]  
(12.38)

Inserting typical ground values \( (N = 288, T = 273 \, K, p = 1000 \, hPa) \) yields a ratio:

\[ \frac{\sigma_e}{\sigma_T} \approx \frac{1}{5} \]  
(12.39)

Typical ground values of water vapor pressure at mid latitude are around 2 hPa; if the desired accuracy should be around 20% uncertainty in water vapor, the temperature has to be known to within an error of 2 K.

### 12.4 Resolution of Radio Occultation Measurements

The obtainable resolution of radio occultation measurements is limited by Fresnel diffraction. The derivation of bending angles is based on geometric optics, assuming the wavelength approaches zero. The radio signal originates from a point source, propagates through the atmosphere and is detected by the receiver. A thorough study reveals that the atmosphere acts like a weak inhomogeneous lens and the radiation detected at the LEO corresponds to an effective cross beam sampling at the limb which is centered on the ray path. The effective area is given by the first Fresnel zone (Born and Wolf, 1993), which is about 1.5 km in the stratosphere. The resolution increases gradually to about 0.5 km at the surface, due to the exponential increase in the refractivity. The corresponding horizontal resolution can be calculated as the maximum length of the ray path at the tangent point within a shell that has the width of the first Fresnel zone. For the stratosphere, a resolution of about 280 km follows, while the resolution in the troposphere is about 160 km (Melbourne et al., 1994).
The vertical resolution can be improved by applying a diffraction correction based on synthetic aperture principles (Gorbunov and Gurvich, 1998), as for example discussed in Mortensen and Høeg (1998), where a Fresnel inversion technique is used. This approach is not considered in this text and consequently the chosen retrieval resolution is 0.5 km in the troposphere and degrades to 5 km in the upper stratosphere/lower mesosphere. This lower resolution compared to the 1.5 km caused by diffraction is a result of the low signal-to-noise ratio.
13 Retrieval of atmospheric Parameters from Radio Occultation Data

Retrieval of atmospheric parameters like temperature and water vapor concentration from radio occultation data can be performed directly by a matrix inversion technique, Steiner (1998) utilized this method to derive the refractivity from the bending angle measurements. In this work, the OEM (see Chapter 3) is used to derive the atmospheric parameters from bending angle measurements, since OEM offers a rigorous error analysis, which is not provided by the direct inversion.

13.1 Setup

The retrieval is based on two programs, the forward program simulates the measurement, while the inversion program retrieves the atmospheric parameters of interest from the measurement. Inputs to the program are described in this section.

The five standard atmospheres, shown in Figure 1.1, are used as representative examples of the variability of the Earth’s atmosphere to evaluate the retrieval errors under different atmospheric conditions.

13.1.1 Forward Program

The forward model for radio occultation was developed by the author within this study and validated with results of the End-to-end GNSS Occultation Performance Simulator (EGOPS) (Kirchengast, 1998). Input parameters are temperature and water vapor profiles, output are the bending angles at certain altitudes. The altitude spacing can be defined by the user, the resolution used in this study is based on the possible retrieval resolution, which is limited by diffraction (see Section 12.4). The forward resolution should always be higher than the retrieval resolution, to avoid systematic errors. Table 13.1 shows the different altitude intervals chosen and the corresponding resolutions, along with the assumed errors of the measurement. These errors are estimated based on the specifications for the future GNSS Receiver for Atmospheric Sounding (GRAS), which is currently developed by the European Space Agency; for more information please refer to EUMETSAT (1997). In comparison, the GPS/MET instrument error is about a factor 2 higher for this resolution.

Table 13.1: Resolution used in the GNSS simulated measurement calculation and corresponding errors. Above 60 km no appreciable contributions from a radio occultation instrument is expected.

<table>
<thead>
<tr>
<th>Range [km]</th>
<th>Resolution [km]</th>
<th>Error [grad]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 ≤ x ≤ 25</td>
<td>0.25</td>
<td>4.0</td>
</tr>
<tr>
<td>25 ≤ x ≤ 40</td>
<td>0.50</td>
<td>2.8</td>
</tr>
<tr>
<td>40 ≤ x ≤ 60</td>
<td>1.00</td>
<td>2.0</td>
</tr>
</tbody>
</table>

The refractivity is calculated according to Eq. (1.40) and the bending angles follow from Eq. (12.14), where a pole free version of that integral can be found in Hocke et al. (1997).

13.1.2 Inversion Program

The inversion program is a slightly modified version of the one described in Section 3.3. Inputs to the program are:

Measurement: the bending angles of the five scenarios are calculated with the forward program described above
Measurement noise: as given in Table 13.1
A priori temperature profile: taken from the CIRA 86 model, according to the scenario chosen
13.1 Setup

**Temperature profile a priori error:** given in Table 13.2, unless otherwise indicated.

**Temperature profile retrieval resolution:** given in Table 13.2.

**A priori water vapor profile:** taken from the FASCODE package, according to the scenario chosen.

**Water vapor profile a priori error:** 100% unless otherwise indicated.

**Water vapor profile retrieval resolution:** 0.5 km between 0 km and 20 km.

**Reference pressure:** only retrieved if indicated, value at 30 km is given.

A priori pressure error: 10%.

<table>
<thead>
<tr>
<th>Range [km]</th>
<th>Resolution [km]</th>
<th>A priori error [K]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 ≤ x ≤ 30</td>
<td>0.5</td>
<td>10.0</td>
</tr>
<tr>
<td>30 ≤ x ≤ 40</td>
<td>1.0</td>
<td>10.0</td>
</tr>
<tr>
<td>40 ≤ x ≤ 60</td>
<td>5.0</td>
<td>10.0</td>
</tr>
</tbody>
</table>

The pressure profile is calculated with the reference value, using the hydrostatic equation. The water vapor profile is retrieved in logarithmic coordinates, hence the a priori error is given in logarithmic units. The assumed error corresponds to about 100% in linear units, refer to Bühler (1999) for a detailed discussion.

Note: the inversion setup is an a priori equals true one, this has the advantage of quick convergence in an iterative inversion without loosing any information about the error of the retrieval. The inversion of radio occultation data is an almost linear problem, iterative retrievals are in general not necessary, and consequently only one iteration is performed. The a priori equals true setup is nevertheless kept in order to ease the readability of the retrieval result plots.

13.2 Water Vapor Retrieval

Figure 13.1 shows the water vapor retrieval results for the mid-latitude summer scenario, where only water vapor is retrieved and the temperature profile is assumed to be perfectly known.

The error ratio and the averaging kernel functions indicate that water vapor information up to an altitude of about 12 km can be derived from a measurement. Note that the FWHM of the presented retrieval is equal to the spacing of the retrieval levels, indicating that a higher altitude resolution of the retrieval is possible. However, the diffraction effects discussed in Section 12.4 limit the attainable resolution, except if sophisticated ‘diffraction-correction’ pre-processing is employed (Gorbunov and Kornblueh, 2000).

The contributions from water vapor to the bending angles $\alpha$ and to the refractivity $N$, as well as the error ratio of the retrieval for all five scenarios are presented in Figure 13.2. Retrieval of water vapor profiles is possible up to 12.5 km for the tropical and the mid-latitude scenario, the other scenarios allow retrievals up to 10.5 km, if one sets the limit of a meaningful retrieval to an error ratio of 0.5. This corresponds to contributions from water vapor to $\alpha$ of about 0.2%.

While the contribution to the bending angle are integrated through the whole atmosphere, contributions of water vapor to the refractivity are at a specific altitude. These contributions are shown in Figure 13.2 at the top left. The integrated contribution of water vapor to $\alpha$ are about 50% for a tropical atmosphere at the ground, while contributions to $N$ are only 30%.

13.3 Temperature Retrieval

Figure 13.3 shows the retrieval results for a temperature only profile retrieval of a mid-latitude summer scenario. No water vapor retrieval is performed.

The retrieval levels in Figure 13.3 are so close, that the averaging kernels hardly separate in the upper right figure. The error ratio figure at the lower
Run: mid_summer_H2O, Species: h2o

Figure 13.1: Water vapor retrieval of a mid-latitude summer scenario. Please refer to Section 3.4 for a general description of the individual plots.
13.3 Temperature Retrieval

Run: mid_summer_T_2, Species: T

Figure 13.3: Temperature retrieval of a mid-latitude summer scenario. Please refer to Section 3.4 for a general description of the individual plots.

left side indicates, that temperature retrieval is possible up to about 40 km for this measurement and retrieval setup.

Figure 13.4 gives some additional information about the temperature retrieval. The relative response $RR_i$ at a retrieval level $i$ is defined as:

$$RR_i = \left( \frac{\alpha(T_i) - \alpha(T_i + 1\, \text{K})}{\alpha(T_i + 1\, \text{K})} \right) \times 100 \% \quad (13.1)$$

$RR_i$ gives information about the relative response of the bending angle $\alpha$ to an increase of the temperature by 1 K at level $i$. And, since the derivative of the forward model with respect to the retrieval parameter is generated with a 1 K offset, the values of $RR$ are related to the diagonal elements of the weighting function matrix $K$.

Additionally, one must consider the error of the bending angles, expressed as the signal-to-noise ratio $\text{SNR}_i$:

$$\text{SNR}_i = \frac{\alpha(T_i)}{\sqrt{S_y[i, i]}} \quad (13.2)$$

where $S_y[i, i]$ is the corresponding element of the covariance matrix of the measurement.

The figure on the top left side shows the $RR$ to a 1 K offset in the temperature profile. It is about 1.5 % to 2 % for all 5 standard atmospheres. The structure of the $RR$ visible in Figure 13.4 is caused by the combination of the exponentially varying pressure profile and the temperature profile, as given by the first term on the right hand side of Eq. (1.40). Without an error in the bending angles $\alpha$, retrieval of the temperature profile is possible even above 60 km. But the figure on the top right side shows the exponentially decreasing SNR, which reaches 1 at 60 km. An improvement of a factor of 20 is necessary in the SNR to retrieve temperatures at 60 km with an error of 4 K, which is achieved at 40 km with the current measurement errors given in Table 13.1. The bottom left figure shows the ratio of the retrieved and the a priori error. Except for the subarctic winter scenarios, all error ratios are very similar.
Relative Response

Signal-to-Noise Ratio

Error Ratio

Figure 13.4: Upper Left: Relative Response of bending angles $\alpha$ to a 1 K offset; Upper Right: Signal-to-Noise Ratio of a 1 K offset; Lower Left: Error ratio of only temperature retrievals

13.4 Simultaneous Water Vapor and Temperature Retrieval

Figures 13.5 and 13.6 show the retrieval results of a combined temperature and water vapor retrieval for a mid-latitude summer scenario. The measurement error and the resolution as indicated in Table 13.1, the retrieval levels for temperature are the one given in Table 13.2, the water vapor ones are given in Section 13.2.

The derivation of a temperature and water vapor profile from bending angle measurements, using the OEM, is performed by retrieving an additional reference pressure at a certain altitude from which the pressure profile is generated according to Eq. (6.2). The calculation of the pressure profile for a temperature only retrieval is straightforward, since the first term in Eq. (1.40) is proportional to the density. This simple situation is not given for bending angles measurement that include a significant amount of water vapor, since both terms on the right hand side of Eq. (1.40) are pressure dependent. A reference pressure at an altitude of 30 km for the generation of the hydrostatic atmosphere is therefore introduced to the retrieval.

The error ratio of the temperature retrieval in Figure 13.5 is almost 0.8 at ground level, indicating that virtually no information about the temperature is available from measurements at 0 km. The error correlation plot shows that temperature and water vapor are highly correlated here. Above 0 km, the error ratio and the correlation with water vapor are decreasing, reaching a minimum at about 3 km. The retrieval is able to separate the two terms on the right hand side of Eq. (1.40), since the first term varies inversely with temperature, while the second one varies with $1/T^2$. In addition, one has to keep in mind that both terms are pressure dependent, and pressure is correlated with temperature via the hydrostatic equation. The retrieval algorithm is not able to separate the two term effectively above about 3 km and the error ratio and the correlations with water vapor increase. The decreasing influence of water vapor on the bending angles leads to a maximum on the error ratio at about 7 km. The temperature retrieval
Run: mid_summer_TH2O_1, Species: T

0.0-25.0 km: 4.0 µrad
25.0-40.0 km: 2.8 µrad
40.0-60.0 km: 2.0 µrad

p_ref = 13.153 +/- 0.088 hPa

Retrieval

0.0-25.0 km: 4.0 µrad 25.0-40.0 km: 2.8 µrad 40.0-60.0 km: 2.0 µrad , p_ref = 13.153 +/- 0.088 hPa
is almost unaffected by the simultaneous water vapor retrieval above 11 km, where no water vapor information is available.

Figure 13.6 shows the results for the water vapor profile retrieval. Water vapor retrieval at the ground is possible, despite the fact that almost no temperature information is available here, indicating that the sensitivity towards water vapor retrieval is higher than the one towards temperature. The error ratio and the correlations with temperature have a minimum at 3 km. The error ratio increases above, reaching 1 at an altitude of 11 km. The correlations with temperature are 1 at the ground and above 7 km, the retrieval is unable to separate the two terms in Eq. (1.40).

This result seems to be in contradiction to the calculation performed in Section 12.3.4. Two reasons are responsible for the much better retrieval errors obtained with the OEM. Firstly, the assumption of uncorrelated errors does not hold, correlations represent additional information, and, secondly, OEM uses a priori knowledge.

The reference pressure is retrieved at an altitude of 30 km, the error of the retrieval is below 1%. The pressure is positively correlated with the temperature retrieval, especially between 12 km and 30 km. Generally, the pressure is correlated with the temperature via the hydrostatic equation. For temperature profile and reference pressure at 30 km retrieval only, there would be strong correlations for all altitudes below 30 km and decreasing correlations above, since the retrieval sensitivity decreases. Including the water vapor profile retrieval leads to almost no correlations between temperature and the reference pressure for all altitudes where water vapor information is present. This is caused by pressure information available from both retrieved species.

The tiny peak in the correlations at 25 km is caused by the changing measurement error and resolution at this altitude (see Table 13.1), and can be seen in the error ratio plots as well; it is thus of no physical relevance.

The error ratios of temperature and water vapor for all five atmospheric scenarios are shown in Figure 13.7. The error ratios for temperature have all a very similar structure, as already seen in the described mid-latitude summer scenario. The error increases near the surface and reaches about 8 K at the surface. Above, the error varies between 0.5 K and 2 K for tropospheric altitudes. The actual altitudes of the minimum and maximum in the error ratios for altitudes below 10 km are dependent on the scenario, since the temperature and water vapor profile between the scenarios vary. The same holds for the altitude where the presence of water vapor does not affect the error ratio of the temperature retrieval.

The error ratios for water vapor in a combined retrieval are deteriorated compared to a water vapor only retrieval (see Figure 13.2). If one sets the criterion for a meaningful retrieval to achieve error ratios below 0.5, the different scenarios allow retrieval of water vapor only up to 8 km (tropical, mid-latitude summer scenario), and up to 5 km for a subarctic-winter scenario, respectively.

The obtainable retrieval error as a function of the a priori error of the temperature is given in Figure 13.8. It is assumed that the temperature profile at all altitudes is given with the indicated a priori error. Calculations with varying a priori error, e.g., 2 K a priori error for all altitudes below 15 km and 10 K error above, show no significant difference.

Even very tight constrains like 1 K on the a priori error of the temperature profile show no substantial improvements in the retrieval accuracy for water vapor. Either very accurate knowledge of the temperature profile is required to improve the water vapor accuracy, or the a priori error of the water vapor has to be reduced.

13.5 Ignoring Water Vapor in Temperature Retrieval

The effect of ignoring the presence of water vapor and perform a temperature only retrieval can be seen in Figure 13.9, where two calculations are performed, one with temperature retrieval altitudes from 0 km to 60 km, and one where altitudes below 5 km are ignored. A reference pressure at 30 km is additionally retrieved.

Ignoring water vapor in the temperature retrieval leads to a cold bias in the retrieved temperatures near the surface, see Figure 13.9 left. The bias can exceed 30 K in the case of a moist atmosphere (tropical scenario), but is only a few K for a dry atmosphere (subarctic winter scenario). The error
Figure 13.7: Combined temperature – water vapor retrieval. Left: Error ratios for temperature; Right: Error ratios for water vapor.

Figure 13.8: Combined temperature – water vapor retrieval, error ratios of water vapor for different a priori errors of temperature.
Figure 13.9: Effect of ignoring the presence of water vapor in temperature retrieval, deviation between the true temperature profile and the retrieved one. Left: For retrieval altitudes from 0 km to 60 km; Right: For retrieval altitudes from 5 km to 60 km.
14 Part Summary and Conclusion

The retrieval of temperature and water vapor profiles from measurement simulations based on the radio occultation method has been performed. The characteristics of the instrument are derived from a future radio occultation instrument, currently developed at the European Space Agency. The basic atmospheric quantity in radio occultation is the bending angle, the retrieval of temperature and water vapor from this quantity is based on the OEM. Despite the fact that a direct inversion is possible with radio occultation data, the OEM has been used, since it offers a rigorous error analysis.

Five observation scenarios have been defined to cover the expected variability of the measurements, namely a tropical, a mid-latitude summer, a mid-latitude winter, a subarctic summer, and a subarctic winter one.

The retrieval of temperature and water vapor is first performed separately, assuming that the other quantity is perfectly known. This does not correspond to a realistic situation but shows the maximum accuracy achievable. Water vapor retrieval with error ratios better than 0.5 is possible up to altitudes of 12 km for a moist atmosphere, assuming the temperature is perfectly known. Temperature retrieval with error ratios below 0.5 is possible up to altitude of 45 km. The error ratio varies with altitude, the best performance is achieved at low altitudes, where errors smaller than half a Kelvin are obtained.

A realistic combined retrieval of temperature and water vapor changes the retrieval errors of both species, water vapor retrieval is only possible up to altitudes of 7 km for a moist atmosphere. Temperature retrieval is affected at altitudes below 12 km, the error varies between 0.5 K and 2.0 K for altitudes above 2 km, below, large errors of up to 8 K are found.
Part IV

MASGRAS
15 Combination of Radio Occultation and Passive Microwave Data

The simultaneous retrieval of data from different instruments requires the extension of the retrieval algorithm as presented in Chapter 3. The OEM combines in an optimal way the information of different instruments so that the accuracy of the retrieved temperature profile is maximized over the full range of the detected altitude range. The necessary modifications are outlined in this chapter, followed by the setup of the observation scenario for a combination of a MAS and a GRAS sensor.

15.1 Retrieval Method

The concept of the optimal estimation retrieval method is not restricted to one instrument alone, it is straightforward to extend the measurement vector \( y \) to include different data from different instruments (Rodgers, 1990); (Rodgers, 1976). For combining the two measurement methods discussed in this text, the total \( y \) vector consists now of the measurement of the passive microwave (PMI) and the radio occultation instrument (ROI):

\[
y = \begin{pmatrix}
y_{\text{PMI}} \\
y_{\text{ROI}}
\end{pmatrix}
\]

This combination has the major advantage that information of both instruments is mutually used, while a single retrieval performed for each instrument alone does not include information of the other instrument. With more and more satellite platforms carrying several instruments, the development of retrieval algorithms that include all available information seems necessary. A similar combination is performed in the assimilation of measurements into numerical weather prediction models.

The weighting function matrix \( K \) in Eq. (3.2) is now generated with two different forward models (described in Chapter 5 for the passive microwave instrument and in Section 12.2.1 for the radio occultation instrument):

\[
K = \begin{pmatrix}
K_{\text{PMI}} \\
K_{\text{ROI}}
\end{pmatrix}
\]

The same applies to the covariance matrix of the measurements \( S_y \), which holds the errors of both instruments.

With these extensions of the matrices, the usual OEM can be performed, either in a linear case, as given be Eq. (3.4), or by the iterative approach as given by Eq. (3.7).

15.2 Measurement Simulation Setup

Both instruments are assumed to be mounted on the International Space Station (near-circular orbit at \( \approx 400 \text{ km height with } \approx 53^\circ \text{ inclination} \), reflecting a relevant radio occultation - passive microwave hybrid sensor proposal by Hartmann et al. (1997). It is assumed that both instruments are observing in opposite-flight direction, with the passive microwave sensor ('MAS') continuously measuring the atmospheric emissions while the radio occultation instrument ('GRAS') acquires setting occultation events in roughly the same atmospheric space. The hybrid instrument is referred to as 'GRASMAS sensor' in this context. Utility and performance studies for such a GRASMAS sensor have been performed by Kirchengast and Ramsauer (1998) and Engeln et al. (1999); the work published in the latter is strongly related to the contents of this chapter.

The retrieval error of the temperature profile depends on the magnetic field strength and the angle between the magnetic field and the observation direction, as discussed in Section 7.4. Consequently, the error of the retrieval varies with the geographic location, and a statistical approach is necessary to define the expected retrieval errors.
The position and time of the occultation events as well as the quasi-realistic bending angle measurements are computed with the End-to-End GNSS Occultation Performance Simulator (EGOPS), a radio occultation mission simulation software (Kirchengast, 1998). More than 160 useful setting events of either GPS or GLONASS covering the required altitude range of 0 km to 80 km were found for a single day. For the investigation in this paper, 30 events out of the 160 were quasi randomly chosen to cover the Earth appropriately and allow statistics to be performed. The positions of all 163 events are shown in Figure 15.1 (top), the 30 selected cases are shown at the bottom.

The passive microwave measurement data are generated at the occultation location of the GRAS instrument, assuming that both instruments observe the same atmospheric space. This assumption is not unrealistic, since the occultation events are in general acquired along the flight/opposite-flight direction of the satellite, as are in general the passive microwave limb measurements.

The error characteristics for the radio occultation instrument are unchanged from Chapter 13, and are given in Table 13.1. The passive microwave instrument characteristics have basically been derived from the original MAS. Only the temperature band around 61.15 GHz including information from the image band is used. Three different values have been set for $T_{\text{sys}}$, 1500 K, reflecting the original MAS characteristics, and two values for modern instruments: 1000 K and 500 K. A longer integration time of 0.3 s is assumed for two reasons. Firstly, the instrument is at a higher altitude than the Space Shuttle, secondly, the horizontal resolution has been degraded to improve the signal-to-noise ratio in the mesosphere. For further improvement of the mesospheric temperature retrievals, a different but reasonable modern antenna has been assumed, which has already been applied in Chapter 9. The original MAS instrument allowed temperature retrieval with 10 km resolution in the mesosphere (see Chapter 3), with the improvements, a resolution of 5 km is possible (see Chapter 9).

1 The original MAS has an integration time of 0.04 s.
15.3 Retrieval Setup

Two different retrieval calculations are performed; one assuming that either water vapor is not present or perfectly known and retrieving a ‘dry’ temperature profile. The other calculation is realistic, with water vapor included, retrieving a water vapor and a ‘wet’ temperature profile simultaneously. Additionally, the reference pressure at a tangent altitude of 30 km is retrieved, from which the pressure profile is generated by employing the hydrostatic equation (see Section 6.2).

The two sensors are highly synergistic for the retrieval of a hybrid temperature profile, since there is an overlap interval of about 40 km for tangent altitudes between 20 km and 60 km, where both sensors contribute information. The passive microwave instrument has its greatest potential above the troposphere, while the radio occultation provides temperature measurements way into the troposphere.

This synergistic effect does not hold in this sense for the retrieval of water vapor, since water vapor information is almost entirely provided by the radio occultation instrument for altitudes < 8 km, if only the MAS 61 GHz band is used. Also the addition of the dedicated water vapor channel of the MAS (see Chapter 4) to the MASGRAS instrument would not directly yield a synergistic effect with an overlap region, owing to the water vapor continuum, which restricts retrievals to altitudes above 8 km (Bühler, 1999). Therefore, only three selected cases are investigated for the ‘wet’ atmosphere, covering a dry, a medium, and a moist scenario.

The resolution of the temperature profile retrieval has been determined by an optimization process, assuring that the major part of the information comes from the measurements. The different intervals are presented in Table 15.1. Compared to a radio occultation only retrieval, the resolution has been increased from 5 km to 2.5 km between 40 km and 60 km, owing to the contribution of both instruments. In addition, the a priori error is given in Table 15.1. The error of the temperature profile varies with altitude, roughly reflecting our typical prior knowledge of a temperature profile. The ambiguity in the bending angles at low altitude, caused by the water vapor content, is partly overcome by incorporating very accurate a priori temperature information (see Figure 13.8). A priori data on temperature from short-range forecasts of modern numerical weather prediction models (NWP) are accurate within 2 K in the troposphere (Palmer, 1998). Hence exploitation of radio occultation data focused on information about the water vapor content and good-quality a priori temperature profiles obtained from NWP forecasts are used. It is assumed in this study that a priori temperature information up to about 8 km is provided with an error of 2 K. Errors of up to 5 K can be expected for altitudes between 8 km and 25 km, between 25 km and 60 km information from models is accurate to within 10 K, while practically only zonal mean information is available above (Palmer, 1998). A conservative estimate is around 15 K for the a priori error at these altitudes.

Table 15.1: Temperature retrieval resolution and corresponding a priori errors used for the MASGRAS sensor

<table>
<thead>
<tr>
<th>Range [km]</th>
<th>Resolution [km]</th>
<th>A priori error [K]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 ≤ x ≤ 8</td>
<td>0.5</td>
<td>2.0</td>
</tr>
<tr>
<td>8 &lt; x ≤ 25</td>
<td>0.5</td>
<td>5.0</td>
</tr>
<tr>
<td>25 &lt; x ≤ 30</td>
<td>0.5</td>
<td>10.0</td>
</tr>
<tr>
<td>30 &lt; x ≤ 40</td>
<td>1.0</td>
<td>10.0</td>
</tr>
<tr>
<td>40 &lt; x ≤ 60</td>
<td>2.5</td>
<td>10.0</td>
</tr>
<tr>
<td>60 &lt; x ≤ 90</td>
<td>5.0</td>
<td>15.0</td>
</tr>
<tr>
<td>90 &lt; x ≤ 100</td>
<td>10.0</td>
<td>15.0</td>
</tr>
</tbody>
</table>

The water vapor profile is retrieved between 0 km and 8 km for the three selected cases, with a resolution of 0.5 km. Above 8 km, the contributions of water vapor to the bending angles α do not allow meaningful determination of the water vapor profile in a combined retrieval (see Section 13.4). The a priori error of the water vapor is set to 25 % uncertainty, the a priori error of the reference pressure to 10 %.
16 Instrument Combination Results

The two different methods of detecting the temperature profile of the atmosphere are combined in this chapter, to retrieve one hybrid 'dry' temperature profile, spanning an altitude interval of 0 km to 90 km. This can be achieved with a hybrid MASGRAS sensor as introduced in Chapter 15. In addition, 'wet' retrieval are performed, where both, the water vapor and the temperature profile are retrieved. This reduces the accuracy of the temperature retrieval at altitudes where water vapor is present, as discussed in Section 13.4. Depending on the type of atmosphere, information about the water vapor profile below 5 – 8 km can be derived.

16.1 ‘Dry’ Temperature Results

The results for a 'dry' temperature retrieval are shown in Figure 16.1. Retrieval parameters are the temperature profile and the reference pressure at an altitude of 30 km. Additionally, a 'dummy' water vapor profile is retrieved, where the profile values are zero for all altitude level. The retrieval of this ‘dummy’ profile is introduced as a check whether the retrieval gets all its information from the temperature profile, and does not vary the ‘dummy’ profile within the iterations.

Temperature retrieval is possible up to an altitude of 90 km with a MASGRAS sensor, the averaging kernel at 90 km is well developed, the one at 100 km is already breaking down. The error of this particular retrieval is always below 8 K even for a system noise temperature of 1500 K. The features of the radio occultation instrument are dominating the profile for altitudes up to 40 km, while the passive microwave sensor is dominating for altitudes above 60 km. The correlations with the 'dummy' water va-
por profile are zero throughout the altitude range as required, while the
reference pressure retrieval shows varying correlations.

16.2 Mean ‘dry’ Temperature Results

The accuracy of the combined retrieval varies with location, owing to the
varying ‘dry’ temperature profile, the different magnetic field strengths,
and the different observation geometries with respect to the magnetic field.
The accuracy of the radio occultation instrument varies only slightly with
the temperature profile, the main latitudinal dependence is introduced by
the passive microwave instrument.

The mean error of the temperature retrieval for the 30 selected events is
shown in Figure 16.2. Calculations are performed for three different system
noise temperatures.

The retrievals performed with a system noise temperature of 1500 K show
an error of about 8 K for altitudes around 85 km, while the error at 90 km is
around 6 K. The same feature is visible for all system noise temperatures,
the increasing errors for altitudes above 65 km, with a maximum around
85 km, are caused by the diminishing influence of the pressure broadening
of the oxygen line, while the instrument channels at the center of the line
saturate at an altitude of 90 km, leading to a decrease in the errors. The
influence of different system noise temperatures is negligible up to altitudes
of 35 km, the major information at these lower altitudes comes from the
radio occultation instrument.

A further increase in the accuracy could be obtained by the suppression
of the image band, which doubles the observed brightness temperature
at altitudes above 30 km. This approach neglects information out of the
image band that could be used for tropospheric temperature retrieval, but
the radio occultation instrument is much better suited for this task.

16.3 Combined Temperature and
Water Vapor Retrieval

The presence of water vapor will affect the error of the temperature profile
retrieval from radio occultation data, as pointed out in Section 13.4. The
passive microwave instrument is almost unaffected by water vapor if one
only considers the oxygen band of the instrument. The influence of water
vapor will be visible in radio occultation data at low altitudes where a
significant amount of water vapor is present.

Figure 16.3 shows the results of the temperature retrieval and Figure 16.4
the ones for the water vapor one, both for the case of a medium-moist
atmosphere. The error profile of the temperature retrieval is affected by the
presence of water vapor at altitudes below 10 km, temperature and water
vapor retrieval are strongly correlated in this altitude region, while the
Figure 16.3: Medium-moist atmosphere, simultaneous temperature and water vapor retrieval: temperature results. Please refer to Section 3.4 for a general description of the individual plots.

Figure 16.4: Medium-moist atmosphere, simultaneous temperature and water vapor retrieval: water vapor results. Please refer to Section 3.4 for a general description of the individual plots.
correlations with the reference pressure disappear. The results for the water vapor retrieval show that the retrieval is possible up to altitudes of about 7 km. Water vapor has a strong correlation with the temperature retrieval, but almost none with the reference pressure. The retrieved profile shows slight deviations from the true profile, which should not be present in a 'true equals a priori' setup. The deviations are a result of the three dimensional water vapor field, which entered the calculation of the measurement. The measurement is generated with the EGOPS tool, while the retrieval is based on a one dimensional profile of water vapor. The a priori profile corresponds to the true profile at the tangent point of the occultation event.

The temperature and water vapor results for all three cases are summarized in Figure 16.5. Note that the a priori error of the temperature retrieval is set to 2 K, hence retrieval of temperature information close to the ground is hardly possible in a combined retrieval, since most information enters the water vapor retrieval.

Information about contributions of a single instrument can be deduced from the retrieval results. The single AKMs $A_{\text{ROI}}$ and $A_{\text{PMI}}$ for each instrument can be derived from the weighting function matrix $K$, the a priori covariance matrix $S_0$, and the measurement error covariance matrix $S_y$.

by separating them into a radio occultation and a passive microwave part. First, the respective contribution function matrices $D$ are calculated by inserting the corresponding sub-matrices of $K$ and $S_y$ into the following formula:

$$D = (S_y^{-1} + K^T S_y^{-1} K)^{-1} K^T S_y^{-1}$$

where $K^T$ denotes the transpose of $K$. The matrices $A_{\text{ROI}}$ and $A_{\text{PMI}}$ are then calculated by:

$$A_{\text{ROI}} = D_{\text{ROI}} K_{\text{ROI}}$$

$$A_{\text{PMI}} = D_{\text{PMI}} K_{\text{PMI}}$$

These two matrices give information about the contributions of the individual instruments. The resulting rows for the medium-moist atmosphere of these matrices are shown in Figure 16.6 (temperature part) and 16.7 (water vapor part) for a system noise temperature of 1500 K. Note: The total AKM $A$ is not the sum of these two matrices, since the information of both instruments is combined in an optimal way. Nevertheless, the individual matrices show the major source of the information.

The averaging kernels of the MAS instrument for the temperature retrieval are very small at altitudes below 20 km, indicating that temperature information is very limited at these altitudes. Almost all the information below 25 km comes from the radio occultation instrument. The obtained retrieval error for calculations including contributions from the MAS instrument below 25 km have been compared to the errors obtained, when these levels are avoided in the weighting function matrix calculation for the MAS instrument; no significant difference was found. Hence it is justified to avoid these levels in the MAS computation and reduce the computer intensive calculation of the weighting matrix. The effect on the retrieval error is below 0.1 K.

Above 25 km and up to 40 km the averaging kernels are below 0.5, this indicates that the individual instrument is unable to retrieve temperature with this high resolution, while the averaging kernels are well developed from 40 km upward, where most of the information is provided by the MAS instrument. The error profile at the bottom shows that the individual error
Run: MoistAtmSample-80a_092b, Species: T, PMI ROI

Figure 16.6: Medium-moist atmosphere, separated contribution of the MAS (left hand side) and the GRAS instrument (right hand side) to temperature retrieval

Run: MoistAtmSample-80a_092b, Species: h2o, PMI ROI

Figure 16.7: Medium-moist atmosphere, separated contribution of the MAS (left hand side) and the GRAS instrument (right hand side) to water vapor retrieval
of the MAS instrument is identical to the a priori error for altitudes up to 10 km. Above this altitude, where the averaging kernels are not well developed, oscillations, up to altitudes of about 35 km, are present. The right hand side visualizes, that the GRAS instrument is contributing for altitudes below 50 km.

The results for water vapor illustrated by Figure 16.7 show no averaging kernels for the passive microwave instrument, no influence of water vapor is present in the measurement. The radio occultation instrument shows well developed averaging kernels up to altitudes of about 7 km. Above, no satisfactory information about the water vapor profile can be derived from a radio occultation instrument.
17 Part Summary and Conclusion

A combined MASGRAS sensor allows the retrieval of a hybrid temperature profile with an error of about 4 K in the mesosphere. Information in this altitude region comes from the MAS instrument, while mainly the GRAS instrument allows the determination of the temperature profile up to 35 km with an error below 1 K. The region between 35 km and 60 km is sampled by both instruments and the retrieval error gradually goes from 1 K to 4 K with increasing altitude. Note that the passive microwave instrument is a double sideband receiver, following the original MAS. Further improvements in the stratospheric and mesospheric temperature retrieval is possible by using either a single sideband receiver, or by the observation of another strong oxygen line in the other sideband, see Chapter 9.

The retrieved atmospheric state was made hydrostatic by retrieving a reference pressure at 30 km altitude, this retrieval was possible with an error < 1 %. The water vapor profile was retrieved from the GRAS instrument alone, since the temperature band of the MAS instrument allows no determination of water vapor. An additional MAS band dedicated to water vapor would not provide a hybrid profile, since the two instruments have no overlap for water vapor retrieval. The retrieval of water vapor from GRAS data is possible up to an altitude of about 7 km for a moist atmosphere, and up to about 4 km for a dry one.
Part V

Overall Summary and Conclusion
18 Overall Summary and Conclusions

This text has been focusing on two different approaches of detecting the atmospheric temperature profile remotely. One instrument is using passive microwave emissions of the atmosphere, the source of the signal can be modeled by Planck’s radiation law and the knowledge of the spectroscopic lines of the atmospheric species. Since molecular oxygen has a known and constant volume mixing ratio up to altitudes of 100 km, lines of molecular oxygen around 60 GHz are used to derive the temperature profile. The other instrument is based on radio occultation of GNSS satellites signals to probe the atmosphere. The temperature profile is derived from the bending of the ray, caused by the change in refractivity of the atmospheric density field along the line of sight.

The retrieval process has been performed with the optimal estimation method for both instruments. This method incorporates a priori knowledge in a very transparent way and has shown excellent results. The second great advantage of optimal estimation is the combination of different instruments in the retrieval process. This advantage has been used to combine the two instrument and derive a hybrid temperature profile. Mutual information is used in an optimal way to achieve the highest possible accuracy of the retrieved profile.

18.1 Passive Microwave

A passive microwave instrument allows the derivation of the temperature profile between about 20 km and 90 km from oxygen lines. The detection of temperatures at the upper altitude border requires a strong line, because the signal-to-noise ratio is decreasing with altitude. The lower border is given by the saturation of the received signal in the detected band and could be expanded by the observation of weak oxygen lines.

The initial instrument characteristics were derived from the passive microwave instrument Millimeter-Wave Atmospheric Sounder (MAS), which was flown on the Space Shuttle in the years 1992, 1993, 1994. The instrument observed three oxygen lines around 60 GHz, two of them with a low resolution to correct the inaccurate tangent altitude position determination of the shuttle. The line at 61.15057 GHz was observed with high resolution and consequently the main focus here has been on this line.

A thorough investigation on the possible temperature retrieval accuracy from this line was first performed. The accuracy is affected by the Earth’s magnetic field parameters, the actual temperature profile of the Earth, and the a priori information. Generally, temperature retrieval is possible with an error below 5 K for the mesosphere, and below 3 K for the upper stratosphere. The lower stratosphere and troposphere is only poorly sampled, owing to the saturation of the received signal in the detected band.

The developed retrieval algorithm has been used to retrieve temperature profiles from measurements of the MAS. The first performed retrievals showed problems near the tropopause, where too low temperatures were retrieved. This problem was overcome by the introduction of two filters, that remove most of the signal emerging at low altitudes. MAS temperature retrieval was therefore restricted to altitudes above 30 km.

The retrieval results of a MAS track obtained 1992 over Saudi Arabia and Iran, was taken for a validation with other satellite data. Three instruments on-board the UARS satellite were chosen: MLS, CI AES, and ISAMS. The stratospheric temperature results of the UARS instruments agree in general with the MAS results, all instruments were detecting lower temperatures, compared to model results. The upper mesospheric temperatures are very variable, caused by temperature inversion layers. Only the ISAMS instrument was detecting temperatures in the upper mesosphere, both, MAS and ISAMS detected lower temperatures than model data.

Possible improvements of a MAS-like instrument with respect to the line selection, antenna pattern, the system noise temperature, the filter-channel width, and the band width have been investigated. A reasonable, modern instrument was assumed, with an orbit at 820 km altitude.
All lines between 0 GHz and 3000 GHz were investigated for the best line selection. The detection of mesospheric temperatures requires a strong line, whereas the oxygen line at 61.15057 GHz proves to be well suited, since it is the strongest line in this frequency region. Weaker lines show better accuracies in the troposphere, because the received signal saturates at lower altitudes.

Improvements in the retrieval accuracy are possible by employing a antenna pattern with a finer FWHM, but only a substantial decrease shows an increase in accuracy of about 1 K. Technically easier to achieve and thus more promising is a decrease in the system noise temperature, resulting in a direct accuracy gain at all altitudes.

Retrieval accuracy at sub-Kelvin level is provided by a band width of 10 GHz, centered at 60 GHz. This band includes all strong lines within 60 GHz and the temperature retrieval accuracy is below 1 K between 15 km and 40 km. The band was sampled with different filter channel widths to assess the impact. A channel width of 6 MHz is sufficient for stratospheric temperature retrieval, but mesospheric temperature retrieval is only possible with high resolution filter-channels. The MAS high resolution channels of 0.2 MHz have proven to be sufficient, only a substantial reduction in the width would result in an increase of the retrieval accuracy at mesospheric altitudes.

The optimal choice for a MAS-like instrument is a double sideband receiver, that observes a strong line in one sideband, while a weak one should be present in the other. The strong line provides information about the mesospheric temperature, while both lines give information about the stratospheric temperatures. The weak line will additionally allow tropospheric retrieval. The actual width of the band should be 600 MHz, the original MAS band width was 400 MHz.

18.2 Radio Occultation

A radio occultation instrument is currently being developed at the European Space Agency. The characteristics of this instrument were used in an analysis of the possibilities of radio occultation.

Focusing on temperature retrieval, a radio occultation instrument allows the derivation of the temperature profile up to altitudes of 45 km, above the signal-to-noise ratio is too low. The accuracy is almost independent of the actual temperature profile, sub-Kelvin accuracies are possible between 0 km and 30 km, above a nearly linear increase of the error up to altitudes of 60 km, where no information is provided, can be observed.

Radio occultation signals possess an ambiguity at low altitudes, where two sources contributing to the signal can be distinguished. One is the actual density, mainly given by nitrogen and oxygen, the other one is given by the amount of water vapor present, owing to its large permanent dipole moment. Water vapor can be retrieved up to altitudes of 12.5 km for a moist atmosphere, and up to 10.5 km for a dry scenario, under the ideal condition that the temperature profile is perfectly known.

More realistic though is the simultaneous retrieval of water vapor and temperature. This limits the retrieval of water vapor to altitudes of up to 7 km for a moist, and up to 5 km for a dry scenario. The accuracy of the temperature profile retrieval is affected at altitudes where a significant amount of water vapor is present. Almost no information is available near the surface. A varying error up to 2 K is found for altitudes below 12 km, above the error in temperature is unaffected by water vapor.

Water vapor is highly variable in the troposphere, while the tropospheric temperature profile can be calculated quite accurately, using numerical weather prediction models. The exploitation of radio occultation data in the troposphere could therefore concentrate on the retrieval of water vapor, while a temperature profile based on model calculations will be incorporated in the retrieval process. Calculations with varying a priori error on the temperature profile revealed that model data accurate within 2 K are needed to increase the detectable upper altitude of water vapor from 7 km to 8 km, knowledge with an error of 1 K expands the range up to about 9 km for a moist atmosphere. Thus, very accurate temperature knowledge is
required in order to increase the range where water vapor can be detected. Tight constraints on the temperature profile in order to retrieve water vapor are therefore not very efficient. The retrieval should best be performed with respect to both, temperature and water vapor. This is sometimes also referred to as 1DVAR (one-dimensional variational assimilation) approach.

Ignorance of water vapor and retrieving temperature only is possible by neglecting all altitude levels where significant amounts of water vapor are present. Neglecting altitudes below 5 km in a moist scenario will still lead to a cold bias in the detected temperatures at the 5 km level of about 10 K.

18.3 Passive Microwave and Radio Occultation

A combination of data from a passive microwave instrument and a radio occultation one was performed by using optimal estimation. The two instrument types are highly synergistic, since the radio occultation instrument has its main potential in the troposphere and lower stratosphere, while the passive microwave instrument is sensitive to temperature throughout the stratosphere and mesosphere.

It was assumed that both instruments are mounted on the International Space Station at about 400 km altitude with an inclination of 53°. Compared to the MAS, a different antenna was employed, the integration time was increased, and three different system noise temperatures were calculated.

The accuracy of the passive microwave instrument depends on the magnetic field, which is determined by the geographic location. A statistical approach was therefore taken to assess the averaged accuracy of the temperature retrieval. The radio occultation instrument is almost independent of the location, only minor variations caused by the different temperature profiles entering the retrieval are introduced. The actual position of the events were determined by the radio occultation instrument. More than 160 events were found for a single day, out of which 30 events covering the Earth were chosen. The passive microwave observation were assumed to be taken at the same locations.

Under ‘dry’ atmospheric conditions, the determination of a hybrid temperature profile, spanning an altitude interval from 0 km to 90 km, is possible with this instrument constellation. An accuracy better than 4 K in the mesosphere is achieved and below 1 K up to about 35 km. The presence of water vapor will affect the accuracy in the same way as described for the radio occultation instrument, since no tropospheric water vapor information is provided by the passive microwave instrument.
Acknowledgments

I want to express my gratitude to my supervisors: Prof. K. Künnzi, who encouraged me to take on this project and ensured its realization by giving me the opportunity to do research at various locations in Europe, Prof. G. Kirchengast, who made me feel at home in his group in Graz/Austria right from the beginning and whose help concerning the radio occultation method has been invaluable, and Dr. Jörg Langen (ESTEC/Netherlands), for discussions that have been a special source of inspiration. This work would not exist without their continued support and encouragement.

Within the Microwave Limb Sounding group at the University of Bremen, I would like to acknowledge my colleague and friend Dr. Stefan Bühler, who helped me during the course of research, giving invaluable suggestions and thorough and detailed criticism of the manuscript.

To Dr. Olav Wehahn for spending his precious time with proof reading of this work.

I would like to thank the following ex-members of the Microwave Limb Sounding group: Drs. Björn-Martin Sinnhuber, Joachim Urban, and Tobias Wehr.

Members of the Institute for Geophysics, Astrophysics, and Meteorology at the University of Graz I am indebted to include: Dr. Ulrich Feelsche, Heinrich Grillhofer, Dr. Jeffrey Lerner, Werner Pötzi, Dr. Josef Ramsauer, and Dr. Andrea Steiner.

I wish to thank the European Space Agency for the opportunity to get an inside view of the ESTEC establishment in the Netherlands where I worked 18 months in the Earth Sciences Division under the Young Graduate Traineeship (especially to the people in the Earth Sciences Division).

Furthermore, I thank the PI of the MAS experiment Dr. G. Hartmann, MPI für Aeronomie, Lindau/ Harz, for his efforts put into MAS and for partial funding during the MASGRAS investigations.

Persons I would like to thank for Lidar data supply are:

John Bird, Center for Research in Earth and Space Technology, Canada
Fernando Congeduti, Instituto di Fisica dell’ Atmosfera, Italy
Alain Hauchecorne, Observatoire de Haute-Provence, France
Thierry Leblanc, Jet Propulsion Laboratory, USA

Satellite data of the UARS instruments are freely available on the Internet, which is of great help for data comparison.

Software to read MLS, CLAES, ISAMS and HALOE data was also freely available on the Internet. The software package was developed by Hugh C. Pumphrey, Department of Meteorology at the University of Edinburgh.

Finally, I wish to thank everyone who invited me to speak about my work in progress, which allowed me to refine my ideas.
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