An Advanced Sky Background Model for
the European Southern Observatory

Dissertation

by

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I would like to dedicate my thesis to all my friends and family that have supported me on this adventure.
Preface

My thesis work was funded by the Austrian Ministry of Science as part of the University of Innsbruck In-kind group for the Austrian contribution to the European Southern Observatory (ESO). We were tasked to develop software packages for ESO to improve their Exposure Time Calculator and data reduction. The development of the software has been completed and most of them have already been implemented by ESO. This has resulted in several group publications describing the different types of software that were designed. The main software has been the sky background model. My work focused on improving the scattered moonlight portion of the sky background model. With our comprehensive sky background model, there are many applications in data reduction tools and atmospheric science. Here, my work has been on testing the use of the scattered moonlight model to attain aerosol properties from astronomical observations.
Abstract

In the current era of precision astronomy, a complete sky background model is crucial, especially as the telescopes become even larger in the next decade. Such a model is needed for planning observations as well as understanding and correcting the data for the sky background. We have developed a sky model for this purpose, and it is the most complete and universal sky background model that we know of to date (Article A). It covers a wide range of wavelengths from 0.3 to 30 microns up to a resolution of 1,000,000 and is instrument independent. Currently it is optimized for the telescopes at Cerro Paranal and the future site Cerro Armazones in Chile. Its original purpose was to improve the ESO (European Southern Observatory) ETC (Exposure Time Calculator) used for predicting exposure times of observations with a given signal to noise ratio for a set of conditions, as part of the Austrian contribution to ESO. Improving the ETC allows for better scheduling and telescope efficiency, and our new sky model has already been implemented by ESO.

The brightest natural source of optical light at night is the Moon, and it is a major contributor to the astronomical sky background. We have an improved scattered moonlight model (Article B and G), where all of the components are computed with physical processes or observational data with less empirical parametrizations. This model is spectroscopic from 0.3 to 2.5 microns and was studied and verified with observations. To our knowledge, this is the first spectroscopic model extending into the near-infrared.

There are several applications of the sky background model. We have developed two tools for data reduction, skycorr (Article C) and molecfit (Article E and F). Additionally, the sky background model can be used in atmospheric science. Since the model is more physical, we can use the scattered moonlight to determine the distribution of aerosols (Article D). We can also investigate airglow.
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Chapter 1

Introduction

1.1 History

For thousands of years people have admired and wondered about the various sources of light in the night sky. They have pondered the meaning and origin of these lit objects. The Milky Way Galaxy, seen in dark skies, appears as a dimly lit band across the sky (see Fig 1.1). It was given its name from the ancient Greeks. They thought it looked like split milk. They believed that Zeus was secretly letting baby Hercules breast feed on Hera. She awoke in the night, surprised to find Hercules there, and threw him, squirting milk into the sky. The Egyptians also thought it looked like milk but from a divine cow.

![Milky Way Galaxy](http://antwrp.gsfc.nasa.gov/apod/ap070508.html)

Figure 1.1: Panoramic image of the Milky Way galaxy as seen from Death Valley National Park (image credit: Dan Duriscoe, for the U.S. National Park Service, http://antwrp.gsfc.nasa.gov/apod/ap070508.html).

The concept of the Zodiac is also quite old, from the Babylonian era. They first divided the ecliptic into various zodiacal regions. Many past cultures noticed that the planets and the Moon tend to follow the same path across the sky, in what is now known as the ecliptic plane, or the plane of our solar system. This region of the sky is the Zodiac and is known today for the Zodiac constellations, popular in astrology. There is also some reflected light that can be seen along the ecliptic in dark skies.
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skies, called zodiacal light (see Fig 1.2).

Figure 1.2: Image of the night sky before twilight at Nemrut Heritage site. In the middle is the Milky Way galaxy and on the left side is the reflected light off of the ecliptic plane called zodiacal light (image credit: "Zodiacal Light and Nemrut Heritage" by Tunc Tezel, www.twanight.org).

The brightest celestial object in the night sky is the Moon, and it has also inspired many myths over the ages. In Greek mythology, the goddess Selene is the personification of the Moon, and in Roman mythology she is Luna. Galileo Galilei was the first person to observe the Moon with a telescope. He discovered that the Moon did not seem perfect and smooth as it was assumed to be. Previously people thought that the Moon should be perfect, round, and smooth since it was a celestial body and part of the heavens. The terminator, the line between day and night on the Moon, seemed ragged as it passed over the lighter parts of Moon compared to the darker regions, known as Maria. Fig 1.3 shows a sketch of different moon phases made by Galileo. This was one of many observations from Galileo that started shifting our view of the Universe. During Galileo’s time, people believed that the Earth was in the center of the Universe and the sky contained the heavens orbiting around us. The lunar observations amongst others contradicted this notion. In modern times, we know that Sun is instead the center of our solar system and that the Moon does indeed have a rough surface.

These various sources of light that have been long observed, such as the Milky Way, stars, Zodiac, and the Moon, are all part of the sky background flux which we have modeled.
Figure 1.3: Sketch of different moon phases from Sidereus Nuncius (1610) by Galileo Galilei.

1.2 Motivation

When an astronomer wants to observe an object in the sky, they must decide with what instrument and for how long. The choice of instrument relies on the science they wish to achieve from the
observation and what is available. The exposure time depends on the desired signal to noise ratio (S/N). The S/N describes the quality of the signal with respect to the background noise or contamination that is also present in your image. The European Southern Observatory (ESO) has a tool which calculates how long one should observe an object under certain conditions for a given S/N. This tool is called the Exposure Time Calculator (ETC).

Figure 1.4: Two images of M42 where the only difference is the exposure time. The image on the left was taken with 5 minutes and on the right with 10 seconds. The image on the left has many more details visible, including the surrounding nebula gas (image credit: Rogelio Bernal Andreo, www.deepskycolors.com).

The signal to noise ratio (S/N) can be calculated depending on the flux from the signal divided by the square root of the flux from the signal and noise. Therefore the longer the exposure time, in general, the higher the S/N. The higher the S/N the better the signal is compared to the noise, and, therefore, better statistics can be performed. According to ESO, a S/N of two to three means that the object is barely detected. With a S/N of five the object is detected and at ten science and measurements can be conducted. A S/N of 100 is considered an excellent measurement by ESO. An example of an image of M42 (Orion Nebula) taken with two different exposure times is shown in Fig 1.4. The longer 5 minute exposure clearly has a higher S/N. More details can be seen in this image compared to the shorter 10 second exposure.

"ESO is the pre-eminent intergovernmental science and technology organisation in astronomy. It carries out an ambitious programme focused on the design, construction and operation of powerful ground-based observing facilities for astronomy to enable important scientific discoveries. ESO also plays a leading role in promoting and organising cooperation in astronomical research (www.eso.org)." In short, ESO is the group that manages many observing facilities.

The Austrian contribution to ESO from the University of Innsbruck (UIBK) is known as the UIBK in-kind group. Its members are Stefan Kimeswenger (head), Stefan Noll, Wolfgang Kausch, Marco Barden (former), Ceszary Szyszka (former), and myself, Amy Jones. We were tasked to help improve the ETC by developing a comprehensive sky background model. By better understanding the background noise, the ETC can more accurately estimate the exposure times. This improvement in turn makes the telescope scheduling more efficient. Telescope time is expensive and precious at the larger observing facilities. According to Buton et al. (2013), "For many studies accurate
flux calibration is critical for deriving the maximum amount of information from observations with these telescopes, and correction for the optical atmospheric and instrumental transmissions is one fo the main limitations of astronomical flux measurements from the ground.

Two of the major observing sites of ESO are the Very Large Telescope (VLT, Fig 1.5) at Cerro Paranal and the future European Extremely Large Telescope (E-ELT, Fig 1.6) at Cerro Amazones. Both of these are located in the Atacama desert in Chile. For these sites, the sky background model must be instrument independent and valid from 0.3 to 30 \( \mu \text{m} \).

Figure 1.5: Image of the VLT at Cerro Paranal, with the four 8 m class telescopes (image credit: ESO).
1.3 Previous Work

For all major observatories, some form of a sky background model has been developed. The sky and observing conditions need to be characterized at the site. These conditions for determining the quality of an observing site depend on many things, including typical humidity, wind speed, location, and maintenance. The sky background is also an important condition. For example, many observatories are located at high altitudes to have less atmospheric turbulence.

Other observatories have characterized the sky extinction and flux for their observing sites. The standard extinction curve for the observatories at Mauna Kea are mostly from Krisciunas et al. (1987); Boulade (1987); Bélard et al. (1988). These studies where of photometric night sky brightness and do not include measurements of the entire optical spectrum. In light of the new
astronomical surveys that will be conducted at Mauna Kea, like the Nearby SuperNova Factory, a recent survey of the optical extinction was performed by Buton et al. (2013).

Two other major observatories in the Atacama desert in Chile, Cerro Tololo and La Silla, also had the atmospheric extinction properties studied. Cerro Tololo became an observatory site in 1962 and the more recent studies of the extinction were done by Gutierrez-Moreno et al. (1982); Stone & Baldwin (1983); Gutierrez-Moreno et al. (1986); Stritzinger et al. (2005), and for La Silla by Tüg (1977); Sterken & Jerzykiewicz (1977); Rufener (1986); Sterken & Manfroid (1992); Grothues & Gochermann (1992); Burki et al. (1995).

For Cerro Paranal, the location of the ESO VLT, there have also been several studies. The first photometric sky brightness survey for this site was done by Patat (2003, 2008), where they monitored the sky for six years. They found that there is a seasonal effect and dependence on the solar activity. They also had roughly 1000 optical spectra to compare with. Photometrically, the sky brightness was described and monitored. However, the extinction curve for Cerro Paranal came from the neighboring observatories, Cerro Tololo and La Silla and were measured over 15 years ago. For this purpose, Patat et al. (2011) began the PARanal Spectral Extinction Curve project (PARSEc). PARSEC included 600 optical spectra taken between October 2008 to March 2009. With these observations coupled with a radiative transfer code, they were able to determine the different components of the atmospheric extinction as well as the average extinction curve for this period. For our optical sky background model we used about 1000 optical FORS1 spectra from Patat (2008) and the aerosol extinction curve from Patat et al. (2011).

From the previous studies of the sky brightness at Cerro Paranal mentioned above, it was shown that the sky brightness is highly variable on various timescales. A need for a good sky background model to predict and estimate the sky brightness for any given observation was needed, especially with the E-ELT being built. This is where the Austrian contribution comes in and the UIBK in-kind was tasked with developing such a model.

1.4 Sky Background Model

The sky background model can predict how much sky background flux and extinction will be observed for a given target and exposure time. The original purpose was for the ESO ETC to help astronomers estimate how long they should observe a target for a desired S/N ratio. The ETC application must, therefore, be computational quick and adaptable. The sky background model has evolved past this original application and there is a more sophisticated version for non-ETC applications. It can also be modified for other locations. Nevertheless, the sky background model was designed to be quick, and was split into two modules. Module 1 contains all of the computational expensive parts and is only needed to be run once (Fig 1.7). Module 2, on the other hand, is run every time and is computationally quick (Fig 1.8).

Fig 1.7 shows the different components of Module 1. The output is a library of synthetic spectra. As input, it needs an atmospheric profile and the HIgh-resolution TRANsmission molecular absorption
database (HITRAN, Rothman et al. 2009). The atmospheric profile is a merged profile from three different sources: Global Data Assimilation System\(^1\) (GDAS), ESO Meteo Monitor (ESO-MM), and a standard profile (Seifahrt et al. 2010). It provides the pressure, temperature, and chemical composition up to 120 km high for a given time at the location of Cerro Paranal (Noll et al. 2012, and references therein). The HITRAN database contains the spectroscopic parameters of many molecules for calculating the transmission and emission of light in the atmosphere. This is then used as input for a line file creation program (LNFL) and the line-by-line radiative transfer code (LBLRTM, Clough et al. 2005). This is done for a range of precipitable water vapor (PWV), seasons, and time of the night to create a library of synthetic spectra. In addition a library of airglow transmission line profiles is also produced in Module 1.

Module 2 is run every time and the ETC version takes a few tenths of a second. It requires the libraries created in Module 1 as input. Module 2 interpolates between the synthetic spectra that are closest to the given observing conditions. The absorption spectrum then is modified by the transmission curve of the atmosphere to produce the sky transmission curve. The emission spectrum is adjusted for the various sources of sky background flux. This includes scattered moonlight,

\(^1\)http://ready.arl.noaa.gov/gdas1.php
scattered and direct zodiacal light, scattered starlight, thermal emission from the telescope, and airglow emission and continuum. These components depend on the location of the sources and target observation, and the time of the observation. An example of the output sky transmission spectrum is shown in Fig 1.9 and of an emission spectrum in Fig 1.10.

There are several components of the sky background model and they theoretical comprise all of the possible sources of background light and extinction at Cerro Paranal. These sources range from extraterrestrial, astronomical objects to chemicals and particles in the Earth’s atmosphere. I will make a general introduction of the most distant to the closest sources here and more detailed introductions are given in the following chapters (Articles A-G). An extensive review of sky background light is given in Leinert et al. (1998).

The Milky Way galaxy, as can been seen in the night sky in clear dark places, is a source of sky background flux. Along the plane of the Milky Way there is an enhancement of dust and starlight. The light from the stars can be scattered off of the dust causing the Milky Way to appear bright compared to the rest of the sky. Fig 1.1 shows the Milky Way galaxy as it would appear in dark skies. This component is spatially and wavelength dependent. If the target object is in the plane of the Milky Way there will be more sky background flux compared to an object that is not near the plane of our galaxy. The light from the Milky Way is not being emitted as a single point source, but rather a collection of many point sources. Therefore it is considered an extended source.
Background starlight is another source of sky background flux. It is also considered an extended source because it is the light coming from all the stars in the sky, and hence is normally called integrated starlight. There is an increase in the amount of stars along the Milky Way. Because the integrated starlight directly correlates with the Milky Way galaxy, these two components are modeled together. Compared with the other sources of background flux, the starlight contributes only a small fraction (unless the observation is in the direction of the Milky Way).

From our solar system, there is also some background light. The plane of our solar system has an increased amount of dust compared to its surroundings. This dust reflects the light from the Sun and is called zodiacal light. In Fig 1.2 on the left side of the photograph one can see the zodiacal light. This light is also an extended source that is spatial dependent with respect to the plane of our solar system. The wavelength dependence can be characterized roughly as a reddened solar spectrum, from the scattering of sunlight off of the dust grains. The zodiacal light is further split into two parts in the model, direct and scattered. These distinctions refer to zodiacal light that passes directly through the atmosphere and that which is scattered in the Earth’s atmosphere.

Within our solar system, our closest, orbiting neighbor, the Moon, is another source of sky background flux. When the Moon is above the horizon it is the brightest source of light in the optical wavelengths. Accurately predicting and estimating the amount of light from the Moon...
was, therefore, an important focus for the sky background model. It was the core of my research. The amount of moonlight depends on several factors. The most intuitive factor is the lunar phase. There is more light reflected by the Moon to the Earth during a full Moon compared to a crescent. In addition, it depends on if the Moon is waxing or waning because there are more Maria on one side of the Moon compared to the other. Near full Moon, the Moon actually appears even brighter due to an effect called gegenschein. This effect is still not fully understood and could be due to an alignment of the dust grains on the surface of Moon causing an increased back scatter. An enhancement of around 35% in the visible at full Moon is observed. The amount of moonlight also depends on the distance between the Earth and the Moon. Finally the moonlight is scattered in the Earth’s atmosphere before reaching the telescope. This depends on the positions of the Moon and target observation (Jones et al. 2013).

The atmosphere plays a crucial role in the sky background model. In the upper atmosphere, chemical reactions emit light known as airglow. Fig 1.11 shows the airglow from space and Fig 1.12 from the VLT. This airglow consists of both emission lines, commonly called sky lines, and a pseudo-continuum. Both pieces are highly variable and can depend on the solar flux, time of night, season, etc (see Noll et al. 2012, and references therein). By looking at 1000s of observations, we have tried to parametrize and better understand this part of the sky background model. Generally, the airglow emission lines were divided into groups, where each group should vary in the same way.
Then with the observations, we investigated how these groups varied depending on e.g. solar flux, time of the year, and time of the night. From this investigation, we can predict the amount of airglow in each group from the given observing conditions.

The atmosphere also scatters and absorbs the light. The scattering can be off of molecules or aerosol particles. Scattering off of molecules can be described by Rayleigh scattering and mostly depends on the height of the observatory and the atmospheric pressure. The aerosol scattering is more complicated. We made the approximation that the aerosol particles are spherical symmetric and used Mie theory to describe the scattering properties. We used both an empirical fit for the aerosol scattering by Patat et al. (2011) and the distributions for remote continental aerosol provided by Warneck & Williams (2012). For the scattering we used a fully 3D single and double scattering code. This considers light that is scattered out of and into the path to the telescope and off of molecules, particles, and the ground. This component depends on the atmospheric composition and the direction of the observation.

The final and closest component is the light coming for the telescope itself. All bodies radiate, and this includes the telescope. It is known as thermal telescope emission and is parametrized as a gray body depending on the temperature of the telescope.

These various sources of sky background flux and extinction have been modeled with the latest experiments and knowledge to achieve the most comprehensive sky background model possible. The sky background model is the topic of Article A. In the optical the Moon is the brightest contaminate when it is above the horizon and therefore was one of the main focuses of my thesis. Therefore it will be further introduced in its own section.

1.4.1 Scattered Moonlight Model

When the Moon is the above the horizon, it is the brightest optical source in the sky background, as can be seen in Fig 1.13 of a moonrise. In Fig 1.10, the emission spectrum from a first quarter Moon is shown and its light dominates the sky background flux in the optical regime. It is therefore important to develop an advanced scattered moonlight model that depends on several factors and is as accurate as reasonably possible.

Previously, there were mainly two scattered moonlight models used by the astronomical community. First one was done by Walker (1987). This consisted of measurements in five different photometric bands of the sky brightness from scattered moonlight at five different lunar phases. It did not take into account the location of the Moon or target observation. These measurements are what was used for the ESO ETC before our sky background model was implemented. For the next generation telescopes, there was a definite need for an improved model of scattered moonlight.

The other widely used scattered moonlight model was by Krisciunas & Schaefer (1991). This model was also only photometric, just in the Johnson V band. It was based on measurements taken at Mauna Kea. A simple parametrization was done for various factors that influence the amount of
scattered moonlight, including lunar phase, positions of the Moon and target observations, and the atmospheric extinction. However, a model providing the full optical spectrum was still lacking.

For the first version of the scattered moonlight model for the sky background model is presented in Noll et al. (2012). We made an extension of the model from Krisciunas & Schaefer (1991). We extended the model with respect to wavelength using the solar spectrum as input (Colina et al. 1996), and optimized the model for Cerro Paranal based on the optical spectra from Patat (2008). This model was purely an empirical parametrization with several scaling factors. Since the Moon is a crucial component in the optical, we decided to design a model which was based more on data and physics. This could also then be extended easily into the near-Infrared (NIR), where there is still some scattered moonlight present.

Our approach for designing a more advanced scattered moonlight model was based on tracing the light from the source to the detector at the telescope. The source of light comes from the Sun, and we used the solar spectrum from Colina et al. (1996). Then the light is reflected off of the lunar surface and towards the Earth. The amount of light reflected depends on the lunar albedo. Kieffer & Stone (2005) presented an empirical fit for the lunar albedo based on over 100 000 images of the Moon. The fit was done for 32 narrow band filters. We did a linear interpolation over wavelength to have a spectrum of the lunar light. This fit depends on the lunar phase, including waxing and waning, libration, and the distance between the Moon and Earth. Finally, the light must pass through the Earth’s atmosphere. Here the light can be both scattered and absorbed. The scattering can occur off of molecules or particles in the atmosphere. We have developed a 3D single and double scattering code, which takes into account light being both scattered into and out of the line of sight, as well as being scattered off of the ground. For light that is scattered more than twice, we use an approximation by comparing the amount of light that is scattered twice to once. Additionally light is absorbed by molecules, like ozone, O$_2$, and water vapor. The scattering and absorption depends on the location of the Moon and the target observation and the atmospheric conditions. For astronomical observations, objects are normally only observed during clear sky conditions, so the types of possible atmospheric conditions are limited. For more details about the scattered moonlight model in the optical, see Article B.

There is also some scattered moonlight present in the NIR. It is a small component and usually astronomers ignore the moonlight at these wavelengths. Nevertheless, we wanted to extend the scattered moonlight to 2.1 µm. Most of the scattered moonlight model naturally extended into the NIR. The lunar albedo fit was done to 2.45 µm, solar spectrum to 2.5 µm, and Raleigh scattering (approximation for scattering off of molecules) is still valid at longer wavelengths. The only issue is with the scattering off of particles, known as aerosol scattering. In the optical there was an empirical fit done by Patat et al. (2011), but it is only valid from 0.4 to $\sim$ 0.9 µm. We have aerosol size distributions for remote continental areas from Warneck & Williams (2012). With these distributions we can calculate theoretical Mie scattering functions (Bohren & Huffman 1983; Grainger et al. 2004). The Mie approximation assumes that the aerosol particles are spherical symmetric. Then we vary the amount of aerosols to create a set of scattered moonlight models. We compare these models with some observations to find which model with a given amount of aerosols fits the best. We have dedicated X-Shooter observations for this purpose. X-Shooter is eschelle spectrograph mounted at the VLT and simultaneously observes from 0.3 to 2.1 µm, with
the K blocking filter (Vernet et al. 2011). The dedicated observations were of the plain sky at six different angular distances from the Moon at three lunar phases. This allows us to verify the scattered moonlight model in the NIR and determine the best prescription for the aerosols. With the three lunar phases we can test the lunar albedo fit. The Mie scattering tends to be strongly forward scattered and the amount of forward scattering is sensitive to the aerosol size distribution. By observing at six different angular distances we are probing the Mie scattering function. For more details on the scattered moonlight model from 0.3 to 2.1 μm, see Article G.
Figure 1.11: View of the atmospheric layers from orbit. The green layer is from airglow (image credit: NASA).
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Figure 1.12: Photo at the VLT. Above the VLT is the Milky Way, and green and red parts of the sky are the airglow (image credit: Y. Beletsky (LCO)/ESO).

Figure 1.13: Photo of moonlight. The Moon illuminates most of the night sky (image credit: Hearts and Minds).
1.5 Applications of the Sky Background Model

There are many possible applications for our comprehensive sky background model. Currently we have explored some of these applications. Two are tools for data reduction called molecfit and skycorr. Another two applications are in atmospheric science: to apply the scattered moonlight model to moonlit observations to determine the amount of aerosols present at the time of observation and to better understand and parametrize airglow.

1.5.1 Molecfit

Molecfit is a data reduction tool that helps correct the absorption features from the atmosphere in spectra, known as telluric features. Normally, a star with a known spectrum, called a telluric standard star, is observed near the target object soon before or after the target observation. Then by comparing the observations of the telluric standard star with its known un-extincted spectrum, one can determine the atmospheric absorption around the time of the science observation. This requires some telescope time to be devoted to observing these telluric standard stars and telescope time is precious in astronomy. Also some features of the atmosphere can vary on short timescales. Thus this process depends on the time difference between the star and science observations. Molecfit corrects the telluric features with a different approach. It uses synthetic spectra, like the ones in Module 1 of the sky background model (Fig 1.7). With a complicated procedure, it scales the various molecules to fit the observed telluric features seen in the science spectrum. The user can choose which molecules it wants to be included and which of those to be fitted to the observed features. It works from 0.3 to 30 \( \mu \text{m} \), and the user can specify which regions to fitted or excluded. Like in Module 1 of the sky background model, molecfit requires the atmospheric profile, HITRAN, andLBLRTM to produce the synthetic spectra. Molecfit was tested on several different instruments, which is shown in Article E along with an introduction of molecfit. It was tested and verified extensively with X-Shooter data, which is discussed in Article F.

1.5.2 Skycorr

Skycorr is another data reduction tool, but in this case it corrects the sky emission lines in observed spectra. Sky lines, or airglow emission lines, are highly variable on short timescales, can vary spatial, and are not yet fully understood. They are mostly emitted from a single atmospheric layer (Fig 1.11). Therefore, an observation of the plain sky along with the science observation is needed to fully correct these emission lines. However, in some cases the object is extended, and no plain sky is seen in the slit of the observation. Skycorr can use any plain sky observation, preferably near the time of the science observation, and scales the sky emission lines from the sky observation to fit the ones seen in the science observation. The airglow lines can be divided into groups that tend to vary in the same way. After carefully removing the continuum, skycorr uses the intensities from the lines within a given group to determine the amount of scaling needed to fit the airglow in the science observation. The analysis and verification of skycorr is given in Article C.
1.5.3 Atmospheric Aerosols

The other applications we have so far explored are related to atmospheric science. Since the scattered moonlight model has physical inputs regarding the aerosol composition, we can then use this in reverse. By using the scattered moonlight model and an observation with scattered moonlight, one can determine the amount of aerosols present at the time of observation. We have a set of possible scattered moonlight models with varying aerosol compositions and compare them with the observation. The aerosol composition depends on a few parameters. There are four main types of aerosols: tropospheric nucleation, accumulation, and coarse, and stratospheric. For each type we assume a log-normal distribution which is described by three parameters: number density, average radius, and the spread of the distribution. Presently we have only varied the number density of each type. In the near future, after private communication with several atmospheric scientists, we plan to fix some of the aerosol types’ distributions and vary the number density and average radius of the other types. Currently, our initial values for the size distributions for remote continental aerosols are provided by Warneck & Williams (2012). In Fig 1.14, we show the distributions of the various aerosols. Also shown in the dotted lines are distributions that were explored for adding to the mix of aerosols. After comparing the scattered moonlight model with some observations, the ones taken near the Moon had more flux than what was reproduced by the model. An explanation for this is that there may be another type of aerosol present. A particle with a 1 \( \mu \text{m} \) radius, would provide the greatest enhancement near the Moon. For this purpose the added aerosol modes (currently with an average radius of 1 \( \mu \text{m} \)) were added and tested. However, this work is still ongoing. The scattered moonlight model is sensitive to changes in amount of aerosols. By finding which model fits the observations best, the amount of aerosols can be determined. We plan to apply this technique to the archival X-Shooter data to detect trends in the aerosol composition over Cerro Paranal. This will be a unique data set in atmospheric science because this includes nocturnal, background aerosols. Most atmospheric science measurements use the Sun as the light source and are done in areas containing lots of urban aerosols. For more details, see Article D.

1.5.4 Atmospheric Airglow

The other atmospheric science project currently happening with our group is using X-Shooter data to study airglow. Since X-Shooter observes simultaneously from 0.3 to 2.5 \( \mu \text{m} \), it allows for multiple airglow features to be studied at once. Most of the instruments dedicated to study airglow only observe in a narrow wavelength range and/or do not have as high of resolution as X-Shooter. Thus, the ESO X-Shooter archive is a treasure for doing airglow research. This is in a sense an extension of the airglow research that was done previously for the sky background model. It will continue to investigate how the airglow varies and compare the different airglow features and emission lines. Some airglow features should theoretically be correlated because they come from the same initial source, such as iron oxide and sodium both originate from meteors (Unterguggenberger et al. 2014). This can now be tested independently from previous studies. Also with this data set, one can explore and compare different methods with the OH vibrational levels for determining the Mesopause temperature (Noll et al. 2014).
Figure 1.14: Aerosol size distributions for the various types of aerosols used in the scattered moonlight model. The solid lines are aerosol size distribution provided by Warneck & Williams (2012) and an added extra coarse mode. The dotted lines are other coarse mode type aerosols that were explored in the analysis to explain the enhanced flux seen at angles close to the Moon.
Acronyms

**E-ELT**: European Extremely Large Telescope

**ESO**: European Space Observatory

**ESO-MM**: ESO Meteo Monitor

**ETC**: Exposure Time Calculator

**FORS1**: FOcal Reducer and low dispersion Spectrograph

**GDAS**: Global Data Assimilation System

**HITRAN**: HIgh TRANsmission molecular absorption database

**LBLRTM**: Line-By-Line Radiative Transfer Model

**LNFL**: Line file creation program

**NIR**: Near-Infrared

**NOAA**: National Oceanic and Atmospheric Administration

**PARSEC**: PARanal Spectral Extinction Curve project

**PWV**: Precipitable Water Vapor

**S/N**: Signal to Noise ratio

**UIBK**: University of Innsbruck

**VLT**: Very Large Telescope
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Article A:
An atmospheric radiation model for Cerro Paranal.
I. The optical spectral range

An atmospheric radiation model for Cerro Paranal

I. The optical spectral range

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ABSTRACT

Aims. The Earth’s atmosphere affects ground-based astronomical observations. Scattering, absorption, and radiation processes deteriorate the signal-to-noise ratio of the data received. For scheduling astronomical observations it is, therefore, important to accurately estimate the wavelength-dependent effect of the Earth’s atmosphere on the observed flux.

Methods. In order to increase the accuracy of the exposure time calculator of the European Southern Observatory’s (ESO) Very Large Telescope (VLT) at Cerro Paranal, an atmospheric model was developed as part of the Austrian ESO In-Kind contribution. It includes all relevant components, such as scattered moonlight, scattered starlight, zodiacal light, atmospheric thermal radiation and absorption, and non-thermal airglow emission. This paper focuses on atmospheric scattering processes that mostly affect the blue (<0.55 μm) wavelength regime, and airglow emission lines and continuum that dominate the red (>0.55 μm) wavelength regime. While the former is mainly investigated by means of radiative transfer models, the intensity and variability of the latter is studied with a sample of 1186 VLT FORS1 spectra.

Results. For a set of parameters such as the object altitude angle, Moon-object angular distance, ecliptic latitude, bimonthly period, and solar radio flux, our model predicts atmospheric radiation and transmission at a requested resolution. A comparison of our model with the FORS1 spectra and photometric data for the night-sky brightness from the literature, suggest a model accuracy of about 20%. This is a significant improvement with respect to existing predictive atmospheric models for astronomical exposure time calculators.

Key words. atmospheric effects – site testing – radiative transfer – radiation mechanisms: general – scattering – techniques: spectroscopic

1. Introduction

Ground-based astronomical observations are affected by the Earth’s atmosphere. Light from astronomical objects is scattered and absorbed by air molecules and aerosols. This extinction effect can cause a significant loss of flux, depending on the wavelength and weather conditions. The signal of the targeted object is further deteriorated by background radiation, which is caused by light from other astronomical radiation sources scattered into the line of sight and emission originating from the atmosphere itself. Since these contributions can vary significantly with time, the achievable signal-to-noise ratio for an astronomical observation strongly depends on the state of the Earth’s atmosphere and the Sun-Earth-Moon system. Therefore, for efficient time management of any modern observatory, it is critical to provide a reliable model of the Earth’s atmosphere for estimating the exposure time required to achieve the goals of scientific programmes. Data calibration and reduction also benefit from a good knowledge of atmospheric effects (see e.g. Davies 2007).

For this reason, various investigations were performed to characterise the atmospheric conditions at telescope sites (see Leinert et al. 1998, for a comprehensive overview). Photometric measurements of the night-sky brightness and its variability were done at e.g. Mauna Kea (Krisciunas et al. 2007), La Palma (Mattila et al. 1996), and Cerro Paranal (Patat 2003, 2008). For Cerro Paranal, Patat (2008) also carried out a detailed spectroscopic analysis, and found that the night sky showed strong variations of more than one magnitude. Also, the sky brightness depends on the solar activity cycle (Walker 1988; Patat 2008). It is related to the variations of the upper atmosphere airglow line and continuum emission, which dominate the near-UV, optical, and near-IR sky emission under dark-sky conditions (Chamberlain 1961; Roach & Gordon 1973; Leinert et al. 1998; Khomich et al. 2008). When the Moon is above the horizon, scattered moonlight dominates the blue wavelengths (Krisciunas & Schaefer 1991). A much weaker, but always present, component is scattered starlight. The distribution of integrated starlight (Mattila 1980; Toller 1981; Toller et al. 1987; Leinert et al. 1998; Melchior et al. 2007) and how it is scattered in the Earth’s atmosphere has been studied (Wolstencroft & van Breda 1967; Staude 1975; Bernstein et al. 2002). A significant component at optical wavelengths is the so-called zodiacal light, solar radiation scattered by interplanetary dust grains mainly distributed in the ecliptic plane (Levasseur-Regourd & Dumont 1980; Mattila et al. 1996; Leinert et al. 1998). For a realistic description of the zodiacal light intensity distribution for ground-based observations, scattering calculations are also required (Wolstencroft & van Breda 1967; Staude 1975; Bernstein et al. 2002). Finally, the wavelength-dependent extinction of radiation from astronomical objects by Rayleigh scattering off of air molecules,
Mie scattering off of aerosols, and absorption by tropospheric
and stratospheric molecules was studied and characterised at
different telescope sites, such as La Silla (Tüg 1977, 1980;
Rufener 1986; Sterken & Manfroid 1992; Burki et al. 2005),
Cerro Tololo (Stone & Baldwin 1983; Baldwin & Stone 1984;
Gutiérrez-Moreno et al. 1982, 1986), and Cerro Paranal (Patat
et al. 2011).

Due to the complexity and variability of the night-sky radi-
ation, a good atmospheric radiation model is crucial for a re-
liable astronomical exposure time calculator (ETC). Currently,
the European Southern Observatory (ESO) uses a sky back-
ground model for its ETC (Ballester et al. 2000), which
includes the photometric night-sky brightness measurements of
Walker (1987) for the optical and Cuby et al. (2000) for the
near-IR. The $U$ to $I$ magnitudes of Walker vary as a function
of Moon phase. For optical spectrographs, a night-sky spectrum
is calculated by scaling an observed, instrument-dependent tem-
plate spectrum to the Walker filter fluxes. The spectroscopic
near-IR/mid-IR model is based on the line atlas of Hanuschik
(2003) and the OH airglow calculations of Rousselet et al.
(2000), thermal telescope emission, an instrument-related con-
stant continuum, and atmospheric thermal line and continuum
emission. The latter is provided as a set of template spectra
computed with the radiative transfer code Reference Forward
Model1 for different airmasses and water vapour column densi-
ties. Since the current ETC is limited in reproducing the variable
intensity of the night sky, we have developed an advanced model
for atmospheric radiation and transmission, which includes scat-
tered moonlight, scattered starlight, zodiacal light, thermal emis-
tion from the telescope, molecular emission and absorption in
the lower atmosphere, and airglow line and continuum emis-
sion, including their variability with time. This “sky model” has
been derived for Cerro Paranal in Chile (2635 m, 24° 38′ S, 70° 24′ W). It is also expected to work for the nearby Cerro
Armazones (3064 m, 24° 36′ S, 70° 12′ W), the future site of
the European Extremely Large Telescope (E-ELT), without ma-
jor adjustments. An example of a spectrum computed by our sky
model is given in Fig. 1. The crucial input parameters are listed
in Table 1. The model will be incorporated into the ESO ETC2
and will be made publicly available to the community via the
ESO web site.

This paper focuses on the discussion of model components
relevant for the wavelength range from 0.3 to 0.92 μm, which
is designated as “optical” in the following. We will discuss scat-
tering and absorption in the atmosphere (Sect. 2), contribu-
tions from extraterrestrial radiation sources (Sect. 3), and the inten-
sity and variability of airglow emission lines and continuum
(Sect. 4). The quality of our optical sky model will be evalu-
ated in Sect. 5. The near-IR and mid-IR regimes will be treated
in a subsequent paper.

If intensity units are not explicitly given in this pa-
er, photons s$^{-1}$ m$^{-2}$ μm$^{-1}$ arcsec$^{-2}$ are taken as the standard.
Magnitudes are always given in the Vega system.

2. Atmospheric extinction

Light from astronomical objects is scattered and absorbed in the
Earth’s atmosphere. For point sources, both effects result in a
loss of radiation, which is usually described by a wavelength-
dependent extinction curve or an atmospheric transmission
curve. The components of such a curve for Cerro Paranal are
discussed in Sect. 2.1. For extended sources, light is not only
scattered out of the line of sight, it is also scattered into it. This
effect causes an effective extinction curve to differ from that of
a point source and depends on the spatial distribution of the ex-
tended emission. To quantify the change of the extinction curve,
we performed three-dimensional (3D) scattering calculations,
which are described in Sect. 2.2.

2.1. The transmission curve

The atmospheric transmission depends on scattering and absorp-
tion. Light can be scattered in dry atmosphere by air molecules
such as N$_2$ and O$_2$ or by aerosols like silicate dust, sea salt,
soot, or droplets of sulphuric acid. The former effect is known
as Rayleigh scattering, and is characterised by a strong wave-
length dependence proportional to $λ^{-4}$ and a relatively isotropic
scattering phase function (a factor of 2 variation for unpolarised
radiation). The latter can be described by Mie scattering if spher-
ical particles are assumed. Aerosol scattering is characterised by
a relatively weak wavelength dependence ($λ^{-1}$ to $λ^{-2}$) and pro-
nounced forward scattering, for which the maximum intensity
can easily be two orders of magnitude higher than at large scat-
ttering angles. Atmospheric absorption in the optical is mainly
caused by bands from three molecules: molecular oxygen (O$_2$),
water vapour (H$_2$O), and ozone (O$_3$). The absorption of O$_3$ is
a function of atmospheric density. While water absorption is most
efficient close to the ground, where the absolute humidity is the
largest, ozone mainly absorbs at stratospheric altitudes of about
20 km. The combination of scattering and absorption results in
an extinction curve, which is often given in mag airmass$^{-1}$, or
a transmission curve providing values from 0 (totally opaque)
to 1 (fully transparent). The transmission $t(λ)$ can be linked to
the zenithal optical depth $τ(λ)$ and zenith extinction coeffi-
cient $k(λ)$ by

$$t(λ) = e^{−τ(λ)X} = 10^{−0.4k(λ)X}.$$  

\[1\]
Table 1. Sky model parameters for optical wavelength range.

<table>
<thead>
<tr>
<th>Parameter*</th>
<th>Description</th>
<th>Unit</th>
<th>Range</th>
<th>Default</th>
<th>Demo run</th>
<th>Section</th>
</tr>
</thead>
<tbody>
<tr>
<td>$90^\circ−\zeta_0$</td>
<td>altitude of target above the horizon</td>
<td>deg</td>
<td>[0, 90]</td>
<td>90.</td>
<td>85.1</td>
<td>2–4</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>separation of Sun and Moon as seen from Earth</td>
<td>deg</td>
<td>[0, 180]</td>
<td>0.</td>
<td>77.9</td>
<td>3.1</td>
</tr>
<tr>
<td>$\rho$</td>
<td>separation of Moon and target</td>
<td>deg</td>
<td>[0, 180]</td>
<td>180.</td>
<td>51.3</td>
<td>3.1</td>
</tr>
<tr>
<td>$90^\circ−\zeta_{moon}$</td>
<td>altitude of Moon above the horizon</td>
<td>deg</td>
<td>[−90, 90]</td>
<td>−90.</td>
<td>41.3</td>
<td>3.1</td>
</tr>
<tr>
<td>$\kappa_{moon}$</td>
<td>relative distance to Moon (mean = 1)</td>
<td>–</td>
<td>(0.945, 1.055)</td>
<td>1.</td>
<td>1.</td>
<td>3.1</td>
</tr>
<tr>
<td>$\lambda_0$</td>
<td>heliocentric ecliptic longitude of target</td>
<td>deg</td>
<td>[−180, 180]</td>
<td>135.</td>
<td>−124.5</td>
<td>3.3</td>
</tr>
<tr>
<td>$\beta$</td>
<td>ecliptic latitude of target</td>
<td>deg</td>
<td>[−90, 90]</td>
<td>90.</td>
<td>−31.6</td>
<td>3.3</td>
</tr>
<tr>
<td>$S_{10.7,cm}$</td>
<td>monthly-averaged solar radio flux at 10.7 cm</td>
<td>sfu$^c$</td>
<td>≥0</td>
<td>130.</td>
<td>205.5</td>
<td>4.2–4.4</td>
</tr>
<tr>
<td>$P_{season}$</td>
<td>bimonthly period (1: Dec./Jan., ..., 6: Oct./Nov.; 0: entire year)</td>
<td>–</td>
<td>0</td>
<td>4</td>
<td>2.1, 4.3, 4.4</td>
<td></td>
</tr>
<tr>
<td>$P_{night}$</td>
<td>period of the night ($x/3$ of night, $x =$ 1, 2, 3; 0: entire night)</td>
<td>–</td>
<td>0</td>
<td>3</td>
<td>4.3, 4.4</td>
<td></td>
</tr>
<tr>
<td>$d_{vac/air}$</td>
<td>vacuum or air wavelengths</td>
<td>–</td>
<td>vac/air</td>
<td>vac</td>
<td>air</td>
<td>2.1, 4.3, 4.4</td>
</tr>
</tbody>
</table>

Notes. $^{(a)}$ We neglect temperature and emissivity of telescope and instrument, because these parameters are irrelevant for the optical spectral range. $^{(b)}$ Used for Table 5. $^{(c)}$ Used for Figs. 1, 6, 13, and 17. $^{(d)}$ Fixed to default value because of its minor importance (see also Sect. 3.1). $^{(e)}$ 1 sfu = 0.01 Mly.

The pressure $p$ can be calculated by the formula of Rozenberg (1966):

$$X = \left(\cos(z) + 0.025 e^{-11 \cos(z)}\right)^{-1},$$

where $z$ is the zenith distance and $X$ converges to 40 at the horizon.

For Cerro Paranal, Fig. 2 shows the annual mean transmission curve at zenith and its components. The extinction at blue wavelengths is dominated by Rayleigh scattering. This component is very stable and can be well reproduced by the parametrisation

$$\tau_R(\lambda) = \frac{p}{1013.25 \times \lambda^{(3.916 + 0.074 (A + 0.50)} \lambda^{-1}},$$

with wavelength $\lambda$ in $\mu$m (see Liou 2002). For the pressure $p$ and the height $H$, we take 744 hPa and 2.64 km respectively.

The pressure corresponds to the annual mean for Cerro Paranal (743.5 ± 1.5 hPa), as derived from the meteorological station of the VLT Astronomical Site Monitor.

At red wavelengths, aerosol scattering becomes as important as Rayleigh scattering. However, the total amount of extinction by scattering is small in this wavelength regime. For Cerro Paranal, Patat et al. (2011) provide an approximation for the aerosol extinction derived from 600 VLT FORS1 spectra observed over six months. The aerosol extinction coefficient is parametrised by

$$k_{aer}(\lambda) = k_0 \lambda^{-\alpha},$$

where $k_0 = 0.013 \pm 0.002$ mag airmass$^{-1}$ and $\alpha = −1.38 \pm 0.06$, with the wavelength $\lambda$ in $\mu$m. Due to an increased discrepancy between the fit and the observed data in the near-UV (see Patat et al. 2011), we use Eq. (4) only for wavelengths longer than 0.4 $\mu$m. For shorter wavelengths, we use a constant value of $k_{aer} = 0.050$ mag airmass$^{-1}$, which corresponds to the fit value at 0.4 $\mu$m. The density, distribution, and composition of aerosols is much more variable than what is observed for the air molecules, which determine the Rayleigh scattering. Patat et al. (2011) find that $k_{aer}$ varies by about 20% at 0.4 $\mu$m. However, these variations are of minor importance for the total transmission of the Earth’s atmosphere, since the aerosol extinction coefficients are small.

Figure 2 exhibits several prominent absorption bands (see also Patat et al. 2011). At wavelengths below 0.34 $\mu$m, there is a conspicuous fall-off of the transmission curve caused by the Huggins bands of ozone. The stratospheric ozone layer is also responsible for the Chappuis absorption bands between 0.5 and 0.7 $\mu$m. The relatively narrow, but strong, bands at 0.688 $\mu$m and 0.762 $\mu$m can be identified as the Fraunhofer B and A bands of molecular oxygen. Finally, the complex bands at 0.72, 0.82, and 0.94 $\mu$m are produced by water vapour.

The molecular absorption bands have been calculated using the Line By Line Radiative Transfer Model (LBLRTM), an atmospheric radiative transfer code provided by the Atmospheric and Environmental Research Inc. (see Clough et al. 2005). This widely used code in the atmospheric sciences computes transmission and radiance spectra based on the molecular line database HITRAN (see Rothman et al. 2009) and atmospheric vertical profiles of pressure, temperature, and abundances of relevant molecules.
transmission curves. Since radiative transfer calculations with (see Eq. (2)) is used as input parameter for the computation of and the less pronounced average, nocturnal variations have been the significant seasonal dependence is included in the sky model of magnitude, i.e. large statistical uncertainties. For this reason, for Cerro Paranal. Second, we use profiles from the Global density of 258 Dobson units, which represents the mean value profile is corrected by a factor of 1.08 to achieve a column data from the MIPAS instrument of the ENVISAT satel-

For Cerro Paranal, we use merged atmospheric profiles from three data sources to reproduce the climate and weather conditions in an optimal way. First, the equatorial daytime standard profile from the MIPAS instrument of the ENVISAT satellite (prepared by Remedios 2001; see Seifahrt et al. 2010) is taken. It provides abundances for 30 molecular species up to an altitude of 120 km. Following Patat et al. (2011), the ozone profile is corrected by a factor of 1.08 to achieve a column density of 258 Dobson units, which represents the mean value for Cerro Paranal. Second, we use profiles from the Global Data Assimilation System (GDAS), maintained by the Air Resources Laboratory of the National Oceanic and Atmospheric Administration (cf. Seifahrt et al. 2010). The GDAS profiles for pressure, temperature, and relative humidity are provided on a 3 h basis for a 1° × 1° global grid. These models are adapted to data from weather stations all over the world and are suitable for weather-dependent temperature and water vapour profiles up to altitudes of 26 km. Third, data from the meteorological station at Cerro Paranal are used to scale the pressure, temperature, and water vapour profiles at the altitude of the mountain. For higher altitudes, the scaling factor is reduced and approaches 1 at 5 km.

For our sky model, we analysed the resulting data set and constructed mean profiles with their 1σ deviations for different periods. We divide the year into six two-month periods, starting with December/January (cf. Table 1 and Sect. 4). The two most extreme mean spectra are shown in Fig. 3. The seasonal variability of the H2O bands is clearly visible. For the driest period (August/September), the mean absorption is only half the amount of the most humid period (February/March). The total intra-annual variability indicates line depth variations of an order of magnitude, i.e. large statistical uncertainties. For this reason, the significant seasonal dependence is included in the sky model and the less pronounced average, nocturnal variations have been neglected. The apart from the two-month period, only the airmass (see Eq. (2)) is used as input parameter for the computation of transmission curves. Since radiative transfer calculations with 3 http://ready.arl.noaa.gov/gdas1.php

![Fig. 3. Variation of molecular absorption for Cerro Paranal. The extreme bimonthly mean transmission curves and 1σ deviations of the annual mean curve (red outer curves) are shown. The highest mean transmission (lowest water vapour content) is found for August/September (green curve), and the lowest arises in February/March (black curve). In contrast to H2O, the variations of the O2 bands are very small. For the identity of the bands, see Fig. 2.](http://example.com/f3.png)

![Fig. 4. Geometry of the scattering in the Earth’s atmosphere (cf. Wolstencroft & van Breda 1967). Point N is at the top of atmosphere and not in the same plane as the other points. The azimuth of N as seen from S is A (not shown). S and T are at an azimuth A0 (also not shown) for an observer at O.](http://example.com/f4.png)
from the entry point in the atmosphere $N$ to $S$ of length $s_1$. The latter includes the scattering of light out of the path (and possible absorption), which depends on the effective column density of the scattering/absorbing particles
\begin{equation}
B(y, \sigma) = \int_0^{\sigma(z, \sigma)} n(\sigma') d\sigma'.
\end{equation}
It also depends on the wavelength-dependent extinction cross section $C_{\text{ext}}(\lambda)$, which can be derived from the optical depth at zenith $\tau_0$ (see Eq. (1)) by means of Eq. (5) and
\begin{equation}
C_{\text{ext}}(\lambda) = \frac{\tau_0(\lambda)}{B_0(0, \sigma_0)}.
\end{equation}
After the scattering at $S$, the intensity is further reduced by the effective column density $B_2(z_0, \sigma)$ along the path $s_2$. Thus, the calculations can be summarised by
\begin{equation}
I_{\text{scat}}(A_0, z_0) = \frac{C_{\text{ext}}(\lambda)}{4\pi} \int_0^{\sigma_2(z_0, \sigma_2)} \int_0^{\sigma_{\text{max}}(\sigma_2)} \int_0^{2\pi} n(\sigma') P(\theta) \times I_0(A, z) e^{-C_{\text{ext}}(\lambda)(B_2(z_0, \sigma) + B_1(0, \sigma_0))} dA \sin \vartheta d\vartheta d\varphi.
\end{equation}
$c_{\text{ext}}$ is the wavelength-dependent scattering cross section, which will deviate from $C_{\text{ext}}$ if absorption occurs. The maximum zenith distance $z_{\text{max}}$ is higher than 90° and depends on the height of $S$ above the ground. The scattering phase function $P$ depends on the scattering angle $\theta$, the angle between the paths $s_1$ and $s_2$. Rayleigh scattering (see Sect. 2.1) is characterised by the phase function
\begin{equation}
P(\theta) = \frac{3}{4} \left(1 + \cos^2(\theta)\right).
\end{equation}
Similar to Bernstein et al. (2002), we neglect the effect of polarisation on the scattering phase function. Even for zodiacal light, where some polarisation is expected (e.g. Staudte 1975), the polarisation does not appear to significantly affect the integrated scattered light. Results of Wolstencroft & van Breda (1967) suggest degeneracies of only a few per cent. For the vertical distribution of the scattering molecules, we use the standard barometric formula
\begin{equation}
n(h) = n_0 e^{-h/h_0}.
\end{equation}
Here, $h = \sigma' - R$, the sea level density $n_0 = 2.67 \times 10^{19}$ cm$^{-3}$, and the scale height $h_0 = 7.99$ km above the Earth’s surface (cf. Bernstein et al. 2002). For the troposphere and the lower stratosphere, where most of the scattering occurs, this is a good approximation. Cerro Paranal is at an altitude of $H_0 = 2.64$ km. For the thickness of the atmosphere, we take $H_{\text{max}} = 200$ km. With these values, $C_{\text{ext}} = 1.75 \times 10^{-20}$ cm$^2$ for $\tau_0 = 0.27$, which corresponds to a wavelength of about 0.40 $\mu$m. For Rayleigh scattering, $C_{\text{scat}} = C_{\text{ext}}$, i.e. no absorption is involved. In the near-UV, where the zenithal optical depth is greater than 0.3, the single scattering approximation becomes questionable. For this reason, we apply a multiple scattering correction derived from radiative transfer calculations in a plane-parallel atmosphere (see Dave 1964; Staudte 1975). We multiply $I_{\text{scat}}$ by the factor
\begin{equation}
F_{\text{MS}} = 1 + 2.2 \tau_0.
\end{equation}
The uncertainty is in the order of 5%. The factor $F_{\text{MS}}$ does not include reflection from the ground. Mattila (2003) reports an average ground reflectance of about 8% in the region near the Las Campanas Observatory in autumn. Since this telescope site is also located in the Atacama desert, we assume this value with an uncertainty of a few per cent. Using the tables of Ashburn (1954), an 8% reflectance translates into an additional $I_{\text{scat}}$ correction factor of about 1.07.

The Mie scattering of aerosols is characterised by a phase function with a strong peak in forward direction. For this study, we take the measured $P(\theta)$ of Green et al. (1971), which covers the peak up to an angle of 20°. The phase function for larger scattering angles is extrapolated by a linear fit in the $\log P – \log \theta$ diagram. This simple approach neglects the increase of the phase function for scattering angles close to 180° (see e.g. Liou 2002). However, since $P$ already decreases by a factor of 30 from 0° to 20°, the details of the phase function at larger angles are not crucial for the scattering of extended emission. The total scattered intensity is completely dominated by the contribution from angles close to the forward direction. For the height distribution of aerosols, we also take $\tau_0 = 1.11 \times 10^5$ cm$^2$ and $h_0 = 1.2$ km. This is the tropospherical distribution of Ellerman (1966). Following Staudte (1975), we neglect the stratospheric aerosol component, which contains only about 1% of the particles. Using Eq. (6) we obtain $C_{\text{scat}} = 3.39 \times 10^{-10}$ cm$^2$ for $\tau_0 = 0.05$, which characterises wavelengths of about 0.4 $\mu$m. Dust, in particular soot, also absorbs radiation. For this reason, $C_{\text{scat}}$ is lower than $C_{\text{ext}}$. The ratio of these is called the single scattering albedo $\omega$. Following the recommendation of Mattila (2003), $\omega = 0.94$ is used for the model, i.e. strong absorbers like soot do not significantly contribute to the aerosol population. We neglect any corrections for multiple scattering and ground reflection for Mie scattering, since the optical depths are low at all relevant wavelengths (see Fig. 2) and forward scattering dominates.

To test our model, we computed scattering intensities for a uniform radiation source of unit brightness. For the surface level and $\tau_0 = 0.052$, we obtain scattering fractions of 0.024 for the zenith and 0.360 for the horizon ($z_0 = 90°$) with the multiple scattering corrections neglected. For Rayleigh scattering, these results can be compared to those of Staudte (1975). Our values are only about 5% higher. This is a good agreement compared to differences between Staudte (1975) and older calculations of Wolstencroft & van Breda (1967) and Ashburn (1954). Figure 5 shows the resulting scattering fractions for Rayleigh and Mie scattering for different optical depths, which have been converted into wavelengths based on the Cerro Paranal mean transmission curve discussed in Sect. 2.1. For zenith distances that are realistic for astronomical observations, wavelengths longer than about 0.45 $\mu$m for Rayleigh scattering, and all wavelengths for aerosol scattering, the scattering fractions stay below 10% for a source of uniform brightness. Scattering by air molecules and the ground surface can be important for lines of sight close to the horizon and near-UV wavelengths. Figure 5 indicates scattering fractions of about 40% under these conditions. Moreover, there appears to be a downturn of the scattering fraction for very high zenith distances (see also Staudte 1975), where the line-of-sight direction becomes nearly opaque. In this case, the light that is not extinguished has to be scattered near the observer and the incident photons have to originate close to the zenith.

The results of scattering calculations for more realistic source intensity distributions will be discussed in Sects. 3.2, 3.3, and 4.3.

3. Moon, stars, and interplanetary dust

Bright astronomical objects affect night-sky observations by the scattering of their radiation into the line of sight. The relevant
Fig. 5. Intensity of scattered radiation for a uniform source of unit brightness using the Paranal extinction curve (see Sect. 2.1). Contributions of scattered light into the line of sight are shown for Rayleigh (solid lines) and Mie scattering (dashed lines) and zenith distances from 0° to 80° in 10° steps plus an extreme value of 85°. Except for Rayleigh scattering at very short wavelengths, the scattering intensities increase with zenith distance.

Initial radiation sources are the Sun and the summed-up light of all other stars. The solar radiation must first be scattered by interplanetary dust grains and the Moon surface to contribute to the night-sky brightness. In the following, we discuss these scattering-related sky model components, i.e. scattered moonlight (Sect. 3.1), scattered starlight (Sect. 3.2), and zodiacal light (Sect. 3.3). Another source of scattered light is man-made light pollution, which can be neglected for Cerro Paranal. Patat (2003) instead, as semi, it is not necessary to perform the scattering calculations for extended sources, as discussed in Sect. 2.2. Instead, a semi-analytical model for the photometric V band by Krisciunas & Schaefer (1991) is used for the sky model, which has been extended into a spectroscopic version.

Based on Krisciunas & Schaefer (1991), we compute the Moon-related sky surface brightness as the sum of the contributions from Rayleigh and Mie scattering

$$B_{\text{moon}}(\lambda) = B_{\text{moon,R}}(\lambda) + B_{\text{moon,M}}(\lambda),$$

where

$$B_{\text{moon,R/M}}(\lambda) = f_{R/M}(\rho) I^*(\lambda) I^{X_{\text{moon}}}(\lambda) \left(1 - t_{R/M}(\lambda)\right).$$

The empirical scattering functions

$$f_{R}(\rho) = 10^{5.70(1.06 + \cos^2(\rho))}$$

for Rayleigh scattering and

$$f_{M}(\rho) = 10^{7.15 - (\rho/40)}$$

for Mie scattering depend on the angular separation of Moon and object $\rho$, which is restricted to angles greater than $10^\circ$. The functions deviate from the ones of Krisciunas & Schaefer (1991) by factors of 2.2 and 10 respectively. These corrections are necessary because of the separation of the two scattering processes in Eqs. (11) and (12), the model extension in wavelength, and an optimisation for the observing conditions at Cerro Paranal. The two correction factors were derived separately from a comparison with optical VLT data (see Sect. 4.2) by using the increasing importance of Rayleigh scattering with respect to Mie scattering for shorter wavelengths and larger scattering angles $\rho$ (see Sect. 2.2). The factor of 10 for Mie scattering is highly uncertain due to a lack of clear constraints from the available data set. The Moon illuminance is proportional to

$$I^* \propto 10^{-0.4(0.026|\phi| + 4.0 \times 10^{-5} |\phi|^2)} \times (d_{\text{moon}})^{-2},$$

where the Moon distance $d_{\text{moon}}$ can vary up to 5.5% relative to the mean value. The lunar phase angle $\alpha = 180^\circ - \phi$ is the separation angle of Moon and Sun as seen from Earth. It can be estimated from the fractional lunar illumination (FLI) by

$$\alpha \approx \arccos(1 - 2 \text{FLI}),$$

since the influence of the lunar ecliptic latitude on $\alpha$ is negligible. $B_{\text{moon}}$ also depends on the atmospheric transmission for the airmass of the Moon $t_{\text{moon}}$, for which the Patat et al. (2011) extinction curve is used (see Fig. 2). Lastly, it depends on a term that describes the amount of scattered moonlight in the viewing direction, which can be roughly approximated by $1 - t_{R/M}^X$, for either Rayleigh or Mie scattering and the target airmass $X_0$. The airmasses of the Krisciunas & Schaefer (1991) model are computed using

$$X = \left(1 - 0.96 \sin^2(\gamma)\right)^{-0.5},$$

which is especially suited for scattered light, because of a low limiting airmass at the horizon (cf. Eq. (2)).

The Krisciunas & Schaefer model was developed only for the V band. It can be extended to other wavelength ranges by using the Cerro Paranal extinction curve (see Sect. 2.1) and its Rayleigh and Mie components for the transmission curves $t_{R}$, $t_{M}$, and $t_{R/M}$ in Eq. (12) and by assuming that the Moon spectrum resembles the spectrum of the Sun (see Fig. 6). The latter is modelled by the solar spectrum of Colina et al. (1996) scaled to the V-band brightness of the moonlight scattering model. For most situations, this approach results in systematic uncertainties of no more than 10% of the total night-sky flux compared to observations. The statistical uncertainties are in the order of 10 to 20% (see Sect. 5). The errors become larger for full Moon and/or target positions close to the Moon ($\rho \lesssim 30^\circ$). The latter especially concerns red wavelengths, where the contribution of Mie forward scattering to the total intensity of scattered light is particularly high. Consequently, the strongly varying aerosol properties have to be known (which is a challenging task) to allow for a good agreement of model and observations. However, optical astronomical observations close to the Moon are unlikely. Therefore, this is not a critical issue for the sky model.

3.2. Scattered starlight

Like moonlight, starlight is also scattered in the Earth’s atmosphere. However, stars are distributed over the entire sky with a distribution maximum towards the centre of the Milky Way. This distribution requires the use of the scattering model for extended...
sources described in Sect. 2.2. Since scattered starlight is only a minor component compared to scattered moonlight and zodiacal light (see Fig. 1), it is sufficient for an ETC application to compute a mean spectrum. This simplification allows us to avoid the introduction of sky model parameters such as the galactic coordinates, which have a very low impact on the total model flux.

For the integrated starlight (ISL), we use Pioneer 10 data at 0.44 μm (Toller 1981; Toller et al. 1987; Leinert et al. 1998). These data are almost unaffected by zodiacal light. The small “hole” in the data set towards the Sun has been filled by interpolation. Since the Pioneer 10 maps do not include stars brighter than 6.5 mag in V, a global correction given by Melchior et al. (2007) is applied, which increases the total flux by about 16%. Scattering calculations are only performed for the distribution of starlight in the B band, i.e., the dependence of this distribution on wavelength is neglected. This approach is supported by calculations of Bernstein et al. (2002), indicating that the shapes of ISL spectra are very stable, except for regions in the dustiest parts of the Milky Way plane. The wavelength dependence of the scattered starlight is considered by multiplying the representative ISL mean spectrum of Mattila (1980) by the resulting wavelength-dependent amount of scattered light (for illustration see Figs. 5 and 6). Since the mean ISL spectrum of Mattila only covers wavelengths up to 1 μm, we extrapolated the spectral range by fitting an average of typical spectral energy distributions (SEDs) for early- and late-type galaxies produced by the SED-fitting code CIGALE (see Noll et al. 2009). Since the SED slopes are very similar in the near-IR, the choice of the spectral type is not crucial. The solar and the mean ISL spectrum are similar at blue wavelengths, but the ISL spectrum has a redder slope at longer wavelengths (see Fig. 6). The differences illustrate the importance of K and M stars for the ISL.

For the desired average scattered light spectrum, we run our scattering code for different combinations of zenithal optical depth, zenith distance, azimuth, and sidereal time for Rayleigh and Mie scattering (see Sect. 2.2). The step sizes for the latter three parameters were 10°, 45°, and 2 h, respectively. Zenith distances were only calculated up to 50°, since this results in a mean airmass of about 1.25 for the covered solid angle, which is typical of astronomical observations. The mean scattering intensities for each optical depth \( \tau_0 \) were then computed. This was translated into a spectrum by using the relation between \( \tau_0 \) and wavelength as provided by the Cerro Paranal extinction curve (see Sect. 2.1). Finally, the mean ISL spectrum (normalised to the B-band flux) was multiplied. The sky model code does not change the final spectrum, except for the molecular absorption, which is adjusted depending on the bimonthly period (see Sect. 2.1). For the effective absorption airmass, the mean value of 1.25 is assumed.

The resulting spectrum shows an intensity of about 13 photons s\(^{-1}\) m\(^{-2}\) μm\(^{-1}\) arcsec\(^{-2}\) at 0.4 μm. At 0.6 μm, there is only half of this intensity (see Fig. 6). The results are in good agreement with the findings of Bernstein et al. (2002).

3.3 Zodiakal light

Zodiacal light is caused by scattered sunlight from interplanetary dust grains in the plane of the ecliptic. A strong contribution is found for low absolute values of ecliptic latitude \( \beta \) and heliocentric ecliptic longitude \( \lambda - \lambda_0 \). The brightness distribution provided by Levasseur-Regourd & Dumont (1980) and Leinert et al. (1998) for 0.5 μm shows a relatively smooth decrease for increasing elongation, i.e., angular separation of object and Sun. A striking exception is the local maximum of the so-called gegenschein at the antisolar point in the ecliptic. The spectrum of the optical zodiacal light is similar to the solar spectrum (Colina et al. 1996), but slightly reddened (see Fig. 6). We apply the relations given in Leinert et al. (1998) to account for the reddening. The correction is larger for smaller elongations. Thermal emission of interplanetary dust grains in the IR is neglected in the sky model, since the airglow components of atmospheric origin (see Fig. 1) completely outshine it. In the optical, zodiacal light is a significant component of the sky model. A contribution of about 50% is typical of the B and V bands when the Moon is down (see Sect. 5.2). At longer wavelengths, the fraction decreases due to the increasing importance of the airglow continuum (see Sect. 4.4).

The model of the zodiacal light presented in Leinert et al. (1998) describes the characteristics of this emission component outside of the Earth’s atmosphere. Ground-based observations of the zodiacal light also have to take atmospheric extinction into account. Since zodiacal light is an extended radiation source, the observed intensity is a combination of the extinguished top-of-atmosphere emission in the viewing direction and the intensity of light scattered into the line of sight (see Fig. 6). The latter can be treated by scattering calculations as discussed in Sect. 2.2. Scattering out of and into the line of sight leads to an effective extinction and this can be expressed by an effective optical depth

\[
\tau_{\text{eff}} = \tau_{\text{ext}} X = f_{\text{ext}} \tau_0 X
\]  
(18)
Fig. 7. Extinction reduction factor $f_{\text{ext}}$ for zodiacal light as a function of the line-of-sight top-of-atmosphere intensity $I_0$ of the zodiacal light in dex. The intensities correspond to those given in Table 17 of Leinert et al. (1998), i.e., the unit is $10^{-8}$ W m$^{-2}$ μm$^{-1}$ sr$^{-1}$ (=1.690 photons s$^{-1}$ μm$^{-1}$ arcsec$^{-2}$ at 0.5 μm). The factors were calculated for different ecliptic longitudes of the Sun, sidereal times, and line-of-sight zenith distances (up to 50° in general and up to 70° for log $I_0 > 2.4$) and azimuths. Only night-time data points with solar zenith distances greater than 108° are considered. For Rayleigh scattering (black “x” symbols), a zenithal optical depth of 0.27 is taken, corresponding to a wavelength of 0.4 μm for the Cerro Paranal extinction curve (see Sect. 2.1). For Mie scattering (green “+” symbols), $\tau_0$ is fixed to 0.01, a value reached at about 1.2 μm. The figure also shows average $f_{\text{ext}}$ in 0.1 dex $I_0$ bins for both scattering modes (Rayleigh: blue circles; Mie: red triangles). The resulting fits based on these average values are displayed by solid (Rayleigh) and dashed lines (Mie).

For an ecliptic longitude of 56°, i.e., for each of the four seasons, one data set was calculated. Scattering calculations were only carried out for solar zenith distances of at least 108°. This restriction excludes daytime and twilight conditions. As for scattered starlight, we consider target zenith distances $z$ up to 50° (see Sect. 3.2). For rare high zodiacal light intensities, we also let 50° $< z \leq 70°$. The $z$ limits do not significantly affect $f_{\text{ext}}$. A test with 0° $\leq z \leq 70°$ showed a variation of $f_{\text{ext}}$ in the order of a few percent only.

For an efficient implementation in the ETC, we searched for a parametrisation of $f_{\text{ext}}$ that simplifies the treatment of scattering and minimises the number of required input parameters. We found that the initial intensity of the zodiacal light in the viewing direction $I_0$ indicates the tightest relation with $f_{\text{ext}}$. The next-best parameter is the ecliptic latitude. Figure 7 shows $f_{\text{ext}}$ versus the logarithm of $I_0$ as provided by Leinert et al. (1998) for Rayleigh and Mie scattering. Since the variation of $f_{\text{ext}}$ with $\tau_0$ can be neglected, the optical depth is fixed to 0.27 for Rayleigh and 0.01 for Mie scattering. These values correspond to the wavelengths 0.4 and 1.2 μm respectively, which represent typical wavelengths dominated by the two different scattering processes (cf. Eq. (1); see also Bernstein et al. 2002). Consequently, the scattering properties of the zodiacal light can be described by the factor $f_{\text{ext}}$ alone. This parameter shows only a weak dependence on $\tau_0$ and, hence, wavelength. For Rayleigh scattering in the range from $U$ to $J$ band, we find an uncertainty of only about 4%. For Mie scattering from $V$ to $J$, a similar variation is found. We obtain this result by calculating $f_{\text{ext}}$ for a grid of optical depths, zenith distances, azimuths, sidereal times, and solar ecliptic longitudes. We take the same grid as for scattered starlight (see Sect. 3.2) plus solar ecliptic longitudes in steps of 90°, i.e. for each of the four seasons, one data set was calculated. Scattering calculations were only carried out for solar zenith distances of at least 108°. This restriction excludes daytime and twilight conditions. As for scattered starlight, we consider target zenith distances $z$ up to 50° (see Sect. 3.2). For rare high zodiacal light intensities, we also let 50° $< z \leq 70°$. The $z$ limits do not significantly affect $f_{\text{ext}}$. A test with 0° $\leq z \leq 70°$ showed a variation of $f_{\text{ext}}$ in the order of a few percent only.

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than 1%. Only at very short wavelengths, the systematic errors become higher. The intersection of the zero line at about 0.4 μm is caused by the selection of τ0 = 0.27 for the \( f_{\text{ext,R}} \) fitting. The \( 1\sigma \) range suggests uncertainties of no more than 3 to 4% for most wavelengths. These results suggest that the parametrisation of \( \tau_{\text{cat}} \) does not cause higher errors than those expected from the uncertainties of the scattering calculations (see Sect. 2.2). The total errors from the simple treatment of multiple scattering and ground reflection, neglect of polarisation, simplified particle distributions, and uncertainties in the aerosol scattering parameters should be in the order of 10% of \( I_{\text{cat}} \). This translates into uncertainties in the transmission of a few per cent at blue wavelengths, which is somewhat higher than the uncertainties from the \( f_{\text{ext}} \) fit.

Finally, the reduction of the zodiacal light intensity by molecular absorption has to be considered. Strong absorption is only important for relatively long wavelengths, where scattering affects only a few per cent of the incoming light (see Fig. 2), assuming zenith distances of typical astronomical observations. Hence, the direct component in the viewing direction is usually much brighter than the scattered light from other directions. For this reason, we can safely assume that the target airmass is well suited to derive the transmission reduction by molecular absorption. Differences between target and effective scattering airmasses can be neglected.

### 4. Airglow emission

Atmospheric emission at wavelengths from the near-UV to the near-IR originates in the upper atmosphere, especially in the mesopause region at an altitude of about 90 km and in the ionospheric F2 layer at about 270 km. In contrast to the thermal radiation in the mid-IR by atmospheric greenhouse gases in the lower atmosphere, this so-called airglow (see Khomich et al. 2008, for a comprehensive discussion) is caused by a highly non-LTE emission process called chemiluminescence, i.e. by chemical reactions that lead to light emission by the decay of excited electronic states of reaction products. Consequently, atmospheric radiative transfer codes like LBLRTM (Clough et al. 2005; see also Sect. 2.1) cannot be used to calculate this emission. Moreover, theoretical analysis is very challenging because of the high variability of airglow on various time scales. The complex reactions are affected by the varying densities of the involved molecules, atoms, and ions in different excitation states. Therefore, airglow can best be treated by a semi-empirical approach. The section starts with a general discussion of airglow extinction (Sect. 4.1). In Sect. 4.2, we present the data set that was used to derive the model. Detailed discussions of the line and continuum components of the model can be found in Sects. 4.3 and 4.4 respectively.

#### 4.1. Extinction of airglow emission

The intensities of airglow lines and continuum rise with growing zenith distance by the increase of the projected emission layer width. This behaviour is expressed by the van Rhijn function

\[
I(z) = \frac{I(0)}{\left(1 - \left(\frac{R \sin(z)}{R + h}\right)^2\right)^{0.5}}
\]

(van Rhijn 1921). Here, \( z \), \( R \), and \( h \) are the zenith distance, the Earth’s radius, and the height of the emitting layer above the Earth’s surface (see Table 2), respectively. The airglow intensity is also affected by scattering and absorption in the lower atmosphere. Since the airglow emission is distributed over the entire sky, we can derive the effective extinction by means of scattering calculations as described in Sect. 2.2. Some modifications have to be applied, since airglow emission originates in the atmosphere itself and because of the van Rhijn effect. The top of atmosphere is reduced from the default \( H_{\text{max}} = 200 \) km to 90 km, which is assumed to be representative of airglow emission layers. The few atomic lines originating in the ionospheric F2 layer are neglected here (see Sect. 4.3). The cut at the lower height is not critical, since the mass of the excluded range is negligible compared to the total mass of the atmosphere (see Eq. (9)). The projected emission layer width (see Fig. 9) is considered by calculating the zenith distance \( z_{\text{ag}} \) of each incoming beam as seen from the corresponding entry point \( N \) at \( H_{\text{max}} \). For our set-up, the resulting beam-specific airglow intensity can be approximated by

\[
I(z_{\text{ag}}) \approx \frac{I_0}{\cos(z_{\text{ag}})}.
\]
since the centres of the scattering path elements $S$ are always located well below the airglow emission layer height, which avoids $z_{ag} = 90^\circ$. The intensity $I_0$ for a perpendicular incidence at $N$ is assumed to be constant for the entire global airglow layer. The scattering calculations only depend on the zenithal optical depth and the target zenith distance.

Like for the zodiacal light (see Sect. 3.3), we can derive an optical depth reduction factor $f_{\text{ext}}$ (Eq. (18)) to describe the airglow extinction properties. The representative optical depths are again 0.27 for Rayleigh scattering (6% uncertainty from $U$ to $I$ band) and 0.01 for Mie scattering (4% variation from $V$ to $J$ band). The only remaining free parameter for $f_{\text{ext}}$ is the zenith distance or airmass. We take

$$X_{ag} = (1 - 0.972 \sin^2(z))^{0.5} \quad (23)$$

(cf. Eq. (17)), which corresponds to the van Rhijn formula (Eq. (21)) for the assumed airglow layer height of 90 km. $X_{ag}$ is better suited for fitting $f_{\text{ext}}$ and Eq. (18) than the Rozenberg (1966) airmass $X$ (Eq. (2)) used for the zodiacal light (see Sect. 3.3), where the $z$ dependence of $f_{\text{ext}}$ was negligible.

Figure 10 shows the extinction reduction factor as a function of the logarithm of $X_{ag}$. There is a strong increase in $f_{\text{ext}}$ with airmass, and the factors for the Mie scattering tend to be about 0.15 lower than those for Rayleigh scattering. These trends are in good agreement with our findings for the zodiacal light. However, the typical values of $f_{\text{ext}}$ are significantly lower. For most zenith distances relevant for astronomical observations, the factors are close to zero. Consequently, the effective extinction of airglow is very low (see Chamberlain 1961). For observations close to zenith, there is even a significant brightening of the airglow emission by the scattering into the line of sight from light with a long path length through the emission layer. Therefore, using a point-source transmission curve for airglow extinction correction will provide worse results than having no correction. As indicated by Fig. 10, a rough correction of airglow emission using the van Rhijn equation is reasonable up to zenith distances of 50$^\circ$ to 60$^\circ$, depending on the ratio of Rayleigh and Mie scattering. At higher zenith distances, the compensation of extinction of direct light by scattered light from other directions becomes less efficient. At the largest $z$, the intensity can be more reduced by extinction than enhanced by the van Rhijn effect. For this reason, there is a zenith distance with a maximum airglow intensity, which depends on the optical depth and, hence, the wavelength. For the Cerro Paranal extinction curve (see Sect. 2.1), we found a $z_{\text{max}}$ of about 70$^\circ$ at 0.35 $\mu$m and 85$^\circ$ at 0.7 $\mu$m.

For the sky model, $f_{\text{ext}}$ was fit up to a zenith distance of 60$^\circ$, where $f_{\text{ext}}$ shows an almost linear relation with the logarithm of $X_{ag}$ (see Fig. 10). A worse agreement at large zenith distances is tolerable, since astronomical observations are rarely carried out at those angles. The parameters obtained by the fits are

$$f_{\text{ext,R}} = 1.669 \log X_{ag} - 0.146 \quad (24)$$

for Rayleigh scattering

$$f_{\text{ext,M}} = 1.732 \log X_{ag} - 0.318 \quad (25)$$

for Mie scattering. For the fixed optical depths and the fitted $z$ range, the fit uncertainties of $f_{\text{ext}}$ are only about 0.01. Figure 11 displays the accuracy of the fits as a function of wavelength. For this plot, the Cerro Paranal extinction curve (see Sect. 2.1) was used to convert optical depths into wavelengths. For the fitted range of zenith distances, the deviations between fitted and the true transmission curves are below 1%, at least for wavelengths longer than 0.4 $\mu$m. As expected, the deviations for $z = 70^\circ$ are significantly larger than for the smaller zenith distances. Nevertheless, for most prominent airglow lines (see Sect. 4.3), the errors are below 2%, which also makes the parametrisation sufficient for large zenith distances.
Apart from scattering, molecular absorption in the lower atmosphere affects the observed airglow intensity. However, in the optical these absorptions are usually small (see Fig. 2). Exceptions are the airglow O$_2$(b-X)(0–0) and O$_2$(b-X)(1–0) bands at 762 and 688 nm, which suffer from heavy self-absorption at low altitudes, and can be observed as absorption bands only. As discussed in Sect. 3.3, the effective molecular absorption can be well approximated by taking the transmission spectrum for the target zenith distance. For the airglow continuum component, this is easily applied. For the line component, this is challenging, since airglow emission as well as telluric absorption lines are very narrow. Therefore, an effective absorption for each airglow line has to be derived at very high resolution. Resolving the airglow lines requires resolutions in the order of 10$^6$. The absorption lines tend to be broader than the emission lines. LBLRTM (see Clough et al. 2005) easily produces spectra with the required resolution. For the airglow emission, we use a line list with good wavelength accuracy, as discussed in Sect. 4.3. In the upper atmosphere, broadening of lines by collisions can be neglected due to the low density (see Khomich et al. 2008). Thus, the shape and width of airglow lines are determined by Doppler broadening, which can be derived by the molecular weight of the species and ambient temperature. The latter is in the order of 200 K in the mesopause region, which explains the low Doppler widths. For example, the full width at half maximum of an OH line (see Sect. 4.3) at 0.8 μm is about 2 picometers (pm). The few lines originating in the thermospheric ionosphere experience distinctly higher temperatures of about 1000 K. The line absorption correction is applied as the multiplication of the initial line intensities by the suitable line of about 1000 K. The absorption lines tend to be less absorbed than the continuum. Hence, the chance to find an airglow line at the centre of a strong absorption feature is relatively low.

4.2. Data set for airglow analysis

The airglow analysis (see Sects. 4.3 and 4.4) and the sky model verification (see Sect. 5) were carried out using a sample of 1186 FORS 1 long-slit sky spectra (see Fig. 12). The FORS 1 data were collected from the ESO archive and reduced by Patat (2008). The spectra were taken with the low/intermediate resolution grisms 600B (12%), 600R (17%), and 300V, the latter with (57%) and without (14%) the order separation filter GG435. The set-ups cover the wavelength range from 0.365 to 0.89 μm. Wavelengths below 0.44 μm are the least covered, since only 600B and 300V spectra without GG435 can be used there. The FORS 1 spectra were taken between April 1999 and February 2005, i.e. observations during a phase of low solar activity are not part of the present data set (see Fig. 12). The mean and standard deviation of the Penticon-OTTawa solar radio flux at 10.7 cm$^6$ (Covington 1969) are 153 and 35 solar flux units (sfu = 0.01 MJy) respectively. The data set is also characterised by a mean zenith distance of 31°. The corresponding standard deviation is only 13° and the maximum zenith distance is 67°. The fraction of exposures with the Moon above the horizon amounts to 26%. 29 spectra were taken at sky positions with Moon distances below 30° (see Sect. 3.1). However, we excluded three spectra from the original sample of 1189 spectra because of unreliable continua concerning strength and shape. The wavelength-dependent results for line-of-sight zenith distances from 0° (black solid line) to 70° (red dashed line) in 10° steps are exhibited.

Fig. 11. Ratio of the airglow transmissions of the fits as shown in Fig. 10 and the full scattering calculations in magnitudes. The wavelength-dependent results for line-of-sight zenith distances from 0° to 70° (red dashed line) in 10° steps are exhibited.

Fig. 12. Date, time, and solar activity for the VLT FORS 1 observations of the Patat (2008) spectroscopic data set. The solar activity is given by the solar radio flux measured at 10.7 cm in sfu. The FORS 1 spectra were taken with different instrument set-ups, which are indicated by different symbols and colours. The plot legend identifies the different set-ups by their covered wavelength ranges in μm. Open symbols indicate that the data were taken with the Moon above the horizon, whereas filled symbols refer to dark-time observations.
exposures affected by strong zodical light contribution are almost completely absent.

The FORS 1 night-sky spectra were not extinction corrected and the response curves for the flux calibration were derived by the Cerro Tololo standard extinction curve (Stone & Baldwin 1983; Baldwin & Stone 1984). We corrected all the spectra to the more recent and adequate Cerro Paranal extinction curve of Patat et al. (2011, see Sect. 2.1), assuming a mean airmass of 1.25 for the spectrophotometric standard stars. This procedure resulted in corrections of +6% at the blue end to −1% at the red end of the covered wavelength range.

4.3. Airglow lines

In the following, we treat airglow lines in detail. At first, the origin of the airglow line emission, the classification of lines, and a derivation of a line list for the sky model are discussed (Sect. 4.3.1). In the second part, we investigate the variability of airglow lines (Sect. 4.3.2).

4.3.1. Line classes and line list

The most prominent optical airglow line is [O I] 5577 (see Fig. 13, panel 1). Its dominant component at an altitude of about 97 km is probably produced by the process described in Barth & Hildebrand (1961). The crucial reactions are

\[ \text{O} + \text{O} + \text{M} \rightarrow \text{O}_2^+ + \text{M}, \]  
\[ \text{O}_2^+ + \text{O} \rightarrow \text{O}_2 + \text{O} \left( ^1\text{S} \right), \]  
\[ \text{and} \]
\[ \text{O} \left( ^1\text{S} \right) \rightarrow \text{O} \left( ^1\text{D} \right) + 557.7 \text{ nm}, \]  
where M is an arbitrary reaction partner. The first reaction (Eq. (26)) also plays an important role for the emission bands of molecular oxygen. In order to start the three body collision, oxygen molecules have to be split by hard UV photons:

\[ \text{O}_2 + h\nu \rightarrow \text{O} + \text{O}. \]  

This process mainly occurs during the day by solar UV radiation, which implies that the oxygen airglow intensity depends on the solar activity and observing time. The O(1D) state can lead to [O I] 6300 emission (see Fig. 13, panel 3). However, in the mesopause the deactivation of this metastable state is mostly caused by collisions. Hence, strong [O I] 6300 emission is restricted to the thermosphere at altitudes of about 270 km. In contrast to the mesosphere, the excitation there is caused by dissociative recombination (Bates 1982), i.e. it depends on the electron density:

\[ \text{O}_2^+ + e^- \rightarrow \text{O} + \text{O} \left( ^1\text{D} \right). \]  

The ionised molecular oxygen is produced by the charge transfer reaction

\[ \text{O}^+ + \text{O}_2 \rightarrow \text{O}_2^+ + \text{O}. \]  

The amount of ionised oxygen and free electrons depends on the solar radiation. The most striking features of the airglow are the Meinel OH bands (Meinel et al. 1954), which dominate at red optical wavelengths and beyond (see Fig. 13, panel 4). The fundamental and overtone rotational-vibrational transitions are mainly produced by the Bates-Nicote (1950) mechanism

\[ \text{O}_3 + \text{H} \rightarrow \text{OH}^+ + \text{O}_2. \]  

Most emission originates in a relatively thin layer at 87 km. Finally, the upper state of the prominent D lines of neutral sodium at 589.0 and 589.6 nm (see Fig. 13, panel 2), which originate in a thin layer at 92 km, is probably excited by

\[ \text{NaO} + \text{O} \rightarrow \text{Na} \left( ^3\text{P} \right) + \text{O}_2 \]  
(Chapman 1939). NaO appears to be provided by

\[ \text{Na} + \text{O}_3 \rightarrow \text{NaO} + \text{O}_2. \]  

For studying airglow intensity and variability, we assigned the optical airglow lines to five classes, for which a similar variability is reasonable or could be proved by a correlation analysis (see Patat 2008). These classes are (1) green O I; (2) Na I D; (3) red O I; (4) OH; and (5) O2 (see Fig. 13). The first three classes correspond to atomic lines, the other two groups comprise molecular bands. The OI lines are divided into two classes. The green OI line at 557.7 nm mainly originates at altitudes slightly below 100 km, while the other significant OI lines (all being in the red wavelength range) tend to originate at altitudes greater than 200 km (see Khomich et al. 2008). Moreover, the kind

Fig. 13. Variability classes for airglow emission lines. The following groups are defined: (1) green O I; (2) Na I D; (3) red O I; (4) OH; and (5) O2. The weak lines (green curves) are scaled by a factor of 30 for Na I D, red O I, and O2, and a factor of 10 for OH.

4.3.2. Line variability

In the second part of this section, we investigate the variability of the airglow lines (Sect. 4.3.2). In the following, we treat airglow lines in detail. At first, the origin of the airglow line emission, the classification of lines, and a derivation of a line list for the sky model are discussed (Sect. 4.3.1). In the second part, we investigate the variability of airglow lines (Sect. 4.3.2).
of chemical reactions are also different, since the high altitude emissions are usually related to reactions involving ions (see above). Another small group consists of the sodium D lines and a weak K I line at 769.9 nm (see Fig. 13, panel 2). By far most of the airglow lines belong to the two classes of molecules which produce band structures by ro-vibrational transitions. The OH electronic ground state (X-X) bands with upper vibrational levels $v \leq 9$ cover the wavelength range longwards of about 0.5 $\mu$m with increasing band strength towards longer wavelengths. There are several electronic transitions with band systems for O₂ in the optical. Relatively weak bands of the Herzberg I (A-X) and Chamberlain (A’-a) systems originate at near-UV and blue wavelengths (see Cosby et al. 2006). At wavelengths longwards of 0.6 $\mu$m, the atmospheric (b-X) band system produces several strong bands. However, those bands related to the vibrational $v = 0$ level at the electronic ground state X are strongly absorbed in the lower atmosphere (see Sect. 4.1). Therefore, the only remaining strong band in the investigated wavelength range is O₂(b-X)(0–1) at about 864.5 nm (see Fig. 13, panel 5). Variability studies of O₂ have to rely on the results from this band. For the identification of airglow lines and as an input line list for the sky model, we use the list of Cosby et al. (2006). It consists of 2805 entries with information on the line wavelengths, widths, fluxes, and line identities. It is based on the sky emission line atlas of Hanuschik (2003), which was obtained from a total of 44 high-resolution ($\lambda \approx 45,000$) VLT UVES spectra. By combining different instrumental set-ups, the wavelength range from 0.314 to 1.043 $\mu$m could be covered. The accuracy of the wavelength calibration is better than 1 pm (cf. Sect. 4.1). The UVES spectra were flux calibrated by means of the Tüg (1977) extinction curve. Since the use of a point-source extinction curve for the airglow leads to systematic errors (see Sect. 4.1) and the La Silla extinction curve was used for Cerro Paranal, we corrected the line extinction by means of the Patat et al. (2011) extinction curve and the recipes given in Eqs. (24) and (25). At the lower wavelength limit, this caused an extreme correction factor of 0.37 and in the range of the O₂(b-X)(0–0) band a maximum factor of 4.5 due to the line molecular absorption correction (see Sect. 4.1). However, for the strongest 100 lines up to a wavelength of 0.92 $\mu$m, we only obtain a mean correction factor of 0.98. In a similar way as discussed in Sect. 4.2 for the Patat (2008) data, we considered how a different extinction curve affects the response curves for flux calibration. Here, we obtain for the 100 brightest lines another correction of 0.97, which is representative of the factors for the entire wavelength range, which range from 0.95 to 1.00. Due to a gap at about 0.86 $\mu$m, the Cosby et al. (2006) line list misses a part of the important O₂(b-X)(0–1) band. There is an unpublished UVES 800U spectrum related to the study of Hanuschik (2003) that covers the gap. We used this spectrum to measure the line intensities. Determined by a few overlapping lines, the resulting intensities were then scaled to those in the line list. For the line identification, we considered O₂ and OH line data from the HITRAN database (see Rothman et al. 2009). For the final line list for the sky model, the intensities of each variability class were scaled to match the mean value derived from the variability analysis (see below). Finally, the line wavelengths were converted from air to vacuum by

$$ \lambda_{\text{vac}} = m \times \lambda_{\text{air}}. $$

The refractive index

$$ n = 1 + 10^{-8} \left( \frac{8342.13}{130 - \sigma^2} + \frac{15997}{38.9 - \sigma^2} \right), $$

where $\sigma = \lambda^{-1}$ and $\lambda$ is in $\mu$m (Edlén 1966). This formula is also used internally in the sky model code if an output in air wavelengths is required (see Table 1).

### 4.3.2. Line variability

In general, airglow lines show strong variability on time scales ranging from minutes to years. This behaviour can be explained by the solar activity cycle, seasonal changes in the temperature, pressure, and chemical composition of the emission layers, the day-night contrast, dynamical effects such as internal gravity waves and geomagnetic disturbances (see Khomich et al. 2006). In order to consider airglow variability in our sky model, we derived a semi-empirical model based on 1186 VLT FORS 1 sky spectra (Patat 2008; see Sect. 4.2). The demands on an airglow variability model are twofold. First of all, it should include all major predictable variability properties. This excludes stochastic wave phenomena like gravity waves. Second, the derived parametrisation should be robust. For studying many variability triggers, about 1000 spectra is not statistically a high number. For this reason, only a few variables can be analysed. Since this neglection leads to higher uncertainties, an ideal set of parameters has to be found that provides statistically significant, predictable variations. For our airglow model, we studied the effect of solar activity, period of the year, and time of the night. The analysis was carried out for each of the five variability classes (see Fig. 13).

The first step for measuring the line and band fluxes was the subtraction of scattered moonlight, scattered starlight, and zodiacal light by using the recipes given in Sect. 3. The resulting spectra were then corrected for airglow continuum extinction as described in Sect. 4.1. For the flux measurements, continuum windows were defined. Their central wavelengths are listed in Table 3. The widths were 4 nm, except for 0.767 $\mu$m, where 0.3 nm was chosen to reduce the contamination by strong OH lines and the O₂(b-X)(0–0) band (see also Sects. 4.1 and 4.4). Then, the continuum fluxes were interpolated to obtain line and band intensities. The hydroxyl bands between 0.642 and 0.858 $\mu$m, i.e. OH(6–1) to OH(6–2), and the O₂(b-X)(0–1) band between 0.858 and 0.872 $\mu$m were measured automatically.

### Table 3. Airglow/residual continuum and its intensity variation relative to the reference wavelength 0.543 $\mu$m.

<table>
<thead>
<tr>
<th>$\lambda$ (nm)</th>
<th>$(\langle I \rangle - I_{0})$</th>
<th>$\sigma_{I}/I_{0}$</th>
<th>$\sigma_{I} / \langle I \rangle$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.535</td>
<td>0.369</td>
<td>0.92</td>
<td>0.13</td>
</tr>
<tr>
<td>0.575</td>
<td>0.387</td>
<td>0.71</td>
<td>0.17</td>
</tr>
<tr>
<td>0.615</td>
<td>0.420</td>
<td>0.69</td>
<td>0.10</td>
</tr>
<tr>
<td>0.655</td>
<td>0.450</td>
<td>0.70</td>
<td>0.11</td>
</tr>
<tr>
<td>0.695</td>
<td>0.480</td>
<td>0.79</td>
<td>0.11</td>
</tr>
<tr>
<td>0.735</td>
<td>0.510</td>
<td>0.70</td>
<td>0.09</td>
</tr>
<tr>
<td>0.775</td>
<td>0.543</td>
<td>0.70</td>
<td>0.00</td>
</tr>
<tr>
<td>0.815</td>
<td>0.575</td>
<td>0.71</td>
<td>0.15</td>
</tr>
<tr>
<td>0.855</td>
<td>0.608</td>
<td>1.40</td>
<td>0.20</td>
</tr>
<tr>
<td>0.895</td>
<td>0.642</td>
<td>1.18</td>
<td>0.19</td>
</tr>
<tr>
<td>0.935</td>
<td>0.675</td>
<td>1.14</td>
<td>0.13</td>
</tr>
<tr>
<td>0.975</td>
<td>0.702</td>
<td>1.32</td>
<td>0.21</td>
</tr>
<tr>
<td>1.015</td>
<td>0.767</td>
<td>1.64</td>
<td>0.46</td>
</tr>
<tr>
<td>1.055</td>
<td>0.820</td>
<td>2.57</td>
<td>0.67</td>
</tr>
<tr>
<td>1.095</td>
<td>0.858</td>
<td>3.56</td>
<td>1.06</td>
</tr>
<tr>
<td>1.135</td>
<td>0.872</td>
<td>3.76</td>
<td>1.12</td>
</tr>
</tbody>
</table>

Notes. The reference continuum intensity at 0.543 $\mu$m is 79.8 photons s$^{-1}$ m$^{-2}$ s$^{-1}$ arcsec$^{-1}$ or 4.27 $\text{R m}^{-1}$. The $\lambda$ values refer to the published models.
In a second iteration, this procedure was improved by subtracting the obtained O$_2$ bands from the OH bands and vice versa before the intensity measurement. This way, the contamination by undesired lines can be minimised. Apart from the bands, the lines [O I] 5577, Na I D, [O I] 6300, and [O I] 6364 were analysed. The continuum fit is very critical for these lines, because of the narrow width of the features and the significant contamination by OH lines. For this reason, the line measurements were also manually performed for a subsample of 15 spectra for each instrumental set-up. The results were then used to derive intensity-dependent correction functions for the automatic procedure. Finally, the resulting band and line fluxes were corrected for the discrepancy between the molecular absorption of continuum and lines (see Sect. 4.1). These corrections were usually very small, since the strongest lines of each class do not overlap with significant telluric absorption.

A variability model can be efficiently determined by deriving a reference intensity and then applying multiplicative correction factors for each variability parameter (cf. Khomich et al. 2008). As a reference value for each variability class, we define the mean intensity at zenith for the five solar cycles 19 to 23, i.e. the years 1954 to 2007. The zenith intensity can be estimated by a correction for the van Rhijn effect (Eq. (21)). The correction factors depend on the target zenith distance and the emission layer height (see Table 2). For describing the solar activity, we take the Penticton-Ottawa solar radio flux at 10.7 cm $S_{10.7\text{cm}}$ (Covington 1969; see also Sect. 4.2). For the defined period, we derive a mean flux of 129 sfu. We can also derive a mean $S_{10.7\text{cm}}$ for the spectroscopic sample. For this purpose, we obtained the monthly $S_{10.7\text{cm}}$ averages corresponding to each spectrum. Due to the delayed response of the Earth’s atmosphere regarding solar activity of up to several weeks (see e.g. Patat 2008), monthly values are more suitable than diurnal ones. In the end, a mean $S_{10.7\text{cm}}$ of 150 sfu could be derived for the entire FORS 1 data set. By performing a regression analysis for the relation between line intensity and $S_{10.7\text{cm}}$ for each line class, we were able to obtain correction factors for a scaling of the lines to intensities typical for the reference solar radio flux. The resulting mean fluxes for the different classes were used to correct the fluxes in the reference line list (see Sect. 4.3.1). To derive the scaling factors, we integrated over all the listed lines in a class that were measured in the spectra. This required adding up the OH intensities of all bands from (6–1) to (6–2) and summing up the fluxes of the [O I] 6300 and [O I] 6364 lines, which have a fixed 3:1 intensity ratio. The extinction-corrected Cosby et al. (2006) intensities had to be corrected by factors between 0.43 for the red O I lines and 1.06 for Na I D lines to reach the intensities for the reference conditions. These reference intensities are given in Table 2. They are slightly lower than those in Patat (2008) due to the lower mean solar radio flux.

The $S_{10.7\text{cm}}$-dependent linear fits to the airglow intensities (see also Patat 2008) are also used to parametrise a correction of solar activity for our sky model. Even though the parametrisation is reasonable (cf. Khomich et al. 2008), there may be systematic deviations for monthly $S_{10.7\text{cm}}$ beyond the data set limits of 95 and 228 sfu (see Sect. 4.2). With the dependence on solar radio flux removed, seasonal and nocturnal variations can be investigated. Since the intensity has a complex dependence on these parameters (see Khomich et al. 2008), we divided the data set into 6 seasonal and 3 night-time bins. In the same way as described in Sect. 2.1 for the transmission curves, the two-month periods start with the December/January combination. The night, as limited by the astronomical twilight, is always divided into three periods of equal length. This means that in winter the periods are longer than in summer. For the latitude of Cerro Paranal (see Sect. 1), the Dec./Jan. night bins are about 30% shorter than the Jun./Jul. bins. Due to the additional consideration of specific averages over the entire year and/or night, the total number of bins defined for the sky model is 28 (see also Table 1). Since the number of spectra in the individual bins differed by an order of magnitude, the average values over several bins could be biased. Therefore, all bins were filled with the same number of spectra by randomly adding spectra from the same bin, i.e. the data were cloned. This approach was also used for deriving the reference intensities. As a consequence, the mean solar radio flux of the data set changed from 153 (see Sect. 4.2) to 150 sfu. Finally, mean values and standard deviations were calculated for the individual and multiple bins using the original and bias-corrected data sets respectively. While the mean value provides an intensity correction factor for seasonal and/or night-time dependence, the standard deviation indicates the contribution of neglected variability components to the measured intensity. It also depends on the data quality, uncertainties in the analysis, and the accuracy of other sky model components. Therefore, the standard deviation of each bin should be an upper limit for the unmodelled airglow variability in the investigated data set.

The results of the airglow variability study are summarised in Table 2, and Figs. 14 and 15. The solar activity strongly influences the intensities of O I and O$_2$, where the slopes are 0.0063 to 0.0087 sfu$^{-1}$. On the other hand, weak or no significant correlations are present for sodium and hydroxyl. These findings are in qualitative agreement with the relations given in Khomich et al. (2008), who provide 0.0025 to 0.0060 sfu$^{-1}$ for the first and about 0.0015 sfu$^{-1}$ for the second group from measurements at different observing sites (mainly in the northern hemisphere). The relatively low value of 0.0025 sfu$^{-1}$ for the green O I line compared to 0.0087 sfu$^{-1}$ from our model is not critical. A more precise latitude-dependent analysis of satellite-based data by Liu & Shepherd (2008) resulted in 0.0065 sfu$^{-1}$ for the latitude range from $-20^\circ$ to $-30^\circ$. For $-30^\circ$ to $-40^\circ$, they even obtain the same slope as in our model. The discrepancies in the results from literature show that quantitative comparisons are difficult with different observing sites, observing periods, instruments, and analysis methods. Solar activity directly affects the Earth’s atmosphere by the amount of hard UV photons. The higher the photon energy, the more the production rate depends on solar activity (see Nicolet 1989). This relation appears to be important for O I and O$_2$ airglow emission, which depends on the dissociation or ionisation of molecular oxygen by hard UV photons (see Sect. 4.3.1).

Significant dependence on the bimonthly period is found for all line classes (see Fig. 14). Na I D and the red O I lines indicate the strongest variability with a maximum intensity ratio of 3.4 and 5.0 respectively, whereas OH shows the weakest dependence with a ratio of 1.4 (see Table 2). Except for OH, the maximum is reached in the autumn months April and May. For the atomic lines, the minimum arises in Dec./Jan., and for the molecular bands, it appears to be in Aug./Sep. The variations found reflect the semi-annual oscillations of the airglow intensity (cf. Patat 2008), which are characterised by two maxima and minima of different strength per year. Complex empirical relations based on long-term observations at many observing sites as given by Khomich et al. (2008) can be used to estimate this intensity variation. However, since these relations depend on rough interpolations and extrapolations, they can only provide a coarse variability pattern for an arbitrary location on Earth. Nevertheless, these relations confirm the amplitude of the variations and the rough
positions of the maxima and minima. For example, the peak-to-peak ratios for green O I, Na I D, and OH are 1.4, 3.8, and 1.3, which agrees well with the sky model values 1.7, 3.4, and 1.4 (see Table 2). Apart from the obvious change of the incident solar radiation, the seasonal variations are related to changes in the layer heights of the atmospheric constituents, changes in the temperature profiles, and the dynamics of the upper atmosphere in general.

Averaged over the year, the dynamical range of the night-time variations is in the order of 20 to 30%, which is distinctly smaller than the seasonal variations. Only the red O I lines show a clear decrease by a factor of 1.4 from the beginning to the end of the night. Usually, the diurnal variations are the largest in airglow intensity with possible amplitudes of several orders of magnitude (see Khomich et al. 2008). Since we exclude daytime and twilight conditions with direct solar radiation, the variability is much smaller. However, an investigation with the unbinned data (see also Patat 2008) and results from photometric studies (Mattila et al. 1996; Benn & Ellison 1998; Patat 2003) confirm the absence of strong trends. Averaging over all bimonthly periods appears to cancel part of the variability. This is illustrated in Fig. 15, which shows the bimonthly dependence of the airglow intensity for each third of the night.

The residual statistical variations of the airglow model, as depicted in Fig. 14, are mainly between 20 and 50% for the lines originating in the mesopause region. The smallest uncertainties are found for OH in summer, whereas the ionospheric O I lines indicate very strong unpredictable variations with an amplitude comparable to the intensity itself (see also Patat 2008). This behaviour is caused by the aurora-like intensity fluctuations from geomagnetic disturbances. This effect is particularly important for Cerro Paranal, because of its location close to one of the two active regions about 20° on either side of the geomagnetic equator (Roach & Gordon 1973).

### 4.4. Airglow continuum

The airglow continuum is the least understood emission component of the night sky. In the optical, the best-documented process is a chemiluminescent reaction of nitric oxide and atomic oxygen in the mesopause region as proposed by Krassovsky (1951):

\[
\text{NO} + \text{O} \rightarrow \text{NO}_2 + h\nu \\
\text{NO}_2 + \text{O} \rightarrow \text{NO} + \text{O}_2.
\]

\[\text{(37)}\]
\[\text{(38)}\]
This reaction appears to dominate the visual and is expected to have a broad maximum at about 0.6 μm (see Sternberg & Ingham 1972; von Savigny et al. 1999; Khomich et al. 2008). Reactions of NO and ozone could be important for the airglow continuum at red to near-IR wavelengths (Clough & Thrush 1967; Kenner & Ogryzlo 1984). In particular, the reaction

\[ \text{NO} + \text{O}_3 \rightarrow \text{NO}_2 + \text{O}_2 \]  

(39)
is expected to significantly contribute to the optical by continuum emission with a broad maximum at about 0.85 μm (Kenner & Ogryzlo 1984; Khomich et al. 2008). Finally, a pseudo continuum by molecular band emission produced by

\[ \text{Fe} + \text{O}_3 \rightarrow \text{FeO}^* + \text{O}_2 \]  

(40)

(West & Broida 1975) could be an important component of the continuum between 0.55 and 0.65 μm (Jenniskens et al. 2000; Evans et al. 2010; Saran et al. 2011).

The airglow continuum was analysed in a similar way as the airglow emission lines. As reported in Sect. 4.3.2, the derivation of line intensities already required the measurement of airglow continuum fluxes in suitable windows (see Table 3). These results were refined by subtracting possible contributions from airglow lines by applying the line emission model as described in Sect. 4.3. For the variability analysis, the Patat (2008) data set (see Sect. 4.2) was restricted to the 874 FORS 1 spectra, where the Moon was below the horizon. This avoids large errors in the continuum flux from the subtraction of a bright and uncertain component (see Sect. 3.1). Even though the absolute uncertainties of the other components are significantly smaller, the derived continuum is a residual continuum. It is affected by uncertainties in zodical light brightness, scattered starlight, airglow line emission, molecular absorption, possible unconsidered minor components, scattered light from dispersive elements, and flux calibration of the spectra. While the other sky model components should cause an uncertainty in the order of a few per cent only (for 0.767 μm this could be somewhat higher, see Sect. 4.3.2), the uncertainty in the flux calibration could be significantly more. Since theoretical components are subtracted from the observed spectra to obtain the airglow continuum, errors in the flux calibration have a larger effect on the resulting continuum than on the total spectra. For example, for a 50% contribution of the continuum to the total flux, a flux error of 10% would convert into a continuum error of 20%.

For the subsequent analysis, we defined a reference continuum wavelength. Due to its availability in all spectroscopic modes and the absence of contaminating emission lines, we selected 0.543 μm. In the following, we studied the continuum relative to this wavelength, i.e. the mean continuum was derived by scaling the fluxes to the reference solar radio flux of 129 sfu.

\(^7\) This effect can cause line profiles with wide Lorentzian wings (see Ellis & Bland-Hawthorn 2008). However, we did not detect significant wings in the profiles of the strong airglow lines or lines in the wavelength calibration lamp spectra. In view of the relatively low contrast between lines and continuum for our spectra (cf. the near-IR regime), we can conclude that a possible continuum contamination of more than a few per cent is unlikely, even at the reddest wavelengths.
Fig. 16. Airglow/residual continuum (solid line) and its variability (dashed line) relative to the reference wavelength 0.543 μm.

(see Sect. 4.3.2) by using only the linear regression results and binning corrections derived for 0.543 μm. This approach means that a fixed shape of the continuum is assumed. This simplification of the model can be more easily used in the sky model. As shown by the last column of Table 3, there are relatively low variations of the continuum flux relative to the reference flux for the investigated data set. For most wavelengths, the standard deviation divided by the mean flux $\sigma_f/\langle f \rangle$ is lower than 20% and only reaches 30% at the reddest wavelengths. In view of all the uncertainties discussed above, which also contribute to these numbers, the assumption of a fixed continuum slope is sufficient for an application of the ETC sky background model. This assumption is also supported by the high correlation factors for different continuum windows measured by Patat (2008). It should be noted that the number of available spectra decreases towards the margins in the analysed spectral range due to the different instrumental set-ups (see Sect. 4.2). In particular, wavelengths shorter than 0.44 μm have only 239 spectra, i.e. 27% of the sample used for 0.543 μm. The change in the sample size as well as different systematic errors in the response curves for the different set-ups cause systematic uncertainties in the airglow continuum shape. By comparing the mean fluxes in overlapping wavelength regions of the different set-ups, we estimate an uncertainty in the order of 10%.

We obtained a mean airglow continuum for Cerro Paranal with an intensity of about 4.3 R nm$^{-1}$ at 0.543 μm (for Rayleigh units see Table 2). The corresponding variability is 1.6 R nm$^{-1}$. Considering the latitude of Cerro Paranal, this result is in good agreement with observations that suggest an increase of the airglow continuum from 1–2 R nm$^{-1}$ at the equator to 10–20 R nm$^{-1}$ in the polar region for similar wavelengths (see Davis & Smith 1965; Khomich et al. 2008). As illustrated in Fig. 16 and listed in Table 3, the mean airglow continuum is characterised by a broad bump at about 0.6 μm and an increase in intensity towards longer wavelengths with a steep slope at about 0.8 μm. The continuum in the bump region appears to be mainly produced by two processes: a relatively smooth NO + O continuum (see Eq. (37)) and a more structured Fe + O$_2$ continuum (see Eq. (40)) showing a peak at about 0.6 μm (see Evans et al. 2010). If the bump, which indicates a width of about 0.1 μm, could be completely explained by the iron oxide reaction, this component would contribute up to 1/3 of the mean airglow continuum flux (see also Sect. 5.1). Towards longer wavelengths, it is not clear whether the observed increase in intensity is mainly caused by relatively narrow peaks or a smooth increase (see Sternberg & Ingham 1972; Sobolev 1978; Content 1996). Up to 0.872 μm, our measurements suggest a monotonic increase beyond the 0.6 μm bump. Intensities of about 15 R nm$^{-1}$, as found by Sternberg & Ingham (1972) and Sobolev (1978) at wavelengths longwards of 0.8 μm, are in good agreement with our mean spectrum, with the same intensity at about 0.86 μm. Also, the intensities of Sternberg & Ingham (1972) and of the sky model mean airglow continuum are very similar at our reference wavelength in the V band. A possible production mechanism for the strong increase at about 0.8 μm could be a reaction of nitric oxide with excited ozone (see Eq. (39)), for which a peak wavelength of about 0.85 μm is expected (see Kenner & Ogryzlo 1984; Khomich et al. 2008).

Then, the strong intensity increase would be the blue wing of the bump from this reaction. The slope does tend to decrease where the peak is predicted, and the continuum variations there relative to 0.543 μm (see $\sigma_f/\langle f \rangle$ in Table 3) are the highest. This could be another argument for different chemical processes producing the emissions at 0.55 and 0.85 μm.

As in the case of the airglow lines, the intensity of the sky model airglow continuum measured at 0.543 μm depends on zenith distance, solar radio flux, period of the year, and period of the night. The results are shown in Table 2, and Figs. 14 and 15. The dependence of the continuum emission on solar radio flux is significant and comparable to O1 (green and red) and O$_2$. Since OH does not indicate a significant dependence on S$10.7\text{cm}$, the continuum must be the main source for the dependence of the broad-band fluxes on solar activity (cf. Walker 1988; Patat 2003, 2008). Concerning the seasonal and nocturnal variations, the continuum at 0.543 μm tends to show the best agreement with OH, i.e. the variability of these parameters is relatively low. The maximum ratio of the bimonthly mean intensities is only about 1.5 (cf. Patat 2008).

5. Discussion

After describing all the optical model components in the previous sections, we now discuss the quality of the sky model as a whole by comparing it to the Patat (2008) data set of sky spectra and results found in the literature. First, sky model spectra and observed spectra are compared (Sect. 5.1). Second, a systematic quality evaluation by means of broad-band photometry of our model with data, and a comparison to the night-sky brightnesses from the literature are discussed in Sect. 5.2. Finally, we evaluate the improvements achieved by our sky model compared to the current ESO ETC sky background model in the optical (Sect. 5.3).

5.1. Comparison of spectra

In order to evaluate the quality of our sky model, spectra were computed for the different instrumental set-ups and observing conditions of the Patat (2008) data set (see Sect. 4.2). A detailed description of the sky model input parameters can be found in Table 1. Before the full data set is discussed, we show a few typical sky model spectra in comparison with the corresponding observed spectra (Figs. 17 to 19).

In the optical, the relevant sky model components are scattered moonlight, scattered starlight, zodiacal light, and airglow lines and continuum of the upper atmosphere (see Fig. 1). Figure 17 compares a typical FORS 1 spectrum exhibiting moderate Moon contribution to the corresponding sky model. This
Fig. 17. Comparison of the sky model (upper panel: thick black line) and an observed FORS 1 300V spectrum (thin red line) with moderate lunar contribution (see Table 1). The uncertainty of the sky model due to airglow variability is also shown (green). The lower panel exhibits the ratio of the sky model and the observed spectrum.

Fig. 18. Comparison of the sky model and an observed FORS 1 300V spectrum with strong lunar contribution. For an explanation of the different curves, see Fig. 17.

and the FORS 1 spectra of the other figures were taken with the 300V grism without order separation filter. This set-up provides the maximum wavelength range. Due to the missing order separation filter, there can be a slight (≤10%) contamination by the second order spectrum at red wavelengths. However, this does not affect the quality of the sky model (see Sect. 5.2), because of the small number of spectra used in the analysis. Figure 17 demonstrates that the different sky model components agree reasonably well with the observed spectrum. Apart from the reddest part of the spectrum, deviations of 10 to 20% are typical. The best agreement is found for the continuum in the visual. Residuals of strong sky lines in the ratio plot in the lower panel appear more prominent than the real values due to slight differences in the instrumental profiles of the model and the observed spectrum.

Figure 18 shows the effect of a strong Moon contribution on the sky model. Scattered moonlight dominates the continuum at all wavelengths in the displayed range. At blue wavelengths, the example spectrum reaches up to 2000 photons s\(^{-1}\) m\(^{-2}\) μm\(^{-1}\) arcsec\(^{-2}\). In contrast, during moonless nights the values are about one order of magnitude lower (see Fig. 19). Even though the deviations between the sky model and the observed spectrum are not larger than 10% for most of the continuum, there is a systematic trend. For a wide wavelength range, the sky model appears to be too bright by a relatively constant factor. Apart from deviations of the Moon illuminance from the model in Eq. (15), this discrepancy could be explained by uncertainties in the Mie scattering model, since this changes slowly with wavelength (see Fig. 2). Moreover, the angular distance between Moon and target ρ = 44° is small enough for significant Mie scattering. Similar trends with positive as well as negative deviations are observed in other cases of high lunar sky brightness. As already mentioned in Sect. 3.1, the amplitude of the differences tends to increase for decreasing ρ. Nevertheless, the uncertainties of the extended Krisciunas & Schaefer (1991) model are usually not critical for spectra with low to moderate lunar contribution, as it is illustrated in Fig. 17.

A spectrum without scattered moonlight is shown in Fig. 19. In this case, the continuum is mainly a combination of zodiacal light and airglow continuum. Scattered starlight only adds a few per cent to the total continuum emission. In the B and V bands, the continuum of dark-time exposures is usually well reproduced by the sky model. At longer wavelengths, the uncertainties increase from the significant (and partly unpredictable) variability of the airglow continuum and the simplifying assumption of a fixed continuum shape (see Sect. 4.4). The three spectra
shown indicate deviations between 20 to 40% at about 0.82 μm. By chance, the sky model is brighter than the observed spectrum in all cases. Airglow emission lines can vary significantly, depending on the line class, observing direction, solar activity, season, and time of night. Even though there is always a stochastic component, which cannot be modelled, the sky model accounts for such variations quite well. The uncertainty of the line modelling for the spectra shown is in the order of 20%. The systematic errors in the model intensities. The standard deviation of the magnitude differences between the model and observed data σ_m, shown in the middle panel of Fig. 20, indicates an interesting wavelength dependence. For the dark-time sample, the continuum uncertainty ranges between 0.16 and 0.24 mag. Including observations with scattered moonlight increases these values to 0.19 and 0.28 mag. The additional variation is mainly caused by a few spectra with large uncertainties in the Mie scattering of moonlight (see above). These results suggest that the relative strong continuum deviations at 0.82 μm, as in Figs. 17 and 19, are relatively high compared to the entire sample. The spectrum of σ_m shows a relatively broad feature at about 0.6 μm, which is reminiscent of the shape of the FeO pseudo continuum (see Jenniskens et al. 2000; Evans et al. 2010; Saran et al. 2011). This result supports the assumption that the airglow continuum bump at 0.6 μm (see Fig. 16) is mainly produced by iron oxide (see Sect. 4.4) and varies different from the underlying NO2 continuum, for which the intensity changes at 0.543 μm are considered by the sky model. Figure 20 indicates a FeO-related variability of about 15%. Since the mean bump contributes about 20% of the total flux at 0.6 μm, the variation is almost comparable to it. These strong variations are in agreement with previous results (see Evans et al. 2010; Saran et al. 2011). A minor source of continuum variability at 0.6 μm is the Chappuis ozone bands (see Fig. 2), which indicate a variation of 0.02 mag airmass⁻¹ (see Patat et al. 2011). The middle panel of Fig. 20 does not exhibit strong signatures of OH bands (see Fig. 13, panel 4). The bands are clearly detectable only in the range of low continuum uncertainty. Consequently, the quality of the OH modelling is comparable or even better than the continuum modelling. This is particularly important for the quality of the full sky model at long wavelengths, where OH emission dominates the spectra. The sky model is less able to model atomic lines, as shown in Fig. 20. The maximum variability of 0.7 mag is found at [OI] 6300. In addition, other lines of the thermospheric ionosphere, which are usually difficult to recognise (see Patat et al. 2011), significantly contribute to σ_m. For example, N1 at 520 nm and O1 at 616, 656, and 777 nm are clearly detectable. This confirms the conclusion of Sect. 4.3.2, stating that the intensities of ionospheric lines are difficult to predict due to their sensitivity to geomagnetic disturbances (see Roach & Gordon 1973).

5.2. Comparison of photometry

To perform a more quantitative comparison of our sky model and observed data, and for an easier comparison to other studies, we derived magnitudes from broad-band filter fluxes. Specifically, we used the standard photometric system consisting of U, B, V, R, and I (see Bessell 1990). For the Patat (2008) data and their corresponding sky models, only a grism-dependent subset of filters can be taken. The spectrum needs to cover greater than 90% of the filter curve. An exception is the U filter, which extends below 0.365 μm, the lower wavelength limit of the bluest spectral set-up (see Sect. 4.2). Therefore, the results for this filter are questionable.

Figure 21 and Table 4 show the results of the computations for the full sample of FORS 1 spectra and a subsample with the Moon below the horizon (cf. Sect. 5.1). Only a small fraction in the upper panel of Fig. 20 suggests that the model quality is similar at all wavelengths. As already discussed in Sect. 4.4, the real accuracy of the model also depends on the quality of the flux calibration of the Patat (2008) data. The uncertainties can be in the order of 10%, and so this appears to be the main source of systematic errors in the model intensities.

![Figure 20](image-url)

**Fig. 20.** Deviations between the sky model and the observed FORS 1 spectra in magnitudes. The mean magnitude difference (upper panel), the standard deviation (middle panel), and the wavelength-dependent number of considered spectra (lower panel) are shown for 1 nm bins. Results for the full spectroscopic data set (red) and for spectra with the Moon below the horizon (black) are displayed.
Fig. 21. Histograms for the deviations of the sky model from the FORS 1 data in mag for the filters $U$, $B$, $V$, $R$, and $I$. The filled histograms show only data with the Moon above the horizon.

($\sim 1/4$) of the spectra contribute to the mean values and standard deviations of the $U$ and $B$ filters. Most spectra cover the range of the $V$, $R$, and $I$ filters. For both samples and all filters, the mean magnitude differences are small ($\lesssim 0.05$ mag). Even though the sky model tends to be slightly fainter at the blue end and slightly brighter at the red end, there are no serious systematic deviations from the observed spectra (cf. Sect. 5.1). The standard deviations $\sigma_{\Delta m}$ are relatively similar for the different filters. For the full sample, they range from 0.19 mag for the $V$-band to 0.24 mag for the $I$ band. Consequently, the accuracy of the sky model is in the order of about 20%. These values can be compared to the magnitude variations in the measured data $\sigma_{\Delta m,\text{obs}}$ which correspond to $\sigma_{\Delta m}$ for an optimum sky model of time-invariant flux. For the full sample, the deviations are distinctly larger. They range from 0.37 to 0.56 mag. These large deviations are mainly due to the observations with a strong moonlight contribution (see Sect. 3.1). For dark-time conditions, $\langle \Delta m \rangle$ ranges from 0.17 mag for $B$ to 0.21 mag for $U$, and $\sigma_{\Delta m}$ indicates differences between 0.18 mag for $B$ and 0.29 mag for $I$. In particular, for the bands $V$ to $I$, a time-invariant sky model would be significantly worse than our sky model (see also Sect. 5.3). This shows the improvements from a variable zodiacal light, airglow lines, and airglow continuum model.

Finally, we compare the sky model to literature data. Magnitudes in the five broad-band filters $U$ to $I$ were calculated using standardised observing conditions. Specifically, zenith, new Moon, ecliptic pole, annual average, and mean solar activity, i.e. 130 sfu (see Sect. 4.3.2), were assumed. The resulting magnitudes are provided in Table 5. For a better comparison with published data, the table also contains sky model results for 90 and 180 sfu. The reference data in Table 5 originate from Mattila et al. (1996) for La Silla, Walker (1987) and Krisciunas et al. (2007) for Cerro Tololo, Benn & Ellison (1998) for La Palma, and Patat (2003, 2008) for Cerro Paranal. In general, there is a good agreement between the sky model and observed sky brightnesses. By comparing magnitudes with similar average solar radio fluxes, we find typical deviations in the order of 0.1 mag. An exception is the $U$ filter with typical differences of about 0.3 mag, which could be explained by the lower quality of the sky model at near-UV wavelengths due to the lack of data (see Sect. 4.2). Also, it is not clear to what extent components like zodiacal light or scattered starlight, which significantly affect short wavelengths, contribute to the observed data. The corresponding intensities can differ from those of the sky model for the assumed ideal conditions. The published photometry appears to confirm the lack of reproducibility of $U$-band magnitudes. Unexpectedly, the sky brightness seems to increase with decreasing solar activity. It should be noted that photometric samples are often too small to cover all of the airglow variability, which causes additional uncertainties. For the airglow continuum, which is a major contribution to the night-sky brightness in the optical, the intensity significantly depends on the geographic latitude (see Davis & Smith 1965). In summary, we can assume that our sky model calculates reliable night-sky brightnesses, at least for the levels of solar activity that could be analysed.

A comparison of the sky model with other studies can also be enlightening in terms of the night-sky variability, particularly the striking dependence of the sky brightness on solar activity (Walker 1988; Mattila et al. 1996; Krisciunas 1997; Patat 2003, 2008). For the range of photometric fluxes in $UV$ under dark-time conditions at zenith, Patat (2008) found 0.9, 1.3, and 1.7 mag. For the same filters, he estimated a flux increase of 0.6, 0.3, and 0.2 mag for a change in the solar radio flux from 80 to 240 sfu. In contrast, Walker (1988) gives $\Delta B \approx 0.8$ mag and $\Delta V \approx 1.0$ mag for a similar solar activity change. About 0.5 mag are reported by Mattila et al. (1996) for blue wavelengths and by Krisciunas et al. (1997) for the $V$ band. For a typical brightness of the zodiacal light of 1.7 times the intensity at the ecliptic pole and the same range of solar radio fluxes as used by Patat (2008), the sky model gives 0.7, 0.5, 0.6, 0.6, and 0.3 mag for the $UBVRI$ filters. These values are consistent with the results from the other studies. The significant discrepancy of 0.3 mag to the Patat (2008) result for the $V$ filter might be explained by the relative small sample of only 148 images and the general difficulties in separating the different sky radiation components by means of photometric data. For $B$ to $R$, the solar activity appears to be responsible for about half the night-sky variability. Since the zodiacal light variations cause a $1\sigma$ uncertainty of about 0.1 mag, as estimated from the FORS 1 data set, seasonal, nocturnal, and unpredictable short-term airglow variations should generate most of the remaining variability in $V$ and the adjacent bands.

5.3. Comparison to current ETC sky model

The main motivation for this study is to achieve a significant improvement over the current ESO ETC for a more efficient use of the VLT time. As discussed in Sect. 1, the current sky emission model for optical instruments consists of the Moon phase dependent, photometric sky brightness table of Walker (1987) and an instrument-specific template spectrum scaled to the flux in

<table>
<thead>
<tr>
<th>Filter</th>
<th>N</th>
<th>(\langle \Delta m \rangle)</th>
<th>(\sigma_{\Delta m})</th>
<th>(\langle \Delta m_{\text{obs}} \rangle)</th>
<th>(\sigma_{\Delta m,\text{obs}})</th>
<th>N</th>
<th>(\langle \Delta m \rangle)</th>
<th>(\sigma_{\Delta m})</th>
<th>(\langle \Delta m_{\text{obs}} \rangle)</th>
<th>(\sigma_{\Delta m,\text{obs}})</th>
</tr>
</thead>
<tbody>
<tr>
<td>U</td>
<td>303</td>
<td>-0.053</td>
<td>0.230</td>
<td>-0.113</td>
<td>0.725</td>
<td>239</td>
<td>-0.042</td>
<td>0.213</td>
<td>0.214</td>
<td>-0.059</td>
</tr>
<tr>
<td>B</td>
<td>303</td>
<td>-0.046</td>
<td>0.205</td>
<td>+0.269</td>
<td>0.430</td>
<td>239</td>
<td>-0.048</td>
<td>0.174</td>
<td>0.182</td>
<td>+0.196</td>
</tr>
<tr>
<td>V</td>
<td>979</td>
<td>0.000</td>
<td>0.192</td>
<td>+0.356</td>
<td>0.409</td>
<td>727</td>
<td>+0.006</td>
<td>0.175</td>
<td>0.255</td>
<td>+0.244</td>
</tr>
<tr>
<td>R</td>
<td>1046</td>
<td>+0.009</td>
<td>0.199</td>
<td>+0.169</td>
<td>0.365</td>
<td>762</td>
<td>+0.009</td>
<td>0.177</td>
<td>0.260</td>
<td>+0.083</td>
</tr>
<tr>
<td></td>
<td>839</td>
<td>-0.003</td>
<td>0.238</td>
<td>0.365</td>
<td>0.413</td>
<td>326</td>
<td>-0.004</td>
<td>+0.008</td>
<td>+0.188</td>
<td>0.295</td>
</tr>
</tbody>
</table>

Notes. Mean values \(\langle \Delta m \rangle\) and standard deviations \(\sigma_{\Delta m}\) for magnitude differences between the model and observed data \(\Delta m = m_{\text{model}} - m_{\text{obs}}\) and standard deviations of the magnitudes of the observed data \(\sigma_{\Delta m,\text{obs}}\) are shown. Moreover, mean values \(\langle \Delta m_{\text{obs}} \rangle\) and standard deviations \(\sigma_{\Delta m,\text{obs}}\) for magnitude differences between the Moon phase related data of Walker and the Patat data are displayed. Results are listed for the full and dark-time samples. The number of spectra involved is indicated by \(N\).

Table 5. Typical sky model and literature night-sky brightnesses in mag arcsec\(^{-2}\) for zenith, no Moon, faint zodiacal light, and different solar radio fluxes.

<table>
<thead>
<tr>
<th>Source</th>
<th>Site</th>
<th>(S_{10.7,\text{cm}})</th>
<th>U</th>
<th>B</th>
<th>V</th>
<th>R</th>
<th>I</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benn &amp; Ellison (1998)</td>
<td>La Palma</td>
<td>80</td>
<td>22.0</td>
<td>22.7</td>
<td>21.9</td>
<td>21.0</td>
<td>20.0</td>
</tr>
<tr>
<td>Walker (1987)</td>
<td>Cerro Tololo</td>
<td>90</td>
<td>22.0</td>
<td>22.7</td>
<td>21.8</td>
<td>20.9</td>
<td>19.9</td>
</tr>
<tr>
<td>Krisicunas et al. (2007)</td>
<td>Cerro Tololo</td>
<td>130</td>
<td>22.1</td>
<td>22.8</td>
<td>21.8</td>
<td>21.2</td>
<td>19.9</td>
</tr>
<tr>
<td>Mattila et al. (1996)</td>
<td>La Silla</td>
<td>150</td>
<td>22.4</td>
<td>22.8</td>
<td>21.7</td>
<td>20.8</td>
<td>19.5</td>
</tr>
<tr>
<td>Sky model(^a)</td>
<td>Cerro Paranal</td>
<td>90</td>
<td>22.3</td>
<td>22.9</td>
<td>22.0</td>
<td>21.2</td>
<td>19.8</td>
</tr>
<tr>
<td></td>
<td></td>
<td>130</td>
<td>22.1</td>
<td>22.8</td>
<td>21.8</td>
<td>21.0</td>
<td>19.7</td>
</tr>
<tr>
<td></td>
<td></td>
<td>180</td>
<td>21.9</td>
<td>22.6</td>
<td>21.6</td>
<td>20.9</td>
<td>19.6</td>
</tr>
</tbody>
</table>

Notes. \(^a\) Solar radio flux measured at 10.7 cm in sfu. \(^b\) See Table 1 for model parameters.

the photometric filter closest to the centre of a given spectral setting. It does not consider any change in the relative contributions of the different sky emission components, which can be quite strong as discussed in the previous sections. Thus, we can expect that the model continuum level significantly deviates from the true one, even if the corresponding filter flux is correct. Our new sky model with variable model components is an important improvement.

For a more quantitative comparison of the current and our new sky model, we derived the Walker (1987) magnitudes for the observing conditions of the Patat (2008) FORS 1 data set (see Sect. 4.2). The resulting \(U\) to \(I\) magnitudes can be compared to the measured ones to analyse the quality of the two models (see also Sect. 5.2). Table 4 exhibits the mean deviation of the Walker model \(\langle \Delta m_{\text{obs}} \rangle\) and the standard deviation of the difference \(\sigma_{\Delta m,\text{obs}}\) for the full and the dark-time sample. Since the Walker magnitudes depend on the Moon phase, one can expect that the model based on his data set would have a lower scatter than an optimum time-invariant model given by \(\sigma_{\Delta m,\text{obs}}\). Except for the \(U\) band, which is difficult to compare (see Sect. 5.2), this is true. For the full data set, the standard deviations are lower by 0.04 \((I)\) to 0.15 mag \((V)\). However, this improvement is small compared to the corresponding results for our sky model. For the \(B\) and \(V\) bands \(\sigma_{\Delta m,\text{obs}}\) is more than twice as large as \(\sigma_{\Delta m}\). Moreover, there are significant systematic mean deviations of 0.1 to 0.4 mag. For our sky model, the maximum value is 0.05 mag. Even though this benefit from the use of the same data for the derivation of the airglow line and continuum model, the offset with the Walker model is striking. It can be explained by the fact that the Moon phase is the only variable parameter. Therefore, the systematic changes of other parameters can cause significant magnitude offsets. For example, the fainter magnitudes of the Walker model can partly be explained by the very low solar activity (about 90 sfu), whereas the Patat (2008) data set has a mean solar radio flux of 153 sfu.

The dark-time data provided by Table 4 show a decrease of \(\sigma_{\Delta m,\text{obs}}\) by 0.02 \((B)\) to 0.08 mag \((R)\) compared to the values for the full sample. Excluding the \(U\) band, the typical scatter of the Walker model is about 0.3 mag. This is worse than the results for our sky model and even a time-invariant model. For the \(B\) band, the difference is more than 0.2 mag. For the \(I\) band, the situation is better, since the Walker model almost reaches the standard deviation of the time-invariant model. Nevertheless, \(\sigma_{\Delta m,\text{obs}}\) of our sky model is still about 0.1 mag lower. The unsatisfactory performance of the Walker model is caused by the unconsidered, varying amount of scattered moonlight during a Moon phase. Even for phases close to full Moon, dark-time observations are possible. For this reason, the scatter of the Walker model is larger than for a time-invariant model. The difference depends on the average contribution of scattered moonlight to the sky brightness, which is higher at shorter wavelengths. This effect causes an overestimation of the sky brightness for dark-time observations, which is indicated by a comparison of \(\langle \Delta m_{\text{obs}} \rangle\) for the full and dark-time samples.

In summary, we can state that our sky model performs better than the current ESO ETC sky model for the optical by about several tenths of a magnitude. The quality difference should be even higher for a single wavelength instead of a broad-band filter. Even if the input parameters of our new sky model (see Table 1) could not optimally be constrained in the planning phase, due to uncertainties in the scheduling of the observations, there would be a significant improvement for the prediction of the signal-to-noise ratio for astronomical observations. This justifies the effort in developing an advanced sky model.
6. Summary and outlook

In this paper, we presented a sky model for the ESO observing site at Cerro Paranal to help predict the effects of the Earth’s atmosphere on astronomical observations in the optical. This sky model includes atmospheric extinction, scattered moonlight, scattered starlight, zodiacal light, and airglow emission lines and continuum.

- The atmospheric extinction is characterised by three components: Rayleigh scattering, aerosol extinction, and molecular absorption. For the former, we use the formula given by Liou (2002). The aerosol extinction is based on the parametrisation of Patat et al. (2011) for Cerro Paranal. The molecular absorption is calculated by the radiative transfer code LBLRTM for atmospheric profiles optimised for the observing site.
- Scattered moonlight is derived from the Krisciunas & Schaefer (1991) model for the V band, which is extrapolated for the entire optical range using the solar spectrum and the Cerro Paranal extinction curve.
- For scattered starlight, a mean spectrum was derived by 3D single scattering calculations with multiple scattering corrections, using the Toller (1981) integrated starlight distribution and the mean spectrum of Mattila (1980).
- The zodiacal light is computed based on the model given by Leinert et al. (1998). Scattering of the zodiacal light in the Earth’s atmosphere is also treated with 3D scattering calculations.
- Airglow emission lines and continuum are highly variable. We used a set of 1186 VLT FORS 1 sky spectra (Patat 2008) taken during a wide range of conditions to parametrise a model for five line and one continuum variability classes. The line wavelengths and intensities are based on the atlas of Hanuschik (2003), improved by the results of the variability analysis. For the airglow scattering, 3D calculations were used as well.

After summing over all the components, we then compared the sky model with observed sky spectra. We found that our model is accurate to about 20%. This could only be achieved by having variable model components, especially the airglow model, which is a significant improvement over previous models. The mean sky brightnesses and variations derived from our model are in good agreement with results from other photometric studies. Compared to the current ETC sky model, the accuracy is increased by several tenths of a magnitude.

There are new results from this sky model study:

- We found scattering scaling relations for the extended radiation sources zodiacal light and airglow. These are new simple relations to derive effective extinction curves. The corresponding correction factors for the point-source extinction curve only depend on the unextinguished line-of-sight intensity of the radiation source.
- We characterised the variability of the airglow line and continuum emission at Cerro Paranal based on several input parameters, such as period of the year, time of night, and solar radio flux.
- We derived long-term mean airglow line and continuum intensities. For the latter, we benefit from the modelling of the intensity of the other sky model components. We could determine the shape of the optical airglow continuum with high accuracy. For the controversial wavelength range longwards of 0.7 μm, we find a smooth intensity increase. This could be produced by chemical reactions different from those dominating the shorter wavelengths. The well-known peak at 0.6 μm was identified as strongly varying.

The model presented in this paper is aimed at the ETC for optical VLT imagers and spectrographs. In the near/mid-IR, thermal emission from the telescope, airglow lines (mainly OH and O2 bands) and continuum and, in particular, emission/absorption bands from greenhouse gases, originating mainly in the lower atmosphere, are dominating the sky background of ground-based observations. The scattering-related components become negligible. The change in significance between the components as well as the necessity to use IR data sets for the analysis requires different modelling techniques to achieve reliable ETC predictions in the IR. The IR sky radiation model will be described in a forthcoming paper.

The sky model can also be used as a basis for procedures aiming at reconstructing data by removing the sky signature. This purpose requires the adaption of the sky model to enable the fitting of observed data. Preliminary studies show promising results for this kind of application, which will also be presented in future papers.

Acknowledgements. We are indebted to F. Patat for providing his FORS 1 data set and his LBLRTM set-up for the calculation of the best-fit Paranal extinction curve. We thank A. Seifarth for his support and helpful comments on the use of LBLRTM and the creation of suitable atmospheric profiles. We are grateful to R. Hanuschik for making his UV spectra available to us. Thanks also go to P. Ballester for his input to the paper and his prudent management of the project on ESO side and A. Smette for fruitful discussions. Finally, we thank the anonymous referee for his detailed and helpful comments. This study was carried out in the framework of the Austrian ESO In-Kind project funded by BM:wf under contracts BMWF-10.490/0009-II/10/2009 and BMWF-10.490/0008-II/3/2011. This publication is also supported by the Austrian Science Fund (FWF).

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Article B:
An advanced scattered moonlight model for Cerro Paranal

An advanced scattered moonlight model for Cerro Paranal*

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ABSTRACT

The largest natural source of light at night is the Moon, and it is the major contributor to the astronomical sky background. Being able to accurately predict the sky background, including scattered moonlight is important for scheduling astronomical observations. We have developed an improved scattered moonlight model, in which the components are computed with a better physical understanding as opposed to the simple empirical fit in the frequently used photometric model of Krisciunas & Schaefer (1991, PASP, 103, 1033). Our spectroscopic model can better trace the spectral trends of scattered moonlight for any position of the Moon and target observation. This is the first scattered moonlight model that we know of which is this physical and versatile. We have incorporated an observed solar spectrum, accurate lunar albedo fit, and elaborate scattering and absorption calculations that include scattering off of molecules and aerosols. It was designed for Cerro Paranal, but can be modified for any location with known atmospheric properties. Throughout the optical range, the uncertainty is less than 20%. This advanced scattered moonlight model can predict the amount of scattered moonlight for any given geometry of the Moon and target, and lunar phase for the entire optical spectrum.

Key words. Moon – atmospheric effects – radiative transfer – scattering – methods: data analysis – techniques: spectroscopic

1. Introduction

The current trend in astronomy has been to build larger and larger telescopes. The operating costs for running these large telescopes are high and careful planning of observations is needed for telescope time is always in demand. This means that more accurate predictions and estimation of the sky background are needed to understand how long an exposure is necessary for a given observation with a certain signal to noise ratio. The brightest natural source of light in the night sky, and therefore the greatest contributor to the sky background noise, is scattered moonlight. Having a reliable model of the moonlight for sky background estimation is critical. Also, many observers are trying to characterize faint objects spectroscopically, and knowing accurately the spectrum of the background would allow astronomers to predict which spectral features are observable within a given exposure time. By improving the scattered moonlight model within a sky background model, we can increase telescope scheduling efficiency.

The long standing scattered moonlight model used by ESO (European Southern Observatory) was by Walker (1987) and provides a table of the magnitudes for five photometric bands of the night sky at five different moon phases. It does not depend on the positions of the Moon or target observation and was measured during solar minimum. This model is limited in producing a scattered moonlight spectrum which is accurate enough for the current and future telescope operations.

The current, widely used model was developed by Krisciunas & Schaefer (1991), with 52 citations (e.g. Davies et al. 2013; Knoetig et al. 2013; Trinh et al. 2013). It is an empirical fit to data in the V-band taken at the 2800 m level of Mauna Kea. Even though the fit was separated into various specific functions, such as initial intensity from the Moon, Rayleigh and Mie scattering, it was still a parametrization based on only 33 observations in one photometric band specifically for Mauna Kea. The accuracy is between 8 and 23% if not near full Moon. In a previous paper, Noll et al. (2012), we presented a spectroscopic extension of the Krisciunas & Schaefer (1991) model. It was optimized for Cerro Paranal and covered the optical regime. The lunar albedo was taken to be constant with respect to wavelength and scaling factors for the different functions were introduced to better fit data from Cerro Paranal.

Our advanced scattered moonlight model works from the UV to the near-IR, but has only been fully tested in the optical, due to a current lack of data. It has been calibrated and investigated with 141 optical spectra and has an overall accuracy of σ ≲ 0.2 mag. The model has been split into physically based modules which are given by either physical models or the best current fits. The present version is optimized for Cerro Paranal, but can be modified for any location with information about its atmospheric properties. Our model is fully 3D and can predict the amount of scattered moonlight for any configuration of the Moon and target. It includes higher order scattering and is therefore still reliable at high zenith distances (when either object is near the horizon). Because our scattered moonlight model produces a spectrum, it can be used for finding spectral features and trends as well as photometric magnitudes.

The original purpose of designing an advanced scattered moonlight model, as part of the full sky background model, was for the Austrian accession to ESO to improve the ETC (Exposure Time Calculator), and thus enhance telescope scheduling and efficiency. Our optical sky background model, but with an older version of the scattered moonlight model, is described in Noll et al. (2012). The full sky background model estimates the amount of background light from 0.3 to 30 micron for Cerro Paranal. It includes all relevant components, such as scattered...
moonlight and starlight, zodiacal light, airglow line emission and continuum, scattering and absorption within the Earth’s atmosphere, and thermal emission from the atmosphere and telescope. Each component was designed with the latest knowledge and results in the field and was thoroughly checked with archival ESO data. The new scattered moonlight model is the topic of this paper. The zodiacal light is found using the prescription from Colina et al. (1996), and the airglow model is based on local observations and semi-empirical modeling (Patat 2008). The scattering and absorption are calculated with two codes, one that is fully 3D for the scattering and a line-by-line radiative transfer code for molecular absorption. The scattering and absorption will also be described in this paper, in the context of the scattered moonlight. The thermal emission is estimated as a gray body. The new sky background model has already been implemented by ESO.

In this paper we will discuss the optical portion of the advanced scattered moonlight model. In a subsequent paper, we will discuss the extension of this model into the near-IR using X-Shooter data (Vernet et al. 2011). For the remainder of the paper, the term “moon model” refers to the scattered moonlight model. In Sect. 2, we describe the moon model. In Sect. 3, we compare our scattered moonlight model with the observations and previous models, and finally in Sect. 4 we present our conclusions.

2. The model

To accurately calculate the scattered moonlight, there are several components that must be considered. The simplest way to account for the various pieces is to follow the path of light from the source to the instrument. The source of the scattered moonlight is the Sun. Then the light is reflected by the Moon which depends on the lunar albedo. This is mainly a function of the lunar phase. Next, the moonlight enters the Earth’s atmosphere, where it is scattered by molecules (Rayleigh) and aerosols (Mie), and absorbed. The light can be scattered multiple times, including off of the ground, before it reaches the telescope. This depends on the properties of the atmosphere and the positions of the Moon and target observation.

In the following subsections, we will discuss each of these steps in more detail. Section 2.1 introduces the calibration data set. In Sect. 2.2 we discuss the solar spectrum, in Sect. 2.3 the lunar albedo, and in Sect. 2.4 a more general discussion of the setup of the radiative transfer equations. Then, we have a more detailed discussion about Rayleigh scattering in Sect. 2.5, Mie scattering in Sect. 2.6, and absorption in Sect. 2.7.

2.1. Calibration data set

We calibrated our full sky background model including the improved scattered moonlight model with a FORS1 (FOcal Reducer/low dispersion Spectrograph) data set from Patat (2008). FORS1 was a low resolution optical spectrograph at Cerro Paranal. The data were taken between 1999 and 2005 with four different observing modes and consist of long-slit spectra, where plain sky could be extracted. For the details about the different observing modes, see Table 1. There are 1186 spectra, but only 26% have moonlight. For the analysis, we considered only 141 spectra with good weather conditions according to ESO’s ambient weather conditions database. The condition of good weather depended on two criteria, humidity and clouds. First, we only considered spectra taken when the humidity was ≤20%. Second, there must not be any detection of possible clouds in the night sky, within 5 h of the observation. Since we are measuring scattered moonlight, the entire sky must be free of clouds to ensure stable atmospheric conditions. Figure 1 shows several properties of the data: the distribution of the humidity with the cutoff, moon distance, lunar phase angles with waxing and waning, and angular distance ρ.

Table 1. Properties of the different observing modes in the FORS1 sky background data set.

<table>
<thead>
<tr>
<th>Grism</th>
<th>Filter</th>
<th>Wav. range (Å)</th>
<th>Resolution (Å FWHM)</th>
<th>Dispersion (Å px⁻¹)</th>
<th>Total #</th>
<th># with Moon</th>
<th># Used</th>
</tr>
</thead>
<tbody>
<tr>
<td>300V</td>
<td>GG435</td>
<td>4300–8900³</td>
<td>12</td>
<td>2.6</td>
<td>676</td>
<td>188</td>
<td>70</td>
</tr>
<tr>
<td>300V</td>
<td>...</td>
<td>3615–8900³</td>
<td>12</td>
<td>2.6</td>
<td>163</td>
<td>36</td>
<td>24</td>
</tr>
<tr>
<td>600B</td>
<td>OG590</td>
<td>3650–6050</td>
<td>5.3</td>
<td>1.2</td>
<td>143</td>
<td>29</td>
<td>18</td>
</tr>
<tr>
<td>600R</td>
<td>GG435</td>
<td>5390–7530</td>
<td>4.5</td>
<td>1.0</td>
<td>207</td>
<td>60</td>
<td>29</td>
</tr>
</tbody>
</table>

Notes. Listed here is the total number of sky spectra, the number of sky spectra with moonlight, and the number of sky spectra with moonlight that was used in the analysis (Sect. 2.1). (³) Order separation filter, fluxes <4400 Å were not used; (²) second-order overlapping, fluxes >6200 Å were not used.
The lunar albedo $A$ depends on several factors, including lunar phase, solar selenographic longitude, and wavelength. We use an empirical fit based on the ROLO survey (Kieffer & Stone 2005). They used over 100 000 images of the Moon in 32 different photometric bands in the optical and near infrared for certain lunar phases. The fit given by Kieffer & Stone (2005) is,

$$\ln A_{\lambda} = \sum_{i=0}^{3} a_{i} \Phi g^{i} + \sum_{j=1}^{4} b_{j,\lambda} \Phi^{j-1} + d_{3,\lambda} e^{-g/p_{3}} + d_{5,\lambda} \cos \left(\frac{g - p_{5}}{p_{4}}\right).$$

The last three terms in Eq. (2) are to correct for the opposition effect (exponential functions) and to minimize the residuals between the data and fit (cosine function). The opposition effect

http://eclipse.gsfc.nasa.gov/TYPE/ephemeris.html
is where the Moon has an enhanced brightness near full Moon (Whitaker 1969). We have neglected the terms that depend on the observer selenographic latitude and longitude. They have a small impact, maximum of ~7% over a full Saros (libration) cycle, and are variables that are not easily available in astronomical data.

The ROLO fit only covers the phase angles between \( g = 1.55^\circ \) and 97°. We extrapolated this fit to \( g = 180^\circ \). For the terms that depend on \( \Phi \), when \( g > 97^\circ \) we took the values of \( \Phi \) at \( g = 97^\circ \). This physically means that we are assuming that the ratio of maria to highlands is the same when \( g > 97^\circ \) as \( g = 97^\circ \). The other terms in Eq. (2) are still well behaved when \( g > 97^\circ \) and fit reasonably well with our data (Patat 2008). It is expected from previous studies that the general dependence of \( A \) on \( g \) is exponential for all values of \( g \) (outside the opposition effect) (e.g. Lane & Irvine 1973), which we see in our extrapolation as well. As \( g \) increases the overall flux from the Moon decreases, and becomes less important compared with the other components of the sky background. Thus, we believe the extrapolation to higher \( g \) is reasonable. In Fig. 3, we show the dependence of the lunar albedo on moon phase including the extrapolation when \( g > 97^\circ \). Also shown is the effect of \( \Phi \) which is a bit larger at redder wavelengths and is over-plotted as a band of values in yellow. At \( g = 97^\circ \), \( \Phi \) can cause deviations of ~6.8%.

The fit from the ROLO data was only done photometrically, however we require a full spectrum of \( P \) for the scattered moonlight model. To attain a fit for the entire optical spectrum, we performed a simple linear interpolation between the fit values provided. This interpolation is shown in Fig. 4 for several different moon phases. In general the wavelength dependence is fairly smooth and becomes less significant towards larger \( g \). There are some small variations where the photometric values are clustered.

According to Velikodsky et al. (2011), there are some discrepancies in the overall flux calibration amongst the various Moon observations. They find that the ROLO data at 603 nm is 13% too faint. They used an interpolation of the ROLO fit to find the albedo at 603 nm to compare it with their observations. Since there is no information about the wavelength dependence for this correction, we divide the albedo at all wavelengths by 0.87.

We currently neglect the effects of polarization. We assume that the change in the resulting scattered moonlight due to polarization is smaller than our current errors. In general the polarization of the lunar surface is small, less than 10% at maximum.

However, the maria can have a decent amount of polarization (~30%) (Dollfus & Bowell 1971).

### 2.4. Radiative transfer

The light from the Moon can be scattered many times or absorbed in the Earth’s atmosphere before reaching the telescope. We have developed a fully 3D single scattering code with estimates for double and higher order scattering. At the various scattering points, an effective airmass is calculated for absorption.

The transmission of light \( t \) can be directly related to the optical depth at zenith \( \tau_0 \) or the extinction coefficient \( k \) and airmass \( X \) by the following,

\[
 t(\lambda) = e^{-\tau_0(\lambda)X} = 10^{-0.4k(\lambda)X}. \tag{3}
\]

We will use this formalism in the following sections to describe the effects of scattering.

#### 2.4.1. Single scattering

The single scattering can be done fully in 3D (Wolstencroft & van Breda 1967; Staude 1975; Bernstein et al. 2002). We wish to obtain the integrated scattered light towards the azimuth \( \Lambda_0 \) and zenith distance \( \zeta_0 \). We take the Moon to be a point source. We consider the scattering path elements of density \( n(\sigma) \), with \( \sigma \) being the radius vector from the center of Earth \( C \) to \( S \). \( S \) is located between the top of atmosphere \( T \) to the observer \( O \), at height \( H_0 \) above the surface (see Fig. 5). The distance between \( O \) and \( C \) is \( \sigma_0 = H_0 + R \), where \( R \) is the radius of Earth (6371 km for the mean radius). For each path element \( S \) at distance \( s_2 \) from \( O \), the contributions of radiation from \( M \), where the moonlight enters the atmosphere, to the intensity at \( S \) along \( s_1 \) are considered. This intensity includes the scattering of light out of the path (and possible absorption), which depends on the effective column density of the scattering/absorbing particles. This is given by,

\[
 B_t(z, \sigma) = \int_0^{s_1(z, \sigma)} n(\sigma') \, d\sigma'. \tag{4}
\]

The scattering intensity also depends on the wavelength-dependent extinction cross section \( C_{\text{ext}}(\lambda) \) of the various processes, Rayleigh, Mie and absorption. They are related to the optical depth \( \tau \) (see Eq. (3)) and Eq. (4) at the zenith by,

\[
 C_{\text{ext}}(\lambda) = \frac{\tau_0(\lambda)}{B_0(0, \sigma_0)} \tag{5}
\]
After scattering at $S$ the light travels along path $S_2$ and is extincted by $B_z(z_0, \sigma)$. The total scattering intensity per solid angle $I_{\text{cal}}$ at $(A_0, z_0)$ for the flux of the Moon $F^*$, related to $I$ (Eq. (1)), is the same as seen by $O$, for Rayleigh and Mie scattering separately, is given by,

$$I_{\text{cal}}(A_0, z_0) = C_{\text{cal}}(\lambda) \int_0^{\cos(z_0 - \sigma)} n(\sigma) P(\theta) \times F^*(A_M, z_M) \exp^{-\tau} d\sigma,$$

(6)

where

$$\tau = (C_{\text{cal}}R + C_{\text{cal}}A) \times (B_{1,R}(z, \sigma) + B_{2,R}(z_0, \sigma_0)) + C_{\text{cal}}M \times (B_{1,M}(z, \sigma) + B_{2,M}(z_0, \sigma_0)).$$

(7)

Equation (7) is for Rayleigh (R), Mie (M), and absorption (A). In Eq. (6), $C_{\text{cal}}$ is the wavelength-dependent scattering cross section, which will deviate from $C_{\text{cal}}$. $H$ absorption occurs. The scattering phase function $P$ depends on the scattering angle $\sigma$, the angle between the paths $S_1$ and $S_2$, and is related to the zenith distances and azimuths at $S$ by,

$$\cos \theta = \cos \tilde{\sigma}_0 \cos \tilde{z}_M + \sin \tilde{\sigma}_0 \sin \tilde{z}_M \cos (\tilde{\theta}_0 - \tilde{A}_M).$$

(8)

Here, $\tilde{z}_0$, $\tilde{\theta}_0$, $\tilde{z}_M$, and $\tilde{A}_M$ are the zenith distances and azimuths of the target and Moon at $S$.

In Eq. (7), the various $C_{\text{cal}}$ are calculated by Eq. (4) for their respective densities. $C_{\text{cal}}A$ is calculated assuming the same particle distribution as Rayleigh scattering. This is optimal for molecular oxygen absorption.

We neglect the effect of polarization on the scattering phase function. Scattered moonlight does have some degree of polarization, similar to scattered sunlight, and has large areas of the sky with very little polarization (Horváth et al. 1998; Gál et al. 2001). The distribution of polarized light is not fully understood and would be difficult to implement.

For the vertical distribution of the scattering molecules, we use the standard barometric formula,

$$n(h) = n_0 \exp(-h/h_0).$$

(9)

Here, $h = \sigma - R$, the sea level density $n_0 = 2.67 \times 10^{-1} \text{ cm}^{-3}$, and the scale height $h_0 = 7.99 \text{ km}$ above the Earth’s surface (Staude 1975; Bernstein et al. 2002). For the troposphere and the lower stratosphere, where most of the scattering occurs, this is a good approximation. Cerro Paranal is at an altitude of $H_0 = 2.64 \text{ km}$. For the thickness of the atmosphere, we take $H_{\text{max}} = 200 \text{ km}$. For Rayleigh scattering, $C_{\text{scat}} = C_{\text{cal}}$, i.e., no absorption is involved.

For the height distribution of aerosols, we also use Eq. (9) with $n_0 = 1.11 \times 10^{-4} \text{ cm}^{-3}$ and $h_0 = 1.2 \text{ km}$. This is the tropospherical distribution of Elterman (1966). Dust, in particular soot, also absorbs radiation, thus $C_{\text{scat}}$ is lower than $C_{\text{cal}}$. We used the OMI (Ozone Monitoring Instrument) satellite data to find the median ratio of 0.97 (range between 0.90 and 0.99) for the area around Cerro Paranal (Levelt et al. 2006). The model is not very sensitive to changes in the molecular or aerosol distribution, because we scale them with the extinction curve.

### 2.4.2. Double scattering

The above scattering equations only deal with single scattering. We also considered double scattering. For this, we divided the path $S_1$ into two different possible paths $S_{1,1}$ and $S_{1,2}$ where scattering and absorption can occur at the path elements $D$ (double scattering), in between the two paths (see Fig. 5). At $D$ the scattering is treated in a similar way as in Eq. (6), but over the additional path elements. To simplify this integral and speed up the computing time, we made an approximation that allowed the integration to become an analytical expression with percent level accuracy (Eq. (4)). We assumed that the Moon coordinates where absolute coordinates with respect to the observer, such that the path $S_2 \ll R$ and the Moon is sufficiently far enough away to disregard slight angular shifts to the Moon coordinates for the different scattering points $S$ and $D$. Near the horizon and when scattering occurs at a far distance from the telescope, this assumption breaks down. However, most of the scattering occurs in the lower troposphere and a few km from the observer (with mean distances of $\sim 10$ km). The calculation was performed along a grid, which exponentially grows with distance. Where $\theta$ is small and therefore the contribution from the forward scattering peak of aerosols is high, we increased the resolution of the grid. For the higher order scattering, including double scattering, absorption by molecules via an effective airmass was no longer considered.

In the case of double scattering, scattering can also occur at the ground, labeled as point $G$ in Fig. 5. Since Cerro Paranal is located at 2635 m in a mountainous region, we took $G$ to be at a height of 2 km, although the exact height has little influence. To estimate the ground reflection, we used the A1 profile from Sutter et al. (2007) based on soil samples taken in the Chilean desert. We then scaled it to the values from OMI (Levelt et al. 2006) at the three provided wavelengths for the region around Cerro Paranal. We followed the procedure of Kleipool et al. (2008) to obtain a proper average ground reflection, since there are many errors associated with this calculation. This gave us a wavelength dependent ground reflection at our desired location, as shown in Fig. 6.
Double scattering is the sum of two different single scattering events, which can be off of molecules, aerosols, or the ground. We sum the contributions from the three different types of scattering to arrive at a final double scattering intensity, called $I_{DS}$. Because the moon model was intended for the ETC, it needed to be computationally quick and the exact position of the Moon is irrelevant. For this purpose, we made additional approximations for $I_{DS}$. We computed weighted averages over both the zenith distance to the target $z_0$ and to the Moon $z_M$. The weighting for $z_0$ was based on all the sky spectra from Patat (2008) and for $z_M$ from theoretical modeling of the positions of the Moon. $I_{DS}$ is then only a function of the angular separation between the Moon and target $\rho$ and the optical depth $\tau$. The average uncertainty for this simplification is on the order of 5%, and is higher at large zenith distances but quickly decreases towards smaller zenith distances.

### 2.4.3. Multiple scattering

We now consider the intensity for multiple scattering, anything higher than two, called $I_{MS}$. The intensity for single scattering will be labeled as $I_{SS}$.

For $I_{MS}$, we compared the contributions for $I_{DS}$ with $I_{SS}$. We assumed that the ratio between $I_{DS}$ and $I_{SS}$ would be the same for each consecutive order of scattering. We then summed over the geometric series and multiplied it by $I_{DS}$,

$$I_{MS} = I_{DS} \left( \frac{1}{1 - I_{DS}/I_{SS}} - 1 \right).$$

We imposed an upper limit for $I_{DS}/I_{SS}$ of 0.9, so $I_{MS}$ would not diverge. Similar to the weighted averages for $I_{DS}$, we calculated a weighted average over the difference between the azimuths for the target and Moon $A_0 - A_M$, which were weighted evenly. With Eq. (8), this gave a weighted average over the angular separation $\rho$. In the end, $I_{MS}$ is only a function of optical depth $\tau$, which can be related to wavelength.

The total scattering intensity for the Moon $I_{MS}$ is simply the sum of the contributions from $I_{SS}$, $I_{DS}$, and $I_{MS}$. With the weighting over the various parameters, we created a table of correction factors $f$ for the added amount of scattering due to $I_{DS}(\tau, \rho)$ and $I_{MS}(\tau)$.

$$I_{MS}(\tau, \rho, z_0, z_M) = I_{SS}(\tau, \rho, z_0, z_M) f(\tau, \rho).$$

The higher order scattering, $I_{DS}$ and $I_{MS}$, typically contribute only a few percent and is strongest at high optical depth. Some typical scattering curves are shown in Fig. 7 for three different wavelengths. At the redder wavelengths, Mie scattering is dominating and the scattering function approaches an exponential. At bluer wavelengths, the characteristic Rayleigh scattering phase function is the most influential.

We have compared our scattering intensities $I_{tot}$ with a radiative transfer code called libRadtran (Mayer & Kylling 2008) for a grid of zenith distances of the Moon and target, and the angular separation $\rho$ in $10^6$ steps for many different optical depths (corresponding to the full optical wavelength range). We have made this comparison to check the validity and accuracy of our scattering code. libRadtran is a widely used third party code for calculating radiative transfer in the atmosphere. It has several different numerical solvers, including the default which uses the plane parallel approximation. With this approximation, libRadtran is not accurate when either the source (Moon) or target are near the horizon. For all of the cases, 85% of $I_{tot}$ from our code and libRadtran agreed within a relative error of 20%. For $I_{tot}$ with zenith angles less than 70°, 75% agreed to within 10% relative error. The comparison between our code and libRadtran is shown in Fig. 8. With zenith angles $\leq 50^\circ$, there is very good agreement. As expected, at higher zenith angles where libRadtran is no longer accurate, the two codes diverge.

In the next three subsections, we will describe how Rayleigh, Mie and absorption are treated within the context of the scattering and absorption equations.

### 2.5. Rayleigh scattering

The scattering off of molecules in the Earth’s atmosphere can be well described by Rayleigh scattering, which assumes the particles are much smaller than the wavelength. Rayleigh scattering is characterized with having a steep dependence on wavelength $\sim \lambda^{-4}$ and at Cerro Paranal it is quite stable (Noll et al. 2012).

For the extinction due to Rayleigh scattering we use the following parametrization from Liu (2002),

$$\tau_R(\lambda) = \frac{P}{1013} (8.6 \times 10^{-3} + 6.5 \times 10^{-6} H) \lambda^{-(3.9 + 0.074 \lambda + 0.050/\lambda)}.$$  

Here, $\lambda$ is in $\mu$m, and $P$ is the pressure at a height $H$ of the observer, which we take to be 744 ± 1.5 hPa and 2.64 km, respectively (Noll et al. 2012).
The phase function for Rayleigh scattering is also well defined and is given by,

\[ P(\theta) = \frac{3}{4} (1 + \cos^2 \theta), \tag{13} \]

where \( \theta \) is the scattering angle.

The Rayleigh scattering is taken at each path element \( S \) and \( D_\alpha \), and is a well described and stable component of the model.

### 2.6. Mie scattering

For the aerosol scattering, we have gathered information from several different sources and tried to build the most physical description. We take the Ångström law derived by Patat et al. (2011) for Cerro Paranal in the optical wavelengths. We then decomposed this fit into several aerosol types given by Warneck & Williams (2012), and produced the phase function using a Mie scattering code for log normal distributions written by G. Thomas based on the Ångström law for single particles (Grainger et al. 2004). With the extinction curves for the various aerosol types along with the fit for Cerro Paranal, we determined how much each curve needed to be scaled down by 25% in LBLRTM to match the observations. The optical depth at Cerro Paranal is very low and the aerosols are almost purely background aerosols, with no urban component (Patat et al. 2011). In the optical, their fit is given by,

\[ k_{\text{opt}} = k_0 \epsilon^3, \tag{14} \]

where \( k_0 = 0.013 \pm 0.002 \) and \( \epsilon = -1.38 \pm 0.06 \) mag airmass\(^{-1}\), valid from 0.4 to 0.8 μm. We use the best fit \( k_0 \) value quoted in Patat et al. (2011) of 0.014 mag airmass\(^{-1}\). The aerosol component can fluctuate significantly, as can be seen in data taken at Mauna Kea (Buton et al. 2013). They have the Ångström exponent of \( \alpha = -1.3 \pm 1.4 \) and state that at 330 nm it can vary as much as 0.4 mag airmass\(^{-1}\).

We are interested in extending the scattered moonlight model into the infrared, as well as wanting a more physical basis for the aerosol extinction to more accurately calculate the phase function. Therefore, we decomposed the Ångström law. We used the size distribution given in Warneck & Williams (2012) for the remote continental tropospheric and stratospheric aerosols. The tropospheric aerosols are split into three types: nucleation, accumulation, and coarse modes. Nucleation consists of newly produced particles from either direct emissions of combustion products or gas-phase condensation reactions. Accumulation is from coagulation of nucleation particles, condensation of products from the gas-phase chemical reactions onto particles, and chemical reactions in the aqueous phase of clouds. The mass of the coarse mode comes from mineral dust, sea salt, and biogenic material. The stratospheric aerosols are in a layer around 25 km above sea level and consist mostly of sulfuric acid particles with an admixture of nitrosyl sulfates and solid granules containing silicates (Warneck & Williams 2012). We use a log normal distribution given by,

\[ \frac{dN}{d\log r} = \frac{1}{\sqrt{2\pi} \log s} \frac{n}{R_s} \exp \left[ \frac{(\log r/R_s)^2}{2(\log s)^2} \right]. \tag{15} \]

\( N \) is the cumulative number density distribution in particles cm\(^{-3}\), and \( r \) is the particle radius in μm. Table 2 provides the values for the parameters \( n, R, \) and \( \log s \) of the various aerosol modes, which represent the number of particles, average radius, and a distribution parameter, respectively. To calculate the extinction curve for each aerosol type we used a Mie scattering IDL code for log normal distributions written by G. Thomas based on Bohren & Huffman (1983) for single particles (Grainger et al. 2004). With the extinction curves for the various aerosol types along with the fit for Cerro Paranal, we determined how much each curve needed to be scaled down to match the overall fit. However, there are degeneracies. The refractive index \( N \) is not known for these background aerosols, so we varied it between 1.3 and 1.5. Varying \( N \) changes the scaling of the different aerosol components needed to match the fit. There is also a degeneracy between two of the aerosol types, remote continental tropospheric coarse mode and stratospheric, because their optical extinction curves are similar. In Fig. 9a we have plotted the various Mie extinction curves. The extinction from the different aerosol types with a range in \( N \) between 1.3 and 1.5 are shown, along with the total curve that is consistent with the observed one. It can easily be seen that the tropospheric nucleation mode has little to no

### Table 2. Aerosol modes.

<table>
<thead>
<tr>
<th>Type</th>
<th>( n ) cm(^{-3})</th>
<th>( R ) 10(^{-3}) μm</th>
<th>( \log s ) 10(^{-1})</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trop nucleation</td>
<td>3.20 × 10(^3)</td>
<td>0.10</td>
<td>1.61</td>
</tr>
<tr>
<td>Trop accumulation</td>
<td>2.90 × 10(^3)</td>
<td>0.58</td>
<td>2.17</td>
</tr>
<tr>
<td>Trop coarse modes</td>
<td>3.00 × 10(^{-1})</td>
<td>9.00</td>
<td>3.80</td>
</tr>
<tr>
<td>Stratospheric</td>
<td>4.49 × 10(^{10})</td>
<td>2.17</td>
<td>2.48</td>
</tr>
</tbody>
</table>

Notes. The values used for Mie scattering of remote continental aerosols from Warneck & Williams (2012) (Sect. 2.6).
out at higher angles, rather than dip to a minimum as in the Mie approximation (e.g. Horvath et al. 2006). Since the forward scattering dominates the back scatter by a few orders of magnitude, we prefer the Mie scattering phase function over the Henyey-Greenstein (Henyey & Greenstein 1941) approximation, which depends on the average asymmetry parameter of the aerosols. Additionally, the majority of the stratospheric aerosols in this region are sulfates, which are in droplets, and so are fairly round. The amount of coarse mode aerosol is low, which is the least round type of aerosol. This will also provide another method to break the degeneracies amongst the various aerosol modes. Finally, in astronomical observations it is rare to have the target and Moon at angular distances $>120^\circ$, where the back scatter peak becomes important. In Fig. 9b, the phase functions for the different aerosol types are plotted along with the total Mie phase functions. Once again each mode is shown with a range of $N$ between 1.3 and 1.5.

### 2.7. Absorption

The absorption is calculated using the radiative transfer code LBLRTM (Clough et al. 2005) with a merged atmospheric profile for Cerro Paranal and the effective airmass $X_{\text{eff}}$ at point $O$ calculated from the single scattering at $S$. LBLRTM is a widely used radiative transfer code in atmospheric sciences and it uses the atomic line database HITRAN (High-Resolution TRANsmission; Rothman et al. 2009). This gives the amount of absorption from the various atmospheric molecules. It requires an atmospheric profile, and we use a merged one, which combines the temperature, pressure, and chemical composition as a function of height from three different sources. We combined MIPAS (Michaelson Interferometer for Passive Atmospheric Sounding) equatorial profile (see Seifahrt et al. 2010) with one from GDAS (Global Data Assimilation System)$^5$, and finally scale the quantities of the lower atmosphere to the local meteorological data taken at Cerro Paranal. The MIPAS profile contains height information on 30 molecular species. The GDAS database, which is based on measurements, provides modeled profiles of temperature, pressure, and the relative humidity up to a height of about 26 km on a 3 h basis with a spatial grid of $1^\circ \times 1^\circ$. The local meteorological data from the ESO MeteorMonitor$^6$ gives the local temperature, relative humidity, and pressure. We currently use bimonthly mean, merged profiles for all the nights.

For each single scattering point $S$, an effective airmass $X_{\text{eff}}$ relative to the direct path from the zenith to observer is calculated to scale the amount of absorption due to the given geometry of the Moon and target. We do not calculate $X_{\text{eff}}$ from the higher order scattering, since this contribution is quite small. $X_{\text{eff}}$ then modifies the transmission from the moonlight as calculated by LBLRTM.

For determining $X_{\text{eff}}$, we compare the intensities with and without extinction, $I^{+1}$ and $I^{0}$, respectively. We first look at a specific path element for a given $S$. We find the column density of that path element for both Rayleigh $B_{\text{R}}$ and Mie scattering $B_{\text{M}}$ (similar to Eq. (4)). Then with $C_{\text{scat}}$ and phase function $P(\theta)$, we calculate $I^{-1}$ by,

\[
I^{-1} = \sum_n I_n^{-1},
\]

where,

\[
I_n^{-1} = C_{\text{scat},B}B_{\text{R}}P_R(\theta_n) + C_{\text{scat},M}B_{\text{M}}P_M(\theta_n).
\]

---

$^5$ http://ready.arl.noaa.gov/gdas1.php

$^6$ http://archive.eso.org/asm/ambient-server
We use the particle distribution from Rayleigh scattering as an approximation for the absorbing molecules, which is optimal for O₂. The water vapor, however, is distributed differently from the main air molecules. The absorption from H₂O mostly occurs at low altitudes. Since the distribution of particles is scaled with the extinction curve, the amount of H₂O is fairly accurate. Changing the profile did not significantly change the resulting modeled spectrum.

The ozone is treated separately using the van Rhijn formula with a height of 25 km, which is given by,

$$X_{oz} = \frac{1}{\sqrt{1 - 0.992 \sin^2 z_M}} \quad (21)$$

Here $X_{oz}$ is the effective airmass for ozone and $z_M$ is the zenith distance to the Moon. There are two assumptions made. The first one is that we treat the ozone only at a height of 25 km and not at a distribution of heights. The thickness can vary with season and geographic location. This assumption allows for a much simpler calculation of $X_{oz}$. The second is that we are only considering the light that is coming along the direct path from the Moon, by using the Moon’s zenith distance. We assume that the majority of the light has not been scattered prior to passing through the ozone layer. Since most of the scattering takes place in the lower troposphere, which is distinctly below 25 km, this appears to be a safe assumption. Following Patat et al. (2011), we multiply the amount of ozone given in the standard atmospheric profile by 1.08.

### 3. Comparison with FORS1 data and previous models

We have compared our model with the FORS1 data (see Sect. 2.1 for details) (Patat 2008) and with the previous moon model from Noll et al. (2012) based on Krisciunas & Schaefer (1991). We found that overall, for the complete sky background model, an uncertainty of $\sigma \sim 0.2$ mag with the FORS1 data set. For the moon model, the uncertainty is -0.15 mag.

Figure 10 shows two examples of how well the model fits the observed data. The spectrum in Fig. 10a has moderate moonlight and is around 1st quarter and (b) has significant moonlight and is near full Moon. The full sky model is consistent with the observed spectrum in both scenarios. Also shown is the scattered moonlight model which is a large portion of the overall sky background flux. For (b), the model tends to slightly overestimate the amount of background light.

To better understand the errors of the moon model, we made a mean and $\sigma$ spectrum of the difference between the FORS1 observations and the full sky model for all the spectra, those with moonlight, and those without moonlight (Fig. 11). The mean spectrum is centered around zero, with increased fluctuations at the redder wavelengths due to airglow emission. The $\sigma$ spectrum without moonlight is slightly lower, but all three groups tend to lie around 0.2 mag, and increase slightly at the red end. Loosely comparing the spectrum with moonlight to those without, gives a rough estimate of the quality of our advanced moon model.

To better evaluate only the scattered moonlight model, we subtracted the other components of the sky background, using the sky background model, from the observations. This, in principle, should provide only an observed scattered moonlight spectrum. We then compare this observed moon-only spectrum with the scattered moonlight model. Such a comparison contains all the errors associated with the full sky background model as well.
as the errors from the moon model. For an estimate of the uncertainty in the other sky background components, we looked at the full sky model without moonlight. We then computed a weighted $\sigma$ to represent the uncertainty from the other sky background components, by comparing the relative flux from the moonlight with full sky background for the Moon observations used in this analysis. If there is less moonlight, then $\sigma$ from the other components should be larger, versus an observation dominated by moonlight where $\sigma$ should mostly come from the moon model. We did this comparison using all the data with a significant amount of moonlight (>100 phot s$^{-1}$ m$^{-2}$ μm$^{-1}$ arcsec$^{-2}$) and decent weather conditions. Also, we ignored one of the observing modes, Grism 600B, which had only 8 data points and the flux calibrations appeared to greatly deviate from the other observing modes. This left us with a total of 82 spectra. The results can be seen in Fig. 12. There is a jump in the mean around 500 nm where the majority of the observations changes from one observing mode to another. We believe this comes from errors in the flux calibration of the Patat (2008) data. For the mean of these spectra to be centered at zero, we needed to multiply the moon model by a factor of 1.2 to correct for the flux calibration. The error bars shown here are the uncertainties from the moon model squared minus the square of the weighted $\sigma$ from the other components. At blue wavelengths $\sigma$ is small, and it gets larger towards the red. The estimated weighted $\sigma$ of the other sky background components is inflated in the UV and red wavelengths. The airglow/residual continuum model probably overestimates the flux, and so the residuals, especially in the red, are large. This causes the Moon contribution to be underestimated and $\sigma$ to be inflated, so the last three continuum nodes are not shown for this reason. In Fig. 11a, this effect due to the airglow model can be seen from the downturn in the mean difference spectra. Also plotted in Fig. 12 with the same analysis is the previous moon model discussed in Noll et al. (2012), which is an extension of Krisciunas & Schaefer (1991) moon model and scaled to Patat (2008) data, labeled as KS91. The mean and $\sigma$ for this previous model are worse than our new advanced moon model. KS91 has a larger $\sigma$ at blue wavelengths and the mean is more off centered at redder wavelengths compared with our work. The mean and $\sigma$ for our new advanced moon model and the previous one, before being corrected for the errors from the other sky background components are shown in Table 3, along with the weighted $\sigma$ from the rest of the sky background.

Fig. 12. Means and uncertainties for the scattered moonlight versus observed data at several 4 nm wide continuum bands. The y-axis is the average of the observed minus modeled fluxes for data with good weather conditions and a significant amount of moonlight. Over-plotted is the same analysis with the previous model from Noll et al. (2012) based on Krisciunas & Schaefer (1991), labeled as KS91. The numbers below each point are the number of spectra considered. See Sect. 3 for more details.

Table 3. Narrow band filter statistics for our new moon model (new), Noll et al. (2012) moon model (old), and the weighted $\sigma$ of the other sky background components (SBC).

<table>
<thead>
<tr>
<th>Filter (nm)</th>
<th># (new)</th>
<th>$\sigma_{\text{new}}$ (old)</th>
<th>$\sigma_{\text{old}}$</th>
<th>$\sigma_{\text{SBC}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>369</td>
<td>16</td>
<td>0.259</td>
<td>0.222</td>
<td>0.102</td>
</tr>
<tr>
<td>387</td>
<td>16</td>
<td>0.100</td>
<td>0.213</td>
<td>−0.038</td>
</tr>
<tr>
<td>420</td>
<td>16</td>
<td>0.137</td>
<td>0.191</td>
<td>−0.081</td>
</tr>
<tr>
<td>450</td>
<td>62</td>
<td>−0.026</td>
<td>0.185</td>
<td>−0.155</td>
</tr>
<tr>
<td>480</td>
<td>62</td>
<td>−0.025</td>
<td>0.192</td>
<td>−0.126</td>
</tr>
<tr>
<td>510</td>
<td>62</td>
<td>−0.060</td>
<td>0.208</td>
<td>−0.136</td>
</tr>
<tr>
<td>543</td>
<td>82</td>
<td>−0.076</td>
<td>0.220</td>
<td>−0.077</td>
</tr>
<tr>
<td>575</td>
<td>82</td>
<td>−0.080</td>
<td>0.299</td>
<td>−0.021</td>
</tr>
<tr>
<td>608</td>
<td>82</td>
<td>−0.106</td>
<td>0.330</td>
<td>0.048</td>
</tr>
<tr>
<td>642</td>
<td>66</td>
<td>−0.150</td>
<td>0.314</td>
<td>0.130</td>
</tr>
<tr>
<td>675</td>
<td>66</td>
<td>−0.143</td>
<td>0.326</td>
<td>0.193</td>
</tr>
<tr>
<td>720</td>
<td>66</td>
<td>−0.084</td>
<td>0.364</td>
<td>0.269</td>
</tr>
<tr>
<td>720</td>
<td>66</td>
<td>−0.084</td>
<td>0.364</td>
<td>0.269</td>
</tr>
<tr>
<td>820</td>
<td>46</td>
<td>−0.152</td>
<td>0.676</td>
<td>0.298</td>
</tr>
<tr>
<td>872</td>
<td>45</td>
<td>0.016</td>
<td>0.761</td>
<td>0.483</td>
</tr>
</tbody>
</table>

Notes. The listed $\sigma_{\text{new}}$ and $\sigma_{\text{old}}$ are before subtracting the uncertainties from the other sky background components.
Fig. 13. Comparison of the full sky background model with the previous moon model based on Krisciunas & Schaefer (1991), labeled as KS91, and then one presented in this paper. a) The observed spectrum along with the full sky background model with the old (KS91) approach and this work. b) This shows the relative residuals for the previous model and the work presented in this paper. See Sect. 3 for more details.

To further show the improvement of our new advanced scattered moonlight model, we have plotted the full sky background model using the extrapolated Krisciunas & Schaefer (1991) moon model (labeled again as KS91) and our new moon model with an observed spectrum in Fig. 13a. It can be clearly seen that the new moon model fits the observed spectrum much better than the previous model. The relative residuals are plotted on panel (b).

4. Conclusion

We have developed an advanced scattered moonlight model. It is based on physical processes and data, and has fewer empirical parametrizations than previous models. It is spectroscopic and traces spectral trends seen in observations. Currently, it has been evaluated for the optical range from 0.36 to 0.89 micron. The uncertainty in the moon model is around 0.15 mag, and the full sky background model has $\sigma \sim 0.2$ mag. There are several advantages of our new moon model:

- More physical than previous models (Krisciunas & Schaefer 1991; Noll et al. 2012).
- Uses a fit for the lunar albedo based on more than 100,000 observations of the Moon (Kieffer & Stone 2005).
- Uses fully 3D single scattering calculations.
- Calculates fully 3D double scattering calculations, including ground reflection, then simplifies for faster computing.
- Approximates multiple scattering by comparing double and single scattering.
- Calculates the absorption and single scattering simultaneously.
- Decomposes the Mie scattering Ångström Law into typical aerosol distributions for Cerro Paranal.
- Calculates the Mie phase function based on the aerosols found by decomposing the Ångström Law.
- Provides a scattered moonlight spectrum, not just photometric magnitudes (Walker 1987; Krisciunas & Schaefer 1991).
- The uncertainties across the entire optical range are much lower than previous (Krisciunas & Schaefer 1991; Noll et al. 2012).

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Article C:
Skycorr: A general tool for spectroscopic sky subtraction

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Skycorr: A general tool for spectroscopic sky subtraction

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ABSTRACT

Context. Airglow emission lines, which dominate the optical-to-near-infrared sky radiation, show strong, line-dependent variability on time scales from minutes to decades. Therefore, the subtraction of the sky background in the affected wavelength regime becomes a problem if plain-sky spectra have to be taken at a different time from the astronomical data.

Aims. In solution of this problem, we have developed a physically motivated scaling of the airglow lines in the plain-sky data to fit the sky lines in the object spectrum. We have developed a corresponding instrument-independent approach based on one-dimensional spectra.

Methods. Our code skycorr separates sky lines and sky/object continuum by an iterative approach involving a line finder and airglow line data. The sky lines, which mainly belong to OH and O\(_2\) bands, are grouped according to their expected variability. The line groups in the sky data are then scaled to fit the sky in the science data. Required pixel-specific weights for overlapping groups are taken from a comprehensive airglow model. Deviations in the wavelength calibration are corrected for by fitting Chebyshev polynomials and rebinning via asymmetric damped sinc kernels. The scaled sky lines and the sky continuum are subtracted separately.

Results. ESO-VLT X-shooter data covering 2.5 h with a good time resolution were selected to illustrate the performance. Data taken six nights and about one year before were also used as reference sky data. The variation of the sky-subtraction quality as a function of time difference between the object and sky data depends on changes in the airglow intensity, atmospheric transparency, and instrument calibration. Except for short time intervals of a few minutes, the sky line residuals were between 2.1 and 5.5 times weaker than for sky subtraction without fitting. Additional tests showed that skycorr performs consistently better than the method of Davies (2007, MNRAS, 375, 1099) developed for ESO-VLT SINFONI data.

Key words. atmospheric effects – radiation mechanisms: non-thermal – instrumentation: spectrographs – methods: data analysis – methods: numerical – techniques: spectroscopic

1. Introduction

For spectroscopic instrument set-ups and observing programmes that do not provide plain-sky spectra simultaneously with the desired object spectra (two-dimensional (2D) spectra where the object only covers a small fraction in spatial direction would be ideal), it is necessary to use sky spectra taken at a different time from the science spectra for the sky correction. This especially affects fiber spectrographs, which include instruments using an integral-field unit (IFU). The strong variability of airglow emission on various time scales from minutes to decades (see e.g. Khomich et al. 2008; Patat 2008; Noll et al. 2012) can cause unavoidable sky-correction residual. Significant changes in the airglow emission can also be expected for angular distances in the order of a few degrees or even less depending on the characteristics of possible wave patterns, such as those caused by internal gravity waves (see e.g. Taylor et al. 1997). Moreover, different telescope positions and ambient conditions may cause drift effects, which result in wavelength shifts of the sky spectrum with respect to the science spectrum. Hence, the reference sky spectrum has to be adjusted in both the flux and the wavelength regime to allow a reasonable sky-background correction.

An illustration of this problem and a solution for the Very Large Telescope (VLT) near-infrared (near-IR) integral-field spectrograph SINFONI (Eisenhauer et al. 2003) of the European Southern Observatory (ESO) has been described by Davies (2007). His airglow correction method is based on using arbitrary sky spectra for the sky subtraction in science data by scaling physically related line groups of the sky spectrum to the corresponding groups in the science spectrum. Subsequently, the newly created scaled spectrum is used for the sky correction. Specifically, Davies’ method groups emission lines from vibrational-rotational transitions resulting from non-thermal excitation processes of the OH molecule (Meinel 1950; Bates & Nicolet 1950; Rousselet et al. 2000; Khomich et al. 2008) and defines wavelength regions where these groups dominate the airglow emission. These wavelength ranges are scaled in the sky spectrum to match the corresponding flux in the object spectrum. This approach only works for the line component of the sky emission. Since object and sky continua cannot satisfactorily be separated, the sky continuum cannot be adapted and has to be subtracted before the scaling procedure for the line emission can start. Davies’ code considers a greybody for the thermal continuum, which is fitted to the data. Other continuum sources that dominate the emission at wavelengths shorter than the K band (e.g. airglow (pseudo-)continua, scattered moonlight, zodiacal light, and instrument-related continua; see Noll et al. 2012) are not taken into account. In the J and H bands covered by the SINFONI data, these contributions are distinctly fainter than the

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airglow lines. Since Davies' method is restricted to OH airglow lines beyond 1 \( \mu m \), it can only be applied to near-IR wavelength regions where other line emission is negligible. Davies’ method has successfully been implemented for the ESO SINFONI data-reduction pipeline (Modigliani et al. 2007).

In this paper, we present the instrument-independent code skycorr\(^2\) for the sky correction based on one-dimensional (1D) spectra. It was inspired by Davies' pioneering method. In comparison, skycorr allows a more accurate subtraction of airglow lines because of its more detailed airglow model (see Noll et al. 2012 for the optical range), the pixel-specific scaling of the lines, and an advanced approach for separating lines and continuum. Moreover, the code can also be applied to optical wavelengths. Section 2 describes the algorithm implemented in skycorr. A test data set for illustrating the performance is presented in Sect. 3. The test results are discussed in Sect. 4. This also involves a comparison with Davies’ method. Finally, Sect. 5 provides a summary and contains our conclusions.

2. Method and use

In the following, we describe the skycorr sky-correction procedure in detail. The algorithm is sketched in Fig. 1. Its main purpose is the removal of sky emission lines in a science spectrum by means of a scaled reference sky spectrum. Any continuum component in the input science and reference sky spectra has to be removed in advance. Hence, as a first step, pixels belonging to lines and continuum have to be identified, separated, and masked accordingly. The line identification is discussed in Sect. 2.1. This procedure also derives the typical line full width at half maximum (FWHM, Sect. 2.2). The next step is a fit of the continuum pixels alone, which is subtracted from the input spectrum to obtain a continuum-free spectrum (Sect. 2.3). In the third step, a weight mask for the different airglow line groups in the reference sky spectrum is calculated, which incorporates an extended version of the sky-radiance model described in Noll et al. (2012) (Sect. 2.4). It is an essential input for scaling the reference sky line spectrum to fit the science line spectrum in the subsequent step (Sect. 2.5). The fitting procedure also allows an optimisation of the wavelength grids (Sect. 2.6). The final step of the sky-correction procedure is the sky subtraction itself. This operation is just the subtraction of the best-fit sky line spectrum and the unscaled sky continuum spectrum from the input science spectrum.

Skycorr has been designed to be instrument independent. It only requires a 1D science and reference sky spectrum as input. Both should be taken with the same instrumental set-up and reduced in the same way. For a good sky subtraction (especially for the unscaled continuum), both spectra should refer to a similar integrated sky area. For slit spectrographs, this depends on the slit width and the extraction in spatial direction. The former is also important for the spectral resolution. For data without flux calibration, the science and sky spectra should correspond to the same exposure time. It is expected that both files have the same format. Skycorr accepts ASCII tables, FITS tables, and 1D FITS images. The corrected output files will have the format of the input files. Several additional files are written to the output directory, which contain results of the algorithm and can be used to evaluate the quality of the sky subtraction. Skycorr has also been designed to minimise user interaction. Nevertheless, there might be code parameters that could be modified to improve the sky-subtraction results. The relevant parameters of the skycorr driver file and their default values are listed in Table 1. They are discussed in the following subsections. More details on the file structures and code parameters can be found in the skycorr user manual, which is provided along with the code.

2.1. Line finder

Spectral lines are identified by an approach that uses the first derivative of the spectrum (see Fig. 2). In this way, line pixels can be recognised by their steep flux gradients. Emission line peaks can be identified by a change from positive to negative values of the first derivative. The approach is insensitive to slowly varying continua. All detected lines are assembled in a line list, which is refined by an iterative method depending on the estimation of the sky line FWHM (see Sect. 2.2). This procedure requires the identification of strong, isolated lines. Therefore, the line finder checks the previously identified line peaks, applying criteria that reject spurious detections and line blends. Lines that are sufficiently separated from other lines and whose peaks have a symmetric shape are marked as isolated. The former criterion can be influenced by the user. The parameter file includes the unitless scaling parameter \( \text{MIN\_LINE\_DIST} \) (see Table 1) that is internally multiplied by the line FWHM in pixels, where a first-guessed value is also included in the configuration file.

\(^1\) Version 2.0 of Davies’ code also allows simple scaling of the strong \( \text{O}_2 \) band at 1.27 \( \mu m \). This feature is not described in Davies (2007).

\(^2\) The code can be downloaded from web pages located at ESO (http://www.eso.org/pipelines/skytools/) as well as from the University of Innsbruck (http://www.uibk.ac.at/eso/software/).
for the required accuracy. The FWHM measurements of all isolated lines are averaged to obtain the typical FWHM of the input spectrum. To avoid blended lines contributing to the resulting mean, a σ-clipping approach is applied to skip suspiciously high FWHM. If fewer than five isolated lines remain after clipping, the median FWHM is taken.

Since the FWHM estimation and the search for isolated lines (see Sect. 2.1) affect each other, an iterative approach is required, where the line finder, continuum subtractor, and FWHM estimator are called in a loop to obtain a stable and trustworthy FWHM. This iterative procedure is terminated if convergence is reached for the mean FWHM. The convergence criterion is provided by the parameter LTOL (see Table 1).

For spectrographs whose spectra show a roughly linear increase of the FWHM with wavelength and cover a wide wavelength range (see Sect. 4.1), one can set the parameter VARGFWHM to 1. In this case, the FWHM estimates of the individual lines are converted to correspond to the FWHM that would be measured at the central wavelength of the full spectrum, assuming a linear change of the FWHM is also assumed for the separation actions in the upper atmosphere involving nitric oxide (Khomich et al. 2008 and references therein; Noll et al. 2012). In addition, an instrument-related continuum due to internal scattering and similar effects could significantly contribute (see e.g. Ellis & Bland-Hawthorn 2008; Vernet et al. 2011). As Fig. 3 indicates,

### Table 1. Skycorr default parameter set-up.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Short description</th>
</tr>
</thead>
<tbody>
<tr>
<td>VAC_AIR</td>
<td>vac</td>
<td>wavelengths in vacuum or air</td>
</tr>
<tr>
<td>FWHM</td>
<td>5.0</td>
<td>initial estimate of line FWHM (in pixels)</td>
</tr>
<tr>
<td>VARGFWHM</td>
<td>0</td>
<td>linear increase of line width with wavelength? (1 = yes, 0 = no)</td>
</tr>
<tr>
<td>LTOL</td>
<td>1e-2</td>
<td>relative FWHM convergence criterion</td>
</tr>
<tr>
<td>MIN_LINE_DIST</td>
<td>2.5</td>
<td>minimum distance to neighbouring lines for isolated lines (in FWHM)</td>
</tr>
<tr>
<td>FLUX_LIM</td>
<td>−1</td>
<td>minimum line peak flux (in median flux of identified lines)</td>
</tr>
<tr>
<td>FITLIM</td>
<td>1e-3</td>
<td>relative convergence criterion for iterative improvement of wavelength grid correction</td>
</tr>
<tr>
<td>XTL</td>
<td>1e-3</td>
<td>relative parameter convergence criterion</td>
</tr>
<tr>
<td>WTOL</td>
<td>1e-3</td>
<td>convergence criterion for iterative improvement of wavelength grid correction</td>
</tr>
<tr>
<td>CHEBY_MAX</td>
<td>7</td>
<td>maximum degree of polynomial for wavelength grid correction</td>
</tr>
<tr>
<td>CHEBY_MIN</td>
<td>3</td>
<td>minimum degree of polynomial for wavelength grid correction</td>
</tr>
<tr>
<td>CHEBY_CONST</td>
<td>0</td>
<td>initial constant term for wavelength grid correction</td>
</tr>
<tr>
<td>REBINTYPE</td>
<td>1</td>
<td>type of rebinning (0 = simple, 1 = asymmetric, damped sinc kernel)</td>
</tr>
<tr>
<td>WEIGHTLIM</td>
<td>0.67</td>
<td>minimum relative weight of the strongest line group of a pixel</td>
</tr>
<tr>
<td>SIGLIM</td>
<td>15</td>
<td>σ limit for excluding outliers</td>
</tr>
<tr>
<td>FITLIM</td>
<td>0.</td>
<td>lower relative uncertainty limit for fitting a line group</td>
</tr>
</tbody>
</table>

**Notes.** Input/output parameters are not listed.
Fig. 3. Components of the Cerro Paranal sky model for wavelengths between 0.3 and 6 μm in logarithmic radiance units. The example with the Moon above the horizon shows the scattered moonlight, scattered starlight, zodiacal light, thermal emission by telescope and instrument, molecular emission of the lower atmosphere, airglow emission lines of the upper atmosphere, and airglow/residual continuum. The (optical) model components are described in Noll et al. (2012) except for the improved scattered moonlight model, which is discussed in Jones et al. (2013).

The main continuum component is the airglow/residual continuum, which dominates shortwards of the thermal regime with the exception of the ultraviolet (UV) and optical if the Moon is up.

The variable airglow continuum (see Noll et al. 2012) and the thermal continuum, which can significantly change by temperature differences of a few degrees, cannot be corrected for by a fitting procedure as is done for the airglow lines (see Sect. 2.4.1), since object and sky continuum cannot be separated in the science spectrum (cf. Sect. 1). Hence, skycorr performs a simple continuum subtraction without scaling. To achieve reliable results, this approach requires that the object continuum is distinctly brighter than the variation in the sky continuum (see Sect. 3.2 for more details). Note that the strong thermal methane and water vapour lines of the lower atmosphere at wavelengths beyond 2.3 μm are also handled as continuum. This can lead to significant sky-subtraction residuals for inaccurate wavelength solutions (see Sect. 2.6).

Skycorr obtains the continua in the input science and sky spectra using line identification flags set in the course of the line search described in Sect. 2.1. All pixels not flagged as line pixels are connected by linear interpolation. If the identification of continuum pixels is reliable, this is the most efficient approach even for line blends that cover wide wavelength ranges.

2.4. Airglow model

The wavelength range from the near-UV to the near-IR is characterised by strong emission lines. Most of them constitute band structures. This airglow (see Khomich et al. (2008) for a comprehensive discussion) mostly originates in the mesopause region at about 90 km. In addition, some lines arise in the ionospheric F2-layer at about 270 km. In general, airglow is caused by chemiluminescence, that is, by chemical reactions that lead to light emission by the decay of excited states of reaction products. Apart from atomic oxygen and sodium, the oxygen (O₂) and hydroxyl (OH) molecules are the most important reaction products in this context. In general, airglow lines show strong variability from time scales in the order of minutes to decades. This behaviour can be explained by the solar activity cycle, seasonal changes in temperature, pressure, and chemical composition of the emission layers, the day-night contrast, dynamical effects such as planetary and gravity waves, or geomagnetic disturbances. The dynamical effects also cause spatial intensity variations. In addition, the airglow intensity depends on the projected emission layer width, which is a function of the zenith distance (van Rhijn 1921; Noll et al. 2012).

Because the airglow is highly variable, the strength of the emission lines in a reference sky spectrum for sky correction has to be adapted. This is achieved by a fitting procedure that is discussed in Sect. 2.5. Since object emission lines should not be reproduced by the optimised sky spectrum and finally removed, it is advisable to scale as many lines as possible by a single fitting parameter. Every group should contain airglow lines that are not affected by object lines and that can be used to determine a realistic correction factor for the reference sky spectrum. The number of lines that can be combined is limited by the fact that they should show an almost identical variability behaviour.

As a basis for the definition of suitable line groups, the airglow model developed for the Cerro Paranal sky-radiance model (Noll et al. 2012) was used. This semi-empirical model consists of a line list with line intensities for mean observing conditions and prescriptions for the correction of the line strength depending on molecular species, solar activity, season, time of night, and zenith distance of the target. The latter three input parameters can be retrieved from the FITS header of the sky spectrum file. The solar activity is traced by the solar radio flux at 10.7 cm, which can be provided either by the parameter SOLFLUX in the configuration file or by the corresponding monthly average (default) in a file offered by http://www.spaceweather.gc.ca. In the wavelength range from 0.3143 to 0.9228 μm, the line list consists of data taken from Cosby et al. (2006). They incorporated the emission line atlas of Hanuschik (2003) based on observations with the VLT high-resolution echelle spectrograph UVES (Dekker et al. 2000). To fill a gap at about 0.86 μm, this list was supplemented by unpublished UVES data of R. Hanuschik. At longer wavelengths, the calculated OH lines of Rousselot et al. (2000) were included. However, their line strengths were corrected for the Einstein factors of Goldman et al. (1998) instead of using the original ones of Mies (1974). This resulted in correction factors for OH band strengths between 0.38 and 2.06. Moreover, the flux decrease of airglow lines by molecular absorption in the lower atmosphere was corrected. To this end, Gaussian profiles for each airglow line with Doppler line widths for typical temperatures of about 200 K were convolved with the high-resolution 4\(\frac{\lambda}{\Delta \lambda} \approx 10^7\) Cerro Paranal annual-mean transmission curve for an airmass of 1.254.

4 Although the atmospheric transmission depends on airmass and weather conditions, only a fixed airglow flux correction was applied to avoid time-consuming calculations at very high resolution and the input of temperature and water vapour profiles. Moreover, the optical airglow atlas of Hanuschik (2003) is also characterised by a fixed transmission correction because the UVES mean spectra were used. For most observing conditions, the deviation of the true airglow absorption from the assumed one is expected to be minor in terms of the results of skycorr.
The Cerro Paranal sky model assigns the listed lines to the five different variability classes (1) green OI, (2) Na ID, (3) red OI, (4) OH, and (5) O2 (see Noll et al. 2012). These variability classes result from analysing a sample of 1189 optical FORS1 spectra (Patat 2008). From this sample, the lines’ dependence on solar radio flux and time of observation was derived. The latter was quantified using a grid of six-two-month periods starting with Dec./Jan. and three night-time bins of equal length. The reference line strengths in the line list represent the mean of the five solar activity cycles 19 to 23, that is, the years 1954 to 2007. The ratios of line strengths of different variability classes can easily vary by a factor of two and more.

Assigning airglow lines to the five classes using the rough predictions from the sky model is not sufficient for achieving a line intensity accuracy on the percent level, which is required for a sky-subtraction procedure like Skycorr. Typically, intensity variations of lines within a variability class are stronger than can be tolerated.

In principle, an identical variability behaviour can be expected for transitions with the same upper state. In this case, the ratios of line intensities should be fixed and only determined by quantities such as Einstein coefficients and statistical weights. On the other hand, the excitation and population of different energy levels depends on variable quantities such as temperature and chemical abundances. Therefore, it is promising to define line groups depending on the upper energy level. However, taking all relevant states of the molecules OH and O2 into account would result in very many line groups. Moreover, each group would consist of only a few significant lines. This would result in statistical fluctuations, which could make the line intensity correction uncertain if crucial lines of a group were affected for example by detector defects or object emission lines (see Sect. 2.5). Fortunately, as their energies are very different, it is possible to separate electronic, vibrational, and rotational transitions of molecules. The electronic/vibrational transition determines the band and the rotational transition identifies a single line or doublet (as in case of OH) within a band. Since the distribution of energy levels is very similar for all bands of an electronic transition, each line can be assigned to two different classes that are defined by the upper vibrational and rotational state. This approach reduces the number of required line groups significantly. Moreover, for OH only the electronic ground state is relevant, which splits up into the sub-levels \( ^3 \Pi_{1/2} \) and \( ^3 \Pi_{3/2} \) because of the coupling of spin and orbital angular momentum (see Rousselot et al. 2000). For O2, the electronic transitions are more important than the vibrational ones, since the intensity differences of the bands of an electronic transition are very large. Consequently, there are only three O2 bands that significantly contribute to the airglow, namely \( \text{O}_2(b-X)(0–1)^g \) (the very strong (0–0) band is almost completely absorbed in the lower atmosphere), \( \text{O}_2(a-X)(0–0) \), and \( \text{O}_2(a-X)(0–1) \) (see Khomich et al. 2008). The O2 bands at near-UV and blue wavelengths are weak and can only be resolved at very high resolution. For most instruments, these bands therefore appear as a pseudo-continuum.

Tables 2 and 3 list the final grouping of airglow lines. Line groups with the same upper electronic/vibrational level are called \( A \) groups and those with the same (OH) or a similar (O2) upper rotational level are labelled \( B \) groups. Most OH bands (apart from a few very weak ones) are identified in Figs. 4 and 5. Although bands such as \( \text{OH}(4–1) \) and \( \text{OH}(4–2) \) have the same upper vibrational level, they represent independent variability groups. Since real data suffer from calibration uncertainties, this procedure is necessary, even though the number of \( A \) groups increases significantly. Because OH bands with the same upper vibrational level are widely separated, it is safer to vary these bands independently. Figures 6–9 show identifications of the rotational \( B \) groups for \( \text{OH}(4–2) \) as an example of an OH band, \( \text{O}_2(b-X)(0–1) \), \( \text{O}_2(a-X)(0–0) \), and \( \text{O}_2(a-X)(0–1) \), respectively. Although the two \( \text{O}_2(a-X) \) bands belong to the same roto-vibrational system, their \( B \) groups were defined separately because of the completely different line flux distribution. This

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5 The calculated OH line spectrum of Rousselot et al. (2000) covers a wider wavelength range (0.614–2.624 \( \mu \)m) than the published atlas related to observations with the VLT spectrograph ISAAC (0.997–2.252 \( \mu \)m).

6 The notation used is as follows: molecule (upper – lower electronic state) (upper – lower vibrational state). The letters \( a \), \( b \), and \( X \) are shortcuts for the states \( \Delta \gamma, \beta \Sigma^+ \), and \( \chi \Sigma^+ \). The vibrational states are numbered depending on the energy and starting from 0 for the lowest level.
Table 2. Description of A groups in the input line list.

<table>
<thead>
<tr>
<th>ID</th>
<th>Nlin</th>
<th>λ range [μm]</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>61</td>
<td>0.314–0.872</td>
<td>green O I at 557.7 nm + unidentified lines</td>
</tr>
<tr>
<td>2</td>
<td>3</td>
<td>0.589–0.770</td>
<td>Na ID + other lines from alkali metals</td>
</tr>
<tr>
<td>3</td>
<td>23</td>
<td>0.389–0.845</td>
<td>red O I at 630.0 nm + other thermospheric lines</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>0.467–0.467</td>
<td>OH(7–0)</td>
</tr>
<tr>
<td>5</td>
<td>8</td>
<td>0.491–0.495</td>
<td>OH(8–1)</td>
</tr>
<tr>
<td>6</td>
<td>22</td>
<td>0.519–0.536</td>
<td>OH(9–2)</td>
</tr>
<tr>
<td>7</td>
<td>12</td>
<td>0.526–0.535</td>
<td>OH(6–0)</td>
</tr>
<tr>
<td>8</td>
<td>23</td>
<td>0.554–0.570</td>
<td>OH(7–1)</td>
</tr>
<tr>
<td>9</td>
<td>41</td>
<td>0.587–0.634</td>
<td>OH(8–2)</td>
</tr>
<tr>
<td>10</td>
<td>49</td>
<td>0.624–0.655</td>
<td>OH(9–3)</td>
</tr>
<tr>
<td>11</td>
<td>2</td>
<td>0.672–0.674</td>
<td>OH(10–4)</td>
</tr>
<tr>
<td>12</td>
<td>27</td>
<td>0.614–0.695</td>
<td>OH(5–0)</td>
</tr>
<tr>
<td>13</td>
<td>83</td>
<td>0.647–0.754</td>
<td>OH(6–1)</td>
</tr>
<tr>
<td>14</td>
<td>113</td>
<td>0.681–0.782</td>
<td>OH(7–2)</td>
</tr>
<tr>
<td>15</td>
<td>111</td>
<td>0.720–0.815</td>
<td>OH(8–3)</td>
</tr>
<tr>
<td>16</td>
<td>72</td>
<td>0.768–0.822</td>
<td>OH(9–4)</td>
</tr>
<tr>
<td>17</td>
<td>7</td>
<td>0.827–0.839</td>
<td>OH(10–5)</td>
</tr>
<tr>
<td>18</td>
<td>85</td>
<td>0.745–0.910</td>
<td>OH(4–0)</td>
</tr>
<tr>
<td>19</td>
<td>113</td>
<td>0.781–0.914</td>
<td>OH(5–1)</td>
</tr>
<tr>
<td>20</td>
<td>111</td>
<td>0.826–0.916</td>
<td>OH(6–2)</td>
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<tr>
<td>21</td>
<td>110</td>
<td>0.873–0.937</td>
<td>OH(7–3)</td>
</tr>
<tr>
<td>22</td>
<td>116</td>
<td>0.931–1.007</td>
<td>OH(8–4)</td>
</tr>
<tr>
<td>23</td>
<td>120</td>
<td>0.994–1.081</td>
<td>OH(9–5)</td>
</tr>
<tr>
<td>24</td>
<td>100</td>
<td>0.965–1.043</td>
<td>OH(3–0)</td>
</tr>
<tr>
<td>25</td>
<td>110</td>
<td>1.015–1.098</td>
<td>OH(4–1)</td>
</tr>
<tr>
<td>26</td>
<td>112</td>
<td>1.069–1.168</td>
<td>OH(5–2)</td>
</tr>
<tr>
<td>27</td>
<td>118</td>
<td>1.129–1.236</td>
<td>OH(6–3)</td>
</tr>
<tr>
<td>28</td>
<td>120</td>
<td>1.197–1.314</td>
<td>OH(7–4)</td>
</tr>
<tr>
<td>29</td>
<td>124</td>
<td>1.275–1.420</td>
<td>OH(8–5)</td>
</tr>
<tr>
<td>30</td>
<td>128</td>
<td>1.366–1.531</td>
<td>OH(9–6)</td>
</tr>
<tr>
<td>31</td>
<td>112</td>
<td>1.392–1.558</td>
<td>OH(2–0)</td>
</tr>
<tr>
<td>32</td>
<td>118</td>
<td>1.461–1.654</td>
<td>OH(3–1)</td>
</tr>
<tr>
<td>33</td>
<td>122</td>
<td>1.537–1.743</td>
<td>OH(4–2)</td>
</tr>
<tr>
<td>34</td>
<td>122</td>
<td>1.622–1.842</td>
<td>OH(5–3)</td>
</tr>
<tr>
<td>35</td>
<td>124</td>
<td>1.717–1.978</td>
<td>OH(6–4)</td>
</tr>
<tr>
<td>36</td>
<td>126</td>
<td>1.825–2.110</td>
<td>OH(7–5)</td>
</tr>
<tr>
<td>37</td>
<td>130</td>
<td>1.951–2.265</td>
<td>OH(8–6)</td>
</tr>
<tr>
<td>38</td>
<td>130</td>
<td>2.101–2.485</td>
<td>OH(9–7)</td>
</tr>
<tr>
<td>39</td>
<td>450</td>
<td>0.314–0.532</td>
<td>O2(A-X) (Herzberg I)</td>
</tr>
<tr>
<td>40</td>
<td>5</td>
<td>0.324–0.410</td>
<td>O2(c-X) (Herzberg II)</td>
</tr>
<tr>
<td>41</td>
<td>396</td>
<td>0.326–0.550</td>
<td>O2(A′–a) (Chamberlain)</td>
</tr>
<tr>
<td>42</td>
<td>65</td>
<td>0.382–0.509</td>
<td>O2(c-b)</td>
</tr>
<tr>
<td>43</td>
<td>208</td>
<td>0.656–0.806</td>
<td>O2(b-X) (v′ &gt; v″)</td>
</tr>
<tr>
<td>44</td>
<td>194</td>
<td>0.761–0.816</td>
<td>O2(b-X) (v′ = v″)</td>
</tr>
<tr>
<td>45</td>
<td>103</td>
<td>0.861–0.922</td>
<td>O2(b-X) (v′ &lt; v″); including atm. 0–1 band)</td>
</tr>
<tr>
<td>46</td>
<td>161</td>
<td>1.240–1.305</td>
<td>O2(a-X)(0–0) (IR atmospheric system)</td>
</tr>
<tr>
<td>47</td>
<td>73</td>
<td>1.555–1.598</td>
<td>O2(a-X)(0–1) (IR atmospheric system)</td>
</tr>
</tbody>
</table>

Fig. 5. A-group identifications of the OH bands (cf. Table 2) in the wavelength range between 0.95 and 2.05 μm. The wavelengths and zenithal mean fluxes tabulated in the input line list are plotted.

Table 3. Description of B groups in the input line list.

| ID | Molecule | Upper state(s) | Remarks
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>OH</td>
<td>X′′11/2, J′ = 1/2</td>
<td>Q2(0.5), P2(1.5)</td>
</tr>
<tr>
<td>2</td>
<td>OH</td>
<td>X′11/2, J′ = 3/2</td>
<td>Q1(1.5), P1(2.5)</td>
</tr>
<tr>
<td>3</td>
<td>OH</td>
<td>X′21/2, J′ = 3/2</td>
<td>R2(0.5), Q2(1.5), P2(2.5)</td>
</tr>
<tr>
<td>4</td>
<td>OH</td>
<td>X′21/2, J′ = 5/2</td>
<td>R1(1.5), Q1(2.5), P1(3.5)</td>
</tr>
<tr>
<td>5</td>
<td>OH</td>
<td>X′21/2, J′ = 5/2</td>
<td>R2(1.5), Q2(2.5), P2(4.5)</td>
</tr>
<tr>
<td>6</td>
<td>OH</td>
<td>X′′11/2, J′ = 7/2</td>
<td>R2(1.5), Q1(3.5), P1(4.5)</td>
</tr>
<tr>
<td>7</td>
<td>OH</td>
<td>X′′11/2, J′ = 7/2</td>
<td>R2(1.5), Q1(3.5), P1(4.5)</td>
</tr>
<tr>
<td>8</td>
<td>OH</td>
<td>X′′11/2, J′ = 9/2</td>
<td>R2(3.5), Q2(4.5), P2(5.5)</td>
</tr>
<tr>
<td>9</td>
<td>OH</td>
<td>X′′11/2, J′ = 11/2</td>
<td>R1(4.5), Q1(5.5), P1(6.5)</td>
</tr>
<tr>
<td>10</td>
<td>OH</td>
<td>X′′11/2, J′ = 11/2</td>
<td>R1(4.5), Q1(5.5), P1(6.5)</td>
</tr>
<tr>
<td>11</td>
<td>O2</td>
<td>σ′ν′, J′ = 0, 2, 4</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>O2</td>
<td>σ′ν′, J′ = 6, 8</td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>O2</td>
<td>σ′ν′, J′ = 8, 12</td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>O2</td>
<td>σ′ν′, J′ = 14, 16</td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>O2</td>
<td>a′Δν′, J′ = 2, 4</td>
<td>v′ = 0</td>
</tr>
<tr>
<td>16</td>
<td>O2</td>
<td>a′Δν′, J′ = 6, 8</td>
<td>v′ = 0</td>
</tr>
<tr>
<td>17</td>
<td>O2</td>
<td>a′Δν′, J′ = 10, 12</td>
<td>v′ = 0</td>
</tr>
<tr>
<td>18</td>
<td>O2</td>
<td>a′Δν′, J′ = 14, 16</td>
<td>v′ = 0</td>
</tr>
<tr>
<td>19</td>
<td>O2</td>
<td>a′Δν′, J′ = 18, 20</td>
<td>v′ = 0</td>
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<tr>
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<td>O2</td>
<td>a′Δν′, J′ = 20, 22</td>
<td>v′ = 0</td>
</tr>
<tr>
<td>21</td>
<td>O2</td>
<td>a′Δν′, J′ = 24</td>
<td>v′ ≠ 0</td>
</tr>
<tr>
<td>22</td>
<td>O2</td>
<td>a′Δν′, J′ = 6, 8</td>
<td>v′ ≠ 0</td>
</tr>
<tr>
<td>23</td>
<td>O2</td>
<td>a′Δν′, J′ = 10, 12</td>
<td>v′ ≠ 0</td>
</tr>
<tr>
<td>24</td>
<td>O2</td>
<td>a′Δν′, J′ = 14, 16</td>
<td>v′ ≠ 0</td>
</tr>
</tbody>
</table>

Notes. \(^{(1)}\) OH rotational transitions (identified by the branch and total angular momentum of the lower state \(J^\prime\)) or lower vibrational level \(v′\) for \(O_2(a-X)\) transitions.

25. Airglow line fitter
To prepare a reference sky line spectrum for the sky subtraction in a science spectrum, the line fluxes have to be adapted. To this end, Davies (2007) divided the wavelength range into sections depending on the OH band structure and subsequently scaled

is caused by self-absorption in the \((0-0)\) band. B groups of \(O_2\) bands consist of lines from two rotational upper levels to ensure that enough lines can be identified for the group scaling (see Sect. 2.5). The weak lines of each band are not included in a B group, since they are difficult to fit. Furthermore, this measure avoids a degeneration of fit parameters.

The described grouping is more complex than that of Davies (2007), since Davies only incorporated near-IR OH bands, \(O_2(a-X)(0-0)\), and two rotational groups resembling our \(B\) and \(B^4\) classes (see Table 3).
Fig. 6. B-group identifications of the transitions of an OH band with the same rotational upper state (cf. Table 3). The tabulated wavelengths and zenithal mean fluxes of the lines of the OH(4–2) band are shown as example. Dashed and solid lines indicate transitions of the $X^2\Pi_{1/2}$ and $X^2\Pi_{3/2}$ state. The figure also indicates the R-, Q-, and P-branches that correspond to transitions with a change of the total angular momentum by −1, 0, and 1, respectively.

Fig. 7. B-group identifications of the transitions of the band $O_2(b-X)(0–1)$ with a similar rotational upper state (cf. Table 3). The tabulated wavelengths and zenithal mean fluxes of the lines of the 4 different branches (2 R- and 2 P-branches) are shown (cf. Fig. 6).

Fig. 8. B-group identifications of the transitions of the band $O_2(a-X)(0–0)$ with a similar rotational upper state (cf. Table 3). The tabulated wavelengths and zenithal mean fluxes of the lines of the 9 different branches (3 R-, 3 Q-, and 3 P-branches) are shown (cf. Fig. 6). The band is strongly affected by self-absorption in the lower atmosphere.

Fig. 9. B-group identifications of the transitions of the band $O_2(a-X)(0–1)$ with a similar rotational upper state (cf. Table 3). The tabulated wavelengths and zenithal mean fluxes of the lines of the 9 different branches (3 R-, 3 Q-, and 3 P-branches) are shown (cf. Fig. 6).

these segments independently according to the sections’ flux ratio of the science and sky spectra. This can be problematic where different line groups have significant overlap. While OH bands in H-band spectra do not significantly overlap and are not blended with strong bands of other molecules, at lower wavelengths the situation is less favourable (see Sect. 2.4). Even so, it is difficult to measure the scaling factors for groups with the same upper rotational level. Here, the flux of individual lines has to be derived, which requires that the selected lines are isolated. Typically, this is not the case for Q transitions, which are characterised by a constant total angular momentum (see Fig. 6). Furthermore, the separation of variability groups becomes even more difficult if the spectral resolution is relatively low.

To overcome these limitations, skycorr uses a completely different approach to obtain the scaling factors for the different line groups defined in Sect. 2.4. In skycorr, the contributions of the line groups to each pixel of the sky spectrum are estimated. Subsequently, the resulting spectra for each line class are scaled. This is performed by applying the airglow model presented in the previous section. The wavelengths and intensities of the lines and their group identifications can be converted into intensities of the different line groups for each pixel. This requires a convolution of the lines from the line list with a kernel similar to the instrumental profile of the observed spectra. The mean FWHM of the sky lines, which was obtained in a previous step (see Sect. 2.2), is used to create a sufficiently realistic Gaussian kernel. To treat intensity ratios of overlapping lines as realistically as possible, the airglow variability model from Noll et al. (2012) (see Sect. 2.4) was included. This allows one to roughly correct for the influence of solar activity, season, and time of night on the main line variability classes green O I, Na I D, red O I, OH, and O2.
When different line groups contribute to the same pixel, the sky scaling factors cannot be derived by a simple division of line fluxes of science and sky spectrum anymore. Instead, each scaling factor of the individual line groups has to be included in a fitting procedure as a free fitting parameter. For this purpose, the C version of the least-squares fitting library MPFIT by C. Markwardt\(^7\) based on the FORTRAN fitting routine MINPACK-1 by Moré et al. (1980) is used. The \(\chi^2\) minimisation procedure of this routine is based on a Levenberg-Marquardt technique, an iterative search algorithm characterised by gradient-controlled jumps in parameter space. Since this technique is potentially prone to find local minima, reasonable start values and constraints on the fit parameters are required. For this reason, the mean ratios of the line peaks in the science and sky spectrum are determined for each line group (see Sect. 2.4). Only the spectrum pixels are included that were identified as line peaks (see Sect. 2.1) or are separated from peaks by not more than half the line FWHM (see Sect. 2.2) and have a relative contribution of the selected line group of at least WEIGHT (default: 0.67; see Table 1). Moreover, pixels with unreasonable flux ratios are rejected by applying a global \(\sigma\) limit that is derived from the full set of line peaks and is provided by the parameter SIGLIM (default: 15; see Table 1). In this way, strong object emission lines can be identified in the science line spectrum and excluded. Finally, the \(\sigma\)-clipping approach with variable \(\sigma\) limit described in Sect. 2.2 is applied to the selected pixels of each group separately to further improve the pixel selection. The remaining pixels of this procedure are taken for the initial line group scaling and fitting algorithm, meaning that only these pixels are considered for the \(\chi^2\) calculation. If suitable pixels cannot be found for a line group, a mean flux ratio of the corresponding system of roto-vibrational bands (e.g. OH; see Sect. 2.4) or a global flux ratio is taken for \(A\) groups and a value of 1 is assumed for \(B\) groups. For most sky spectra, this approach is expected to result in a good first guess sufficient for achieving a rapid convergence to the global minimum.

As an option, the fitting can be restricted to uncertain line groups alone. The decision on the group selection depends on the parameter FITLIM (see Table 1), which provides a limiting ratio of the root mean square (rms) and the mean of the group-specific scaling factors. By default, this value is set to 0, meaning that all fitting line groups are considered.

### 2.6. Correction of wavelength grid

Since the sky lines of the science spectrum are removed by a scaled reference sky line spectrum, it is imperative that the wavelength grids of both spectra are aligned. Differences of less than a pixel can already significantly deteriorate the quality of the sky subtraction. Relatively large deviations can occur if a lamp spectrum taken in daytime at different ambient conditions as the science spectrum is used for the wavelength calibration. However, even subpixel shifts that are routinely observed in data taken under perfect conditions can cause problems.

For this reason, skycorr offers an optional correction of the wavelength grid by applying a Chebyshev polynomial of degree \(n_w\)

\[
\chi^2 = \sum_{i=0}^{n_\text{w}} c_i t_i,
\]

where

\[
t_i = \begin{cases} 1 & \text{for } i = 0 \\ 4 & \text{for } i = 1 \\ 2 \lambda t_{i-1} - t_{i-2} & \text{for } i \geq 2 \end{cases}
\]

and \(\lambda\) ranging from \(-1\) to \(1\). The temporary conversion of the wavelength grid to a fixed interval results in coefficients \(c_i\) independent of the wavelength range and step size of the input spectrum. The wavelength solution is not changed if \(c_1 = 1\) and \(c_i = 0\) for all other \(i\). It is possible to set an individual start value for the constant term \(c_0\) via the parameter CHEBY_CONST (see Table 1). In this way, significant possible shifts between the wavelength grids of the science and the sky spectrum can be considered.

The coefficients \(c_i\) are determined by an iterative procedure. This process is initialised with two subsequent estimates (for a better \(\sigma\)-clipping) and a fit of the line flux correction factors (see Sect. 2.5). During this first iteration the wavelength grid remains untouched. In the next step, the coefficients \(c_0\) and \(c_1\) are fitted using MPFIT. Now, a new \(\sigma\) and the constant radius and the line flux correction factors are fitted again. Then, the next iteration starts by fitting the wavelength grid, now applying a Chebyshev polynomial of degree 2. After that, the line scaling factors are adapted again to incorporate the change of the wavelength grid. Each iteration increases \(n_w\) by 1 and uses the results of the previous iteration as input. The search for the best polynomial degree is controlled by the three input parameters CHEBY_MIN, CHEBY_MAX, and WTOL (see Table 1). The iteration process is stopped once the highest polynomial degree given by CHEBY_MAX is reached. For a value of \(-1\), no wavelength grid correction is performed. The parameter CHEBY_MIN indicates the lowest degree, that is to say, the smallest number of iterations. For \(n_w\) not lower than CHEBY_MIN, the code checks whether the resulting \(\chi^2\) shows a relative \(\chi^2\) improvement of at least WTOL (default: 1 \times 10^{-5}) compared with the best \(\chi^2\), so far. If this is not the case, the procedure stops and the results for the polynomial with the lowest \(\chi^2\) are taken. An exception is when CHEBY_MIN > CHEBY_MAX is chosen. In this case, the code runs until CHEBY_MAX is reached and the corresponding results for this degree are taken, regardless of the results for the lower polynomial degrees. The default values for CHEBY_MAX and CHEBY_MIN are 7 and 3.

Independent of the use of a Chebyshev polynomial, the modified sky spectrum has to be rebinned to the wavelength grid of the science spectrum. For this task, the code offers two options that can be selected by the parameter REBINTYPE (see Table 1). The first method sums the fractional fluxes of input pixels that contribute to the wavelength range of the output pixel. The second approach is based on the convolution of the input spectrum with a pixel-dependent asymmetric damped sinc kernel

\[
f(k) = e^{-\left(\frac{k-\delta}{\delta_0}\right)^2} \frac{\sin(\pi(k-s))}{\pi(k-s)},
\]

with \(k\) being an integer variable ranging from \(-k_{\text{max}}\) to \(k_{\text{max}}\). The damping constant \(\delta\) and the kernel radius \(k_{\text{max}}\) are fitted and have the values 3.25 and 5. The parameter \(s\) is the subpixel shift of the sky spectrum relative to the science spectrum. It is a function of the pixel position and ranges from \(-0.5\) to 0.5. For shifts higher than half a pixel, complete pixels are treated by a simple renumbering of the input pixels in the output spectrum. No convolution is performed for this integer part of the pixel shift. The approach is similar to that used in the IDL routine sshift2d.pro of the Lowell Buie Library\(^8\). However, the

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7 http://www.physics.wisc.edu/~ craigm/idl/cmpfit.html

original programme is only for a constant shift of the entire spectrum. A wavelength-dependent shift is also possible, as long as the shift changes slowly with the spectrum pixels and the pixel size is nearly constant for the whole input and output wavelength grids. These requirements are sufficiently met if inconsistencies of the wavelength grids are in the order of 1 pixel and if the functional dependence of the differences can be described by a low-order polynomial. The relatively complicated rebinning method described above is able to effectively suppress the broadening of spectral lines, which typically occurs if a spectrum is rebinned to a shifted grid of similar pixel size. The line-broadening suppression is achieved by alternating positive and negative contributions to the kernel as incorporated in the sinc shift method. Therefore, the sinc shift method produces the best results if significant subpixel shifts close to half a pixel are frequent. However, for a very good agreement of the wavelength grids with subpixel shifts close to zero, it might be better to use the simple rebinning method. In such a case, the relatively broad sinc kernel influences the spectrum more than simple regridding.

3. Test data set

To illustrate the performance of skycorr, we used data taken with the VLT echelle spectrograph X-shooter (Vernet et al. 2011). This instrument is well suited for testing sky subtraction, since its three arms UVB, VIS, and NIR cover the entire wavelength range affected by significant airglow emission. In fact, wavelengths from 0.3 to 2.5 μm can be observed simultaneously with medium resolution between 3300 and 18 200 depending on the arm and the selected slit widths. Since X-shooter is a slit spectrograph9, the performance of skycorr can be compared with the classical sky-subtraction method based on the interpolation of 2D data.

We also investigated the skycorr performance for data taken with other instruments. The skycorr user manual that is provided along with the code also shows several VLT FORS and SINFONI examples.

3.1. Sample selection and data reduction

To analyse the sky-subtraction quality as a function of time, we searched for a time series of a single target in the ESO archive. We decided to use the observations of the ESO programme 288.D-5015, which was carried out on 25 Dec. 2011 between 0:58 and 3:25 UT and comprises 12 UVB, 24 VIS, and 80 NIR-arm spectra with exposure times of 606, 294, and 100 s, respectively (see Set 1 in Table 4). The observed object was the ultracool white dwarf SDSS 0138-0016 (see Parsons et al. 2012). The spectrum is characterised by a maximum emission at about 1 μm, absorption bands in the near-IR, and also emission lines of the time interval between the mid-exposures of the sky and the object observations.

The X-shooter data were reduced using the ESO public pipeline release V2.0.0 executed with the Reflex workflow V2.3 (see Modigliani et al. 2010). To obtain the sky-subtraction results for the 2D interpolation method, we directly used the output pipeline 1D spectra. For the correction with skycorr, we reduced the data without sky subtraction and extracted the input spectra for skycorr from the resulting 2D spectra. For the object spectrum, we applied a wavelength-independent trace based on the median object flux in spatial direction. Pixels masked by the pipeline were excluded from the extraction, and the summed object flux was scaled to correct for missing pixels using the object profile. This approach is similar to the method used by the pipeline. However, by doing it ourselves, we know the exact sky area that contributes to each wavelength. This information is important for extracting the sky from the 2D spectra. Here, we computed the median along the spatial direction and scaled the resulting spectrum to have the same sky area as the reference object spectrum. The data set was not flux calibrated, since the instrument response and the atmospheric extinction (the latter at least for the VIS and NIR arm) only slowly vary with wavelength and time compared with the defined airglow variability groups (see Sect. 2.4).

To test skycorr for sky data not taken in the same night as the reference object spectrum, we extended our sample by two additional data sets (see Sets 2 and 3 in Table 4). The observations had the same slit widths and long exposure times to avoid that the extracted median sky would be contaminated by a bright object. Set 2 was taken six nights earlier than the reference observations and comprises four spectra in each arm. Set 3 was taken about one year earlier in three subsequent nights and consists of seven exposures in each arm. Since the exposure times deviated from those of the reference data, the resulting 1D sky spectra were corrected for by the exposure time ratio.

3.2. Sample properties

Figure 10 provides an overview of the observing conditions for the investigated spectra. The data for each of the three subsamples (see Table 4) are displayed in separate panels as a function of the time interval between the mid-exposures of the sky and object observations.

The first row of panels (a) shows the change in airmass. The observation of a single target over 2.5 h in the main run results in a significant change in the airmass. This affects the airglow intensity because of the nearly proportional increase of the projected emission layer width (van Rhijn 1921; Noll et al. 2012).

The summed intensity of two P-line bands of the OH 3-1 band is shown in the next row of panels. Apart from the airmass-related van Rhijn effect, the intensity varies on different time scales because of changes of the chemical composition, temperature, and dynamics in the OH emission layer (see Khomich et al. 2008). For the entire data set, a highest ratio of 3 in the intensity can be observed, which illustrates the challenge in correcting for the sky in a science spectrum with data taken at a different

<table>
<thead>
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<th>Par.</th>
<th>Set 1</th>
<th>Set 2</th>
<th>Set 3</th>
</tr>
</thead>
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<td>4, 4, 4</td>
<td>7, 7, 7</td>
</tr>
<tr>
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<td>05:56–07:31</td>
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<td>1.0, 0.9, 0.9</td>
</tr>
<tr>
<td>Texp [s]</td>
<td>606, 294, 100</td>
<td>705, 609, 246</td>
<td>900, 900, 900</td>
</tr>
</tbody>
</table>

Notes. (a) The number of exposures Nexp, the slit width, and the exposure time Texp are given for the three X-shooter arms UVB, VIS, and NIR separated by commas. (b) The time range was derived from the start of the first exposure and the end of the last exposure of all three arms. For Set 3, it was neglected that the observations had been performed on three different nights.

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9 The IFU of X-shooter is an image slicer that converts a 4′′ × 1.8′′ field into a 12′′ × 0.6′′ pseudo-slit.
Fig. 10. Properties of the X-shooter NIR-arm test data and quality of the sky subtraction by skycorr as a function of time. The time difference $\Delta t$ is given relative to the object spectrum to be corrected for sky emission (2011/12/25 00:59:05 UT). The left, middle, and right panels characterise the sky data of the same night, about six nights before, and about one year before the object reference exposure, respectively. From top to bottom, the panels display a) the airmass, b) the summed intensity of two airglow lines of the OH(3–1) band, c) the ratio of the same lines tracing relative B-group variability, d) the ratio of the same rotational line in two different OH bands tracing the relative A-group variability, e) the ratio of two OH lines, which can only vary by effects unrelated to airglow, f) the sky continuum at 1.6 $\mu$m relative to the corresponding measurement in the uncorrected object spectrum, g) a similar ratio for 2.1 $\mu$m, h) the ambient temperature in K, and i) the rms of the sky-subtraction residuals for line pixels relative to the mean line peak flux. The latter is shown for two different minimum degrees of the Chebyshev polynomial for the improvement of the wavelength solution by skycorr. In the middle panel of i), the effect of an initial shift of the wavelength scale by one pixel is also plotted (dotted line).
time. The variations are not only caused by airglow variability. Changes of the instrument performance and calibration data can also have an effect. Moreover, variations in the atmospheric transparency can be important for non-photometric observations. This explains the dip in the intensity about 135 min after the start of the main run, when a small cloud probably covered the sky in the line of sight\textsuperscript{10}. Note that the decrease of the airglow intensity was moderate compared with the almost complete extinction of the object light. The difference is caused by the fact that the observed star is a point source, whereas airglow emission covers the entire sky. This allows a partial compensation of extinction losses by scattering of light from other sky positions into the line of sight (see Chamberlain 1961; Noll et al. 2012). Running skycorr with a sky spectrum taken under such unfavourable conditions is a good test of the applicability of the method in challenging situations.

Panels (c) to (e) of Fig. 10 show the time dependence of different line ratios. They indicate a weaker variability than the intensity. However, variations in the order of 10% for OH can still be critical for a reasonable correction of strong airglow lines. For this reason, the line groups described in Sect. 2.4 were introduced. While (c) shows an example of the time-dependent deviations between different \( B \) groups, (d) and (e) are examples of deviations in the intensity ratios of \( A \) groups. Since the bands in (e) have the same upper vibrational level \( v' = 5 \), the ratio should be constant if the airglow variability alone is considered. Therefore, the significant changes (especially if different observing runs are compared) trace the influence of instrumental effects and atmospheric transparency.

Panels (f) and (g) show the ratio of the sky and object+sky continuum for the wavelengths 1.6 and 2.1 \( \mu m \), respectively. Since the sky continuum cannot be adapted by skycorr (see Sect. 2), the variation of such ratios is critical for the quality of the continuum correction. In the \( H \) band, the sky continuum is weak. Except for the cloud event and the observations that were taken about one year before the object spectrum, the variation of the sky relative to the object is in the order of 1% only. Hence, continuum errors by the sky subtraction in the \( H \) band should be small as long as the observed object is not distinctly fainter than the investigated white dwarf. In the \( K \) band, the thermal emission by the telescope is a strong component. For our test data, the contribution is up to 60% at 2.1 \( \mu m \), which means that the telescope emission is about as strong as the object emission. The flux ratio in (g) is well correlated with the ambient temperature in (h), which determines the mirror temperature. The temperature deviated by up to 4.6 K from the value of 14.7 K for the reference exposure. Because of the strong variability, a good thermal continuum subtraction appears to be difficult to achieve in this wavelength regime if an object is not significantly brighter than the thermal emission, and/or the temperature differences between the object and sky exposures are not distinctly lower than 1 K. At least in the case of X-shooter, the strong variations in the \( K \) band might also partly be related to instabilities of the flat-field lamps (Vernet, priv. comm.). Hence, the continuum subtraction for Set 2 and 3 could be improved by using the same flat-field as for Set 1. For flux-calibrated spectra, which we did not analyse, the use of the same flat-field during the reduction of the science and standard star spectra is the default setting in the X-shooter pipeline Reflex workflow.

4. Results

In the following, we evaluate the performance of skycorr on the data set discussed in Sect. 3. At first, the test approach is described (Sect. 4.1). Then, the performance of skycorr is compared with the 2D sky interpolation method applied by the X-shooter pipeline (Sect. 4.2). This test can only be carried out if there is no time difference between the science and the sky spectra. Next, the performance is analysed for different time intervals by using the entire test data set (Sect. 4.3). Finally, we compare the results of skycorr with those obtained without line scaling (Sect. 4.4) and using the method of Davies (2007) for our test data (Sect. 4.5).

4.1. Test approach

For the test runs, we used a fixed set-up of the parameters listed in Table 1. Since skycorr was optimised to minimise user interaction, most parameter values agree with the listed default values. The parameter VAC\_AIR was set to “air” because the X-shooter pipeline provides wavelengths in air. Since the X-shooter spectra have a sufficiently high resolution, some parameters can be modified to speed up the code without deteriorating the results. Setting FLUX\_lim = 0.005 switches off the iterative search of continuum windows between the lines (see Sect. 2.1) without changing the result. We also modified the FWHM and \( \chi^2 \) convergence criteria LTOL (1 \( \times \) 10\(^{-11} \)) and FTOL (1 \( \times \) 10\(^{-5} \)), which did not negatively affect the sky-subtraction quality. For X-shooter NIR-arm spectra with about 25000 pixels, the run times were measured to be between 12 and 25 s\textsuperscript{11}, mainly depending on the number of calculated polynomials of different degrees (see Sect. 2.6). Without changing the parameters discussed above, the run times would have been between 12 and 36 s. Since X-shooter spectra cover a wide wavelength range that is characterised by a roughly linear increase of the width of the line profile in pixels, we set VAR\_FWHM to 1 (see Sect. 2.2). Finally, we reduced SIG\_LIM (Sect. 2.5) from the default value 15 to 5, since the test spectra show many outliers due to bad pixels and not all of them were masked by the pipeline.

Skycorr produces an output ASCII file that includes the best-fit parameters and several other quantities that can be used to evaluate the sky-subtraction quality. In particular, the file provides the rms of the error-weighted sky-subtraction residuals (no continuum) for line pixels relative to the error-weighted mean line peak flux. The weights depend on the statistical noise and possible systematic errors by bad pixels and similar defects. The selection of line pixels originates from the line–continuum separation discussed in Sect. 2.1. The relative rms, as defined above, has turned out to be a good indicator of the sky line subtraction quality and is used in the following. Good values are in the order of a few per cent.

4.2. Comparison with the 2D sky interpolation method

As a first test of the quality of the sky subtraction by skycorr, we compare the results for \( \Delta t = 0 \), that is to say, the science and sky spectrum taken from the same 2D spectrum, with those of the X-shooter pipeline. Figure 11 shows these resulting spectra in the three X-shooter arms. Both methods produce convincing spectra of the target star (cf. Parsons et al. 2012). In the UVB arm (0.30–0.59 \( \mu m \)), stellar emission lines can be seen. The VIS

\textsuperscript{10} This interpretation is consistent with data from ESO’s Ambient Conditions Database.

\textsuperscript{11} Run on a Core2Quad Q9550@2.83GHz, 8GB RAM, Fedora 19 (64 bit).
arm (0.53–1.02 μm) mainly reveals stellar absorption bands, and the NIR arm (0.99–2.48 μm) shows strong atmospheric absorption of the stellar continuum (essentially by water vapour bands). Note that the spectra are not flux calibrated (see Sect. 3.1). The UVB and VIS-arm spectra are only affected by relatively weak sky features compared with the object continuum (cf. Sect. 2.4). Therefore, a good sky correction is not particularly difficult for the given example. The situation is much more challenging in the X-shooter NIR-arm range, where the sky emission tends to be significantly brighter, reaching up to 1 to 2 orders of magnitude higher intensities than the stellar continuum. For this reason, we focus the tests in Sect. 4 on the NIR arm.

Despite the strong airglow lines, skycorr and the 2D interpolation method produce sky-corrected spectra with relatively smooth object continua. The strongest residuals can be identified as instrumental defects (bad pixels). The most obvious difference between the results of both methods is the deviation continua at the red margin of the NIR arm. This discrepancy can be explained by the very strong thermal background, intensity gradients along the spatial direction in the 2D spectra, and the differences in the extraction of the 1D spectra (see Sect. 3.1). Thus, the deviations are not related to the sky-subtraction quality. For a more quantitative comparison of this quality, we calculated the relative rms defined in Sect. 4.1. Interestingly, the skycorr output NIR-arm spectrum has a significantly smaller rms (0.027) than the corresponding pipeline spectrum (0.040). This result is robust. Modifying the considered wavelength range or the exclusion algorithm for unreliable rms outliers (bad pixels) did not change it significantly. Even though this is just one example and the approach for the extraction of the 1D spectra might influence the rms, skycorr appears to be able to subtract sky emission lines at least as well as a method that benefits from the full 2D spectral information.

4.3. Effect of time differences between science and sky spectra

The main purpose of skycorr is the subtraction of the sky emission in science spectra by means of sky data taken at a different time and sky position. Using the data set described in Sect. 3.1, the quality of this correction can be investigated as a function of time. In Sect. 3.2, we have discussed the sky variability during the selected observing runs on the basis of the data plotted in Fig. 10. The last row of this figure shows the relative rms (see Sect. 4.1) for the NIR-arm spectra of the test data set. For the skycorr parameter set-up listed in Table 1 (black symbols and lines), the left-hand panel indicates a gradual increase of the rms from 0.027 at the beginning, over 0.067 at half of the time, to 0.098 at the end of the run. A special situation occurred at Δt ≈ 132 min with a maximum rms of 0.145. As discussed in Sect. 3.2, a cloud probably covered the sky in the target direction. This caused a significant decrease of the sky-subtraction
quality. However, these results are still better than the sky correction performed with sky data taken six nights before. Here, the relative rms was about 0.26. The most noticeable difference in the atmospheric conditions with the reference object exposure was the OH emission intensity (middle panel in row (b)), which was almost twice as high. This probably contributes to the poorer performance of skycorr. However, a long time difference does not inevitably mean a poor sky-correction quality, as Set 3 in the right-hand panel demonstrates. Although the time interval was about one year, the rms values are between 0.10 and 0.18, which is significantly better than for $\Delta t = -6 \text{ d}$ and even comparable with the end of the main run. The OH intensity for Set 3 was closer to the reference value than for Set 2, but the discrepancies are still quite large. Moreover, rows (d) to (f) of Fig. 10 suggest significant differences in the instrumental properties and calibration (see Sect. 3.2).

To better understand the skycorr performance differences, Fig. 12 shows the sky-subtracted NIR-arm spectra for five different cases: $\Delta t = 0 \text{ min}$ (the reference exposure), $+75 \text{ min}$ (half of the time of the main run), $+132 \text{ min}$ (cloud), $-5.9 \text{ d}$ (first exposure of Set 2), and $-360.7 \text{ d}$ (first exposure of Set 3). In addition, Fig. 13 displays the input sky lines and the corresponding sky-subtraction residuals for the single strong airglow line OH(3–1)P1(2.5) (see Sect. 2.4). Figure 14 shows a similar plot for the only partly resolved O$_2$(a-X)(0–0) band, which is also blended with OH(8–5) lines. The figures confirm that the strongest sky line residuals are found for the cloud event and Set 2. The sky-corrected spectrum for the Set 3 example is an intermediate case. Further implications are discussed in the following paragraphs.

Concerning the continuum correction, the cloud event changed the thermal background in a way that the sky-corrected object continuum is completely wrong in the red part of the $K$ band (Fig. 12). Significant changes in the background can already be observed for $\Delta t = 75 \text{ min}$. Since the sky continuum cannot be adapted to changing observing conditions, the continuum correction especially in the red part of the $K$ band has to be taken with care if the object is distinctly fainter than the background (see Fig. 11).

As already indicated by Fig. 10, the intensities of the OH lines deviated the most from the reference exposure for the cloud event and Set 2. Figure 13 also reveals that these cases show a significant shift of the line centres. In particular, the Set 2 spectrum is shifted by about one pixel. Since the physical changes of airglow line positions are orders of magnitude too small to be visible in the X-shooter data, the shifts are probably caused by instrumental effects related for example to the position of the orders on the chip, variations in the wavelength calibration frames, or uncertainties in the determination of the wavelength solution by the pipeline. As the strong asymmetric residuals for the critical cases suggest, the wavelength shifts appear at least as important for the sky-subtraction quality as the intensity of the lines. Skycorr corrects the input wavelength solution by fitting Chebyshev polynomials, where the degree is increased in an iterative procedure (see Sect. 2.6). The default algorithm is a search that at least checks degree 3 and at most degree 7 (see Table 1). Interestingly, the critical cases were only checked up to the minimum degree CHEBY_MIN = 3. Therefore, we ran the code for CHEBY_MIN = 7, which significantly increased the code run time, but also improved the rms for the...
cloud event and Set 2, as Fig. 10 indicates (red symbols and lines in last row). Surprisingly, the best fit for the critical cases was achieved without changing the input wavelength solution. Hence, the iterative procedure appeared to mainly improve the fitting of the line intensities. The parameter CHEBY_CONST (see Table 1) allows a constant initial shift of the wavelength grid. By setting it to $-8 \times 10^{-5}$, which corresponds to about one pixel for X-shooter NIR-arm spectra, we can compensate for the shift found for the Set 2 example. The resulting rms is also shown in Fig. 10. For the selected Set 2 spectrum, it decreased from 0.26 to 0.11. This striking improvement suggests that the fitting procedure of the standard run did not find the global $\chi^2$ minimum because of strong differences in the airglow intensities and wavelength grids of the input science and sky spectra. In such critical cases, the skycorr parameter set-up can be optimised.

For blended O$_2$ lines, Fig. 14 indicates that the most significant residuals are again found in the cloud case and Set 2. Nevertheless, the situation is different since the O$_2$ lines showed a completely different time dependence as the OH. This can be seen at wavelengths beyond 1.275 $\mu$m, where both kinds of lines are present. At $\Delta t = 0$, the O$_2$ band was distinctly brighter than for all other examples plotted. In particular, the observations of Sets 2 and 3 showed intensities that were lower by a factor of 5 to 6. In view of the required strong intensity corrections and the blending of lines with different variability, the quality of the recovered stellar continuum is remarkably good. Only the spectrum related to the cloud shows significant continuum offsets at the wavelengths where line blending is most critical. The target spectrum retrieval can be more difficult than in the present case if the observed object has a complex spectrum in the range of the O$_2$ band. Then, the separation of blended sky lines and continuum could be systematically wrong, which would be a problem if the airglow lines need to be scaled by factors far from 1. The sky line subtraction at about 1.27 $\mu$m is certainly the most difficult for X-shooter. For lower resolution spectra, additional wavelength ranges with blended sky lines could have similar problems.

The NIR-arm spectrum of SDSS 0138-0016 (see Fig. 11) does not allow the test of how object emission lines would appear after the subtraction of strong sky lines at similar wavelengths. For this reason, we carried out a challenging test by multiplying the strong OH line in Fig. 13 by 1.5 in the object spectrum and running skycorr with the full data set for this modified input spectrum. This modification simulates an object emission line with the position, shape, and 50% of the intensity of the OH line. Figure 15 shows the sky-subtraction results for the five selected cases compared with the expected object spectrum. Apart from the $\Delta t = 0$ and 75 min cases, which indicate different in both panels. The two strong uncorrected lines in the centre and the left margin of the figure were caused by instrumental defects. Longwards of 1.275 $\mu$m, the O$_2$ lines are blended with OH(8–5) lines.

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**Fig. 13.** Subtraction of the strong airglow line OH(3–1)P1(2.5) for several time intervals between the object and the sky spectrum. The upper panel shows the line in the input object (black) and sky spectra (see legend for colour and line type). The lower panel displays the corresponding sky-subtraction residuals. To enhance their visibility, the ordinate was significantly zoomed.

**Fig. 14.** Subtraction of the strong and only partly resolved airglow band O$_2$(a-X)(0–0) (cf. Fig. 8) for several time intervals between the object and the sky spectrum. The upper panel shows the band in the input object (black) and sky spectra (see legend for colour and line type). The lower panel displays the corresponding sky-subtraction residuals. Note that the ordinates are different in both panels. The two strong uncorrected lines in the centre and the left margin of the figure were caused by instrumental defects. Longwards of 1.275 $\mu$m, the O$_2$ lines are blended with OH(8–5) lines.
Fig. 15. Subtraction of the strong OH(3–1)P1(2.5) line from an object spectrum with an artificial emission line (black) at the same position and with the same line shape but only 50% of the strength of the sky line. The sky-correction results are shown for several time intervals between the object and the sky spectrum (see legend for colour and line type).

Fig. 16. Comparison of the rms of the sky-subtraction residuals relative to the mean line peak flux (see Sect. 4.1) by skycorr (red) and without line scaling (black) for the data set of the X-shooter NIR-arm sky spectra taken in the same night as the corrected object spectrum. The results are shown as a function of the time difference between the object and the sky spectrum.

4.4. Comparison with sky subtraction without scaling

Figure 16 shows the resulting rms of Set 1 for skycorr (cf. Fig. 10) and the sky spectrum just subtracted from the science spectrum without scaling. In the first 10 min, the rms was only slightly higher than for skycorr (ratios between 1.2 and 1.5). This indicates that for time intervals of a few minutes, a significant correlation of the sky line intensities can be assumed. Afterwards, the rms ratio was quickly increasing, reaching ratios up to 5.5. For Sets 2 and 3, the rms ratios ranged from 3.3 to 4.1 and from 2.4 to 5.1. These factors demonstrate that skycorr performs significantly better than a simple on-off technique without sky scaling. They also show that the latter method is only reliable for very short time differences.

4.5. Comparison with the Davies method

As far as we know, the method of Davies (2007) is the only existing approach with a similar philosophy and purpose as skycorr. For this reason, it is prudent to compare the performance of this method and skycorr. To this end, we attempted to run Davies’ IDL code for the X-shooter NIR-arm test data set defined in Sect. 3.1. Since the version 1.1 implemented in the currently released ESO SINFONI pipeline (Modgiliani et al. 2007) is already fairly old, we improved the results by using the most recent version 2.0. Since SINFONI is an IFU spectrograph (Eisenhauer et al. 2003), 3D data cubes with the spectra of a spatial 2D grid are required as input. However, Davies’ code also performs the sky line scaling on 1D spectra that are derived from the filtered and integrated cubes for object and sky observations. By replacing the internal 1D arrays for object and sky by the X-shooter input data and writing the sky-subtracted object array into a file (neglecting the subsequent application of the best solution to the object cube), we were able to run Davies’ code and to compare it with skycorr. The runs were performed with default parameters plus the thermal background subtraction and the wavelength scale correction (via cross correlation) switched on.

The test indicates that skycorr outperforms Davies’ algorithm for X-shooter data. The SINFONI-optimised Davies’ code appears to be unstable for the investigated data because of an erratically varying quality of the correction. Possible reasons are the much wider wavelength range than that of SINFONI, the higher resolution, the low S/N ratio, the numerous bad pixels, the use of non-flux-calibrated spectra, and a complex continuum that cannot be fitted by a single greybody. Despite the higher complexity, skycorr was also faster than the 1D part of Davies’ code, which might be related to the use of C instead of IDL.

For a fair comparison of skycorr and Davies’ method, we also considered SINFONI spectra, for which the latter method was designed and works reliably. To illustrate the performance of both codes for SINFONI data, we studied an H-band example (Fig. 17) and a K-band example (Fig. 18). Since we are interested in the results for significant time intervals, we did not use the sky cubes that belong to the object cubes. Instead, we took the sky cubes from other observations of the same observing programmes. In this way, time differences of 39 and 11 min for the H and K band could be achieved. The data were reduced with ESO’s SINFONI

![Image](https://example.com/image1.png)

![Image](https://example.com/image2.png)
pipeline. However, we used version 2.0 of Davies’ code for the sky subtraction, as already mentioned above. The code flags were the same as for the X-shooter data set. To run skycorr and the comparison in Figs. 17 and 18, we used the 1D spectra produced by Davies’ code.

For both examples, the two codes show a good performance, even though the objects are up to two orders of magnitude fainter than the sky. Nevertheless, the skycorr sky line residuals are significantly weaker. For shorter time intervals, the quality of the sky subtraction tends to be more similar, as other tests indicated. The corrected object continua show only slight deviations. For longer time intervals, this might change, as both codes use different algorithms for the continuum correction (see Sects. 1 and 2.3).

In conclusion, the algorithms implemented in skycorr seem to result in a consistently better sky subtraction. Our code is more robust and flexible, which means that it can reliably be applied to data of different instruments and set-ups.

5. Conclusions

We have presented a new method to subtract the sky in 1D spectra by means of optimised plain-sky spectra taken at different times and sky positions. This method, which will be provided to the community as software package skycorr, has been inspired by the approach described by Davies (2007), but it is more sophisticated. Important features are an iterative separation of sky lines and continuum, detailed line grouping based on an airglow model, pixel-based scaling of line groups, and an adaptation of the wavelength solution of the input sky spectra by Chebyshev polynomials and asymmetric damped sinc kernels. The sky correction of an input science spectrum consists of the subtraction of the best-fit scaled airglow lines and the separated continuum of the reference sky spectrum.

We have tested the performance of the instrument-independent code by means of X-shooter spectra. Fixing the object spectrum to be corrected, we have analysed the sky-subtraction quality for different time intervals between the science and plain-sky spectra. This comparison revealed promising results that depend on the change of the airglow intensity, atmospheric transparency, and the instrument calibration. The latter includes changes of the instrument sensitivity and especially the wavelength calibration. Although the best corrections are possible for time intervals of only a few minutes, where the airglow intensities are still very similar, convincing sky corrections were even achieved for time differences of about one year. The skycorr results were also compared with the 2D sky interpolation method of the X-shooter pipeline, Davies’ method, and the simple on-off method without sky fitting. In conclusion, skycorr performed at least as well as the 2D approach and convincingly better than Davies’ SINFONI-optimised code. The latter result was confirmed for two SINFONI examples and is due to the more complex sky optimisation of skycorr, the more robust performance, and the high flexibility in terms of the properties of the input data. Compared with sky subtraction without fitting, the skycorr sky line residuals for the test data set without parameter optimisation were between 2.1 and 5.5 times lower if short time intervals of a few minutes were neglected.

These promising results suggest that skycorr can be a valuable tool for wavelength ranges where airglow emission lines dominate the sky background and instrument set-ups that either offer only 1D data or require additional observations if the 2D science exposure does not provide plain sky. Even for sky subtraction in multi-object spectra without time differences, it might be useful if instrument parameters, such as the slit width and the wavelength coverage, are the same for object and sky spectra.

Skycorr has been developed for Cerro Paranal. However, it is feasible to use it for spectra taken at other observing sites. The specific Cerro Paranal airglow variability model is mainly used for setting the initial weights for the different line groups for each pixel. Since this model only considers five classes, it could only have an influence if there was a significant contribution for instance of an OH and O2 line to a certain pixel. This is relatively rare. Moreover, pixels with a strong blending of line groups are usually excluded from the fitting procedure. Ratios of lines of the same molecule as provided by the model line list can also vary depending on the observing site. However, these changes are distinctly weaker than the overall intensity variations and hardly relevant for the weights. Finally, short-term intensity variations can cause significant deviations from the airglow model. Therefore, any intensity prediction is relatively rough, even for well-studied observing sites. In any case, the largest impact on the sky-subtraction quality is that of the reference sky spectra, which have to be taken individually for each instrumental set-up.

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Article D:
Investigating the aerosol extinction using an advanced scattered moonlight model

Investigating the aerosol extinction using an advanced scattered moonlight model

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ABSTRACT

Determining the atmospheric extinction curve for ground based telescopes is important, especially with the current and future large telescopes. The most complicated component of the extinction curve comes from aerosol scattering. We investigate a new method for measuring the aerosol extinction curve for Cerro Paranal from 0.3 to 2.1 \( \mu \)m. We combine observations of a spectrophotometric standard star with those of scattered moonlight. Using our theoretical sky background model and a grid of possible aerosol size distributions of various types, we can find the extinction curve with the highest likelihood. We present the most likely aerosol extinction curve and the probabilities for the different aerosol size distributions for a night of observations at Cerro Paranal, thus demonstrating the value of this method.

Key words. Moon - Atmospheric effects - Radiative transfer - Scattering - Methods: data analysis - Techniques: spectroscopic

1. Introduction

The current trend in astronomy is to use larger telescopes to resolve fainter objects and reveal more detail. Hence, improved methods for data reduction and correction of the sky signature are crucial. Ground based observations must correct for atmospheric extinction (e.g., Burke et al. 2010). Studies of the effect of the atmosphere have been done for several astronomical sites: Mauna Kea (e.g., Buton et al. 2013), Cerro Paranal (e.g., Patat et al. 2011), Cerro Tololo (e.g., Gutierrez-Moreno et al. 1982), and many more.

Atmospheric extinction is composed of several components: absorption and scattering by molecules and particles. Scattering by molecules can be well approximated with Rayleigh scattering, and the amount of molecules in the air is generally stable (see Noll et al. 2012, and references therein). However scattering off of aerosol particles is more complicated and is usually approximated with Mie scattering, where the particles are assumed to be spherical symmetric. The amount of aerosol particles can vary on timescales of hours. In the optical, the extinction curve can be parametrized by an Ångström Law (Ångström 1929). Patat et al. (2011) have found empirically such a fit verified from 330 to 800 nm for Cerro Paranal. In our method, we use our sky background model with the scattered moonlight and standard star observations to find the most likely distribution of aerosols. We will describe this new method for determining the aerosol extinction curve at Cerro Paranal, from 0.3 to 2.1 \( \mu \)m, and present some results.

2. Method

We are investigating and presenting a new method for determining the aerosol extinction curve from the ultraviolet (UV) to the near-infrared (NIR), by coupling observations of standard stars and scattered moonlight with our sky background model. With the standard star observations we can test the transmission spectrum (Section 2.4) and with the scattered moonlight we are probing the emission spectrum (Section 2.5) for a grid of different aerosol extinction curves and phase functions (Section 2.3). With our unique data set of scattered moonlight observations and a standard star (Section 2.1), together with our sky background model (Section 2.2), we can better determine the aerosol extinction curve and scattering phase function.

2.1. Data Set

We have a unique data set taken with X-Shooter (Vernet et al. 2011) at the Very Large Telescope (VLT) for the purpose of verifying and extending to the NIR our scattered moonlight model. The data includes observations of plain sky taken at six different angular distances \( \rho = (7, 13, 20, 45, 90, \text{ and } 110^\circ) \) from the Moon on the night of 2013-07-23. This night the Moon was in gibbous phase and so there was a significant amount of lunar flux. As an example, Fig. 1 shows an observation at \( \rho = 45^\circ \). Additionally, during the same night, a standard star LTT 7987 was observed at two different airmasses.

For the analysis we selected certain wavelength ranges, hereafter called inclusion regions. These regions are parts of the spectrum that should be free of sky emission lines and absorption features. The number of pixels per arm are 850, 850, and 653 for the UVB, VIS, and NIR arm, respectively, and are non-consecutive (see Fig. 1).

\begin{footnote}
Based on observations made with ESO telescopes at Paranal Observatory
\end{footnote}
2.2. Sky Background Model

As part of the Austrian contribution to ESO, the University of Innsbruck In-kind group developed a sky background model. The model was designed to predict the amount of sky background flux to improve the Exposure Time Calculator, used to estimate how long an exposure of a given astronomical target should be for a desired signal to noise. This sky background model produces both an emission and transmission spectrum for a given set of input parameters. The input parameters describe the conditions of the atmosphere at the time of observation and the geometry of the target and sources of sky background light. Fig. 1 shows an example of the sky background model, the scattered moonlight model, the components of the sky background model other than the moonlight, and the transmission curve. For a full description of the sky background model see Noll et al. (2012), and for the scattered moonlight model see Jones et al. (2013).

2.3. Aerosol Grid

The most uncertain part of the extinction curve for the sky background model is the aerosol scattering because the amount of aerosols can vary on hour timescales. In order to find the most likely distribution of aerosols present during the night of observations, we created a set of sky background models with different amounts of aerosols to compare with the observations. We are sensitive to slight changes in the amount of aerosols due to two aspects of this data set. First, our observations cover a wide wavelength range. Second, we have observations at multiple distances from the Moon taken consecutively to minimize the amount of variation of the atmosphere throughout all the observations. We produced a regular coarse grid for remote continental and stratospheric aerosols (Warneck & Williams 2012). Each aerosol distribution is approximated as a log-normal distribution described by \( n \) the number density of particles, \( R \) the mean radius, and \( s \) which determines the spread in radii of the particles. The default parameters for the various aerosols are listed in Table 1 and the distribution is given by

\[
dN(r) = \frac{1}{\sqrt{2\pi} s} \frac{n}{\log s} \exp\left(-\frac{\log r/R_s^2}{2\log s}\right). \tag{1}\]

For the coarse aerosol grid, we scaled the column density for the various aerosols (except the tropospheric nucleation mode, which is negligible so it was kept at 100%). For the column densities, we used the number densities \( n \) and multiplied them by an effective aerosol layer width of 1 km. We chose 1 km because that is approximately the scale height of the (tropospheric) aerosols in the atmosphere and it is a convenient number to use. We varied the column densities in logarithmic steps of 0.25 from 0.06 to 1.00, and the refractive index \( N \) linearly in 0.05 steps ranging from 1.3 to 1.5. For each set of aerosols distributions, we produced the corresponding Mie phase function using an IDL code based on Bohren & Huffman (1983); Grainger et al. (2004).

When the sky observation was at close angular distances to the Moon, in particular the 7 and 13°, we noticed a significant amount of extra observed flux compared with the modeled flux. We speculated that this could be caused by some additional tropospheric coarse mode which would increase the Mie forward scattering. For this purpose, we added an additional coarse mode. We varied the column density of this new mode in the same logarithmic steps as the others (Table 1).

### Table 1: Aerosol modes

<table>
<thead>
<tr>
<th>Type</th>
<th>( n ) cm(^{-3} )</th>
<th>( R ) (10^{-1} \mu m )</th>
<th>( \log s ) (10^{-1} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trop nucleation</td>
<td>( 3.20 \times 10^7 )</td>
<td>0.10</td>
<td>1.61</td>
</tr>
<tr>
<td>Trop accumulation</td>
<td>( 2.90 \times 10^7 )</td>
<td>0.58</td>
<td>2.17</td>
</tr>
<tr>
<td>Trop coarse</td>
<td>( 3.00 \times 10^6 )</td>
<td>9.00</td>
<td>3.80</td>
</tr>
<tr>
<td>Stratospheric</td>
<td>( 4.49 \times 10^6 )</td>
<td>2.17</td>
<td>2.48</td>
</tr>
<tr>
<td>Added coarse</td>
<td>( 1.00 \times 10^6 )</td>
<td>10.00</td>
<td>1.00</td>
</tr>
</tbody>
</table>

Notes: The values used for Mie scattering of remote continental aerosols from Warneck & Williams (2012), except for the added coarse mode (Section 2.3).

2.4. Standard Star Extinction Curve

To find the ideal extinction curve based on the observations of a standard star, we followed a procedure similar to the Langley plot method commonly used in atmospheric science. We had the same standard star observed at two different times and therefore at two different airmasses. The intensity \( I \) is related to the airmass \( X \) by

\[
I = I_0 e^{-\tau X} = I_0 T. \tag{2}\]

\( I_0 \) is the unextincted intensity, \( \tau \) is the optical depth, and \( T \) is the transmission. We can directly compare \( I_1 \) at \( X_1 \) and \( I_2 \) with \( I_2 \) at \( X_1 \) and \( T_2 \) for the same star, meaning \( I_2 \) is the same, assuming the atmospheric conditions are constant over the time period, so \( \tau \) is the same.

We can relate the ratio of intensities \( I_1/I_2 \) to the respective transmissions \( T_1/T_2 \) (Equation 2). For the various Mie scattering parameters, using our sky background model, we can produce the grid of possible \( T \). Then for our inclusion regions we can compute a reduced \( \chi^2 \) for each \( T_1/T_2 \) compared with the \( I_1/I_2 \).

\[
\chi^2 = \frac{1}{v} \sum \frac{(I_1/I_2 - T_1/T_2)^2}{\sigma^2}, \tag{3}\]

The number of the degrees of freedom \( v \) is approximately equal to the number of included pixels (Section 2.1) and the error \( \sigma \) is comprised of two components that were squared and added. First the observational error provided by ESO for the two intensities is propagated. The second comes from the systematic error associated with the model. For the ratio of transmissions we chose an error of 1%.

2.5. Scattered Moonlight Model Extinction Curve

For the determination of the extinction curve using the scattered moonlight model, we also computed the reduced \( \chi^2 \) for each of the models from the aerosol grid at each angular distance \( \rho \) between the Moon and sky observation. With the sky background model, we produced an emission spectrum with the different Mie phase functions and extinction curves based on the aerosol grid. We then compared these emission spectra with the observed spectra for each \( \rho \). For a quantitative comparison we calculated the reduced \( \chi^2 \) for the inclusion regions of the observed \( O \) and modeled \( M \) spectra.

\[
\chi^2_{\lambda\rho} = \frac{1}{v} \sum \frac{(O_\lambda - M_\lambda)^2}{\sigma^2_{M,\lambda}}, \tag{4}\]
Here, \( n \) is the number of pixels used in the inclusion region. The error \( \sigma_{M, i} \) takes into account the error from the observations as well as the model. The error from the observations is a combination of the error provided with the data from ESO and the standard deviation of the scatter between pixels, using a window of 45 pixels. For the model, we were interested in the error associated with the sky background model other than the scattered moonlight model. Thus, we determined the amount of flux from the other components of the sky background model and multiplied them by 20, 20, and 50% for the UVB, VIS, and NIR arms, respectively. This represents the estimated errors in the model at various wavelength regimes. Fig. 1 shows an example of the total sky background model, scattered moonlight model, and the other components (sky background minus moonlight).

We found that even with the additional coarse mode, we still could not reproduce the extra flux seen in the observations at 7°. There may be some additional flux coming directly from the Moon to the detector, and so we have not used this data in the analysis. We can, however, fit the observations at 13° with the added coarse mode. The rest of the analysis shown in this paper was done with the 13° observations, but without the 7°.

Fig. 1: An example spectrum for the scattered moonlight extinction curve determination. The observed spectrum (black) was taken at \( \rho = 45° \). Overlaid is an example total sky background model (green) with the sky lines removed for clarity and the inclusion regions for the analysis (pink plus). The scattered moonlight model (blue) and the other model components (orange dotted), except the sky lines, are also shown. Below the dotted black line is the transmission curve (light green).

2.6. Extinction Curve Likelihoods

For the relative likelihoods from the standard star observations and the scattered moonlight model, we used two simple approaches of converting the reduced \( \chi^2 \) into likelihoods \( L \). For the first approach, we found the likelihood for each type of observation \( i \) with the following,

\[
L_i = e^{-\frac{(\chi^2_{i} - \chi^2_{min})}{2}}. \tag{5}
\]

By subtracting the minimum \( \chi^2 \) labeled \( \chi^2_{min} \), we normalize each distribution and the one with the lowest \( \chi^2 \) then has a \( L = 1 \). We then multiply the six \( L \) (one from the standard star, and five from the scattered moonlight at 13, 20, 45, 90, and 110°) for each point in the aerosol grid for the final resulting \( L \).

The second approach is similar, but first we calculate the mean \( \chi^2 \) from all the observations \( i \) for each point in the aerosol grid. Then we use the \( < \chi^2 > \) and \( < \chi^2 >_{min} \) for calculating the final \( L \). Both approaches result in the same qualitative results. When not stated, \( L \) is from the second approach, since the range of these \( L \) is more convenient.

3. Results and Conclusions

From the final likelihoods \( L \), we can find the most likely aerosol extinction curve for the night of 2013-07-23. For Fig. 2 and 3 we show four examples of the result for clarity from the full grid of results. Two the examples have the highest final \( L \) to illustrate the minor differences in \( L \). One example is for the lowest \( L \), which has too many aerosols. Then for completion we show the lowest \( L \) that has too few aerosols. In Fig. 2, we show the comparison between the ratios of \( T_1/T_2 \) and \( T_1/T_3 \) from the standard star observations. The ratio of \( T_1/T_2 \) was medium smoothed with a window of 45 pixels for transparency. The difference between the first and second most likely model is difficult to distinguish. However for the least likely model, the two ratios do not match. Fig. 3 shows the same models as in Fig. 2 but with the comparison between the scattered moonlight observations and the sky background model. The 13° fits behave differently from the 20 and 45° observations, perhaps due to some direct moonlight hitting the detector or other unconsidered aerosol modes. Examples of the model having too few and too many aerosols are shown. The 90 and 110° observations are not sensitive to the changes in the aerosols, and show that the other components of the model fit the data well.

The probabilities for the different fractions of the column density for the various aerosols and different \( N \) are shown in Fig. 4, using the two different methods for calculating the likelihood \( L \). The added coarse mode is favored to have a very small contribution, whereas the stratospheric mode is almost degenerate. In Fig. 5, we show the top five most likely aerosol extinction curves for the night 2013-07-23, and in Tab 2 we give \( \tau_aer \) of the most likely model for several wavelengths. The aerosol extinction for
Fig. 3: Four examples of how well the sky background model fits the observations. The observations at the five different angular distances to the Moon (13, 20, 45, 90, and 110°) are shown, offset in flux for clarity. Overlaid for each are the most and least likely models. These are same ones as in Fig. 2. For an explanation of the legend, see Fig. 2.

this night is quite a bit smaller compared with the empirical fit found by Patat et al. (2011). The amount of aerosols can vary significantly from night to night as was seen at Mauna Kea by Buton et al. (2013).

This new technique for determining the aerosol extinction curve seems promising. By coupling the scattered moonlight observations with those of a standard star, we are sensitive to changes in the atmospheric aerosol composition.

Fig. 4: In the left panel, probabilities of the different fractions of the column density for the various aerosols. In the right panel are the probabilities for the different refractive indices N. For both panels, the solid line used the first method for the likelihood calculation and the dashed lines used the second method (see section 2.6).

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Table 2: Most Likely Aerosol Extinction Curve

<table>
<thead>
<tr>
<th>Wavelength (µm)</th>
<th>(\tau_{\text{aer}} (\text{airmass}^{-1}))</th>
<th>Wavelength (µm)</th>
<th>(\tau_{\text{aer}} (\text{airmass}^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.30</td>
<td>0.0130</td>
<td>1.60</td>
<td>0.00559</td>
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<tr>
<td>0.35</td>
<td>0.0128</td>
<td>1.70</td>
<td>0.00530</td>
</tr>
<tr>
<td>0.40</td>
<td>0.0124</td>
<td>1.80</td>
<td>0.00503</td>
</tr>
<tr>
<td>0.45</td>
<td>0.0119</td>
<td>1.90</td>
<td>0.00478</td>
</tr>
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<td>0.0115</td>
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</tr>
<tr>
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<td>0.00893</td>
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<td>0.000918</td>
</tr>
<tr>
<td>0.90</td>
<td>0.00864</td>
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<td>0.000719</td>
</tr>
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<td>0.95</td>
<td>0.00836</td>
<td>10.0</td>
<td>0.000570</td>
</tr>
<tr>
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<tr>
<td>1.50</td>
<td>0.00591</td>
<td>30.0</td>
<td>0.0000246</td>
</tr>
</tbody>
</table>

Fig. 5: Five of the most likely aerosol extinction curves for the night of 2013-07-23. For an explanation of the legend, see Fig. 2. Also plotted is the fit from Patat et al. (2011) for comparison.

References
Ångström, A. 1929, Geografiska Annaler, 11, 156

Article number, page 4 of 4
Article E:
Molecfit: a general tool for telluric absorption correction
I. Method and application to ESO instruments

Molecfit*: a general tool for telluric absorption correction

I. Method and application to ESO instruments**

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Received <date>/ Accepted <date>

ABSTRACT

Context. The interaction of the light from astronomical objects with the constituents from the Earth’s atmosphere leads to the formation of telluric absorption lines in their spectra. Correcting them usually relies on the observation of specific stars close in time and airmass to the science targets, therefore using precious observing time.

Aims. We present molecfit, a tool to correct for telluric absorption lines based on synthetic modelling of the atmospheric transmission. Molecfit is versatile and can be used with data obtained with various telescopes and instruments.

Methods. Molecfit is based on a publicly available radiative transfer code, a molecular line database, various kernels to model the line spread function and atmospheric profiles created by merging a standard atmospheric profile, local meteorological data and dynamically retrieved height profiles for temperature, pressure and humidity.

Results. We show examples of telluric line correction on spectra obtained with various ESO instruments: UVES, FLAMES, X-shooter, CRIRES, SINFONI, VISIR. The residuals RMS after correction of optically thin telluric lines is frequently better than 2% of the continuum.

Conclusions. Molecfit is able to accurately model and correct for telluric lines over a broad range of wavelengths and spectral resolutions. The accuracy reached is comparable or better than the typical accuracy achieved using a telluric standard star observation.

Key words. radiative transfer, atmospheric effects, instrumentation: spectrographs, methods: observational, methods: data analysis, technique: spectroscopic

1. Introduction

Ground-based observations, and in particular, spectroscopy can be strongly affected by absorption caused by molecules in the Earth’s atmosphere. The wavelength ranges involved include – but are not limited to – the near- and mid-infrared. It is a standard practice to correct for such telluric absorption lines in order to recover as much as possible the spectrum (or photometry) of the target as it would appear above the atmosphere. Different approaches have been proposed.

A very common method is to observe either an early type or a G-type star (depending on the specific purpose) soon before or after the observations of the science target. This telluric star should ideally be located close to the science target in the sky. Indeed, early type stars are advantageous because they are mostly featureless, except for hydrogen lines. Spectral regions close in wavelength to the one of hydrogen lines on the other hand are therefore best corrected by G-type stars. The reason to observe both objects angularly close on the sky arises because optically thick and thin telluric absorption lines do not scale with the same function of airmass. In addition, the distribution of molecules in the atmosphere (mainly water vapour) can depend on the pointing direction.

Observations of such telluric standard stars are expensive in observing time and therefore reduce, sometimes considerably, the amount of time dedicated to the main science targets. The quality of the correction can be variable and depends much on the difference of airmass between the science and telluric star observations, as, in the best conditions, a difference of 1% in airmass already introduces a 1% change in the optical depth of optically thin telluric lines. Other problems affect observations of

* Molecfit is available at http://www.eso.org/pipelines/skytools
telluric stars: it may sometimes be impossible to find a suitable star close to the science target, atmospheric conditions may have changed at the end of the science observations, or their signal-to-noise ratio may be insufficient. Use of archival data bring additional problems as observation of a telluric star may be missing or not appropriate for the science goal.

Alternatively, the emergence of freely available radiative transfer codes for atmospheric research provides the possibility to use synthetic transmission spectra instead telluric standard stars. One of the first articles demonstrating the ability of this approach was Bailey et al. (2007), who used the radiative transfer model SMART (Meadows & Crisp 1996) for that purpose. Seifahrt et al. (2010) refined the method incorporating the radiative transfer code LBLRTM (Clough et al. 2005), the line database HITRAN (Rothman et al. 2009), a combination of meteorological data from various sources to achieve synthetic transmission curves, and a model of the line spread function. These were then used to successfully perform telluric absorption corrections of CRIRES (Kaeufl et al. 2004) spectra up to an accuracy of ~ 2 per cent. The code LBLRTM is also used by Hasuer & Ulbrich (2013) who incorporated it to fit an entire input spectrum. A different approach is used by Cotton et al. (2013). Since they investigate solar system planetary atmospheres containing similar molecules as the Earth’s atmosphere, they derive the state of the latter by fitting spectral features of telluric standard star observations. Gardini et al. (2013) used the Radiative Transfer Model1 developed for the SCIAMACHY instrument onboard the ENVISAT satellite to fit water features visible in spectra taken at the Sierra Nevada Observatory. In addition, they used it to determine the amount of precipitable water vapour in the Earth’s atmosphere at the time of observation.

Unfortunately, the poor quality of the correction often impedes the general use of such tools. The deviation of the modelled absorption line from the observed one can be caused by errors in the radiative transfer modelling or a poor representation of the line spread function. In addition, a general tool to the astronomical community is simply not available.

Here we describe molecfit, a tool to model telluric lines. Molecfit retrieves the most appropriate atmospheric profile (i.e., the variation of the temperature, pressure and humidity as a function of altitude) for the time of the given science observations. It uses a state of the art radiative transfer modelling or a poor representation of the line spread function. In addition, a general tool to the astronomical community is simply not available.

The initial development of molecfit was carried out mostly as a set of IDL routines used as drivers for the Reference Forward Model2 radiative transfer code. The goal was to measure the amount of precipitable water vapour (hereafter, PWV) using the ~ 19.5 μm emission line with VISIR, the mid-IR spectrograph and imager at the Very Large Telescope (Smette et al. 2008). The code was then slightly modified to measure the amount of PWV using sky emission line spectra obtained with the cryogenic high-resolution infrared echelle spectrograph CRIRES, as the 5.038 to 5.063 μm range is purely dominated by water vapour.

The code of the fits indicated that generalising the code to absorption lines and other spectral ranges was promising and lead to a well-developed IDL prototype (Smette et al. 2010). Its performances were similar to the one created by Seifahrt et al. (2010) which only focused on CRIRES spectra. This prototype was then ported in a robust way to CPL and further developed and optimised as part of the Austrian in-kind contribution for joining ESO. In the process, the LNFL/LBLRTM code (Clough et al. 2005) was chosen instead of RFM, mainly for its better general performance and maintenance. This paper describes the results of these efforts and shows a variety of applications. In Kausch et al. (2014) (hereafter, Paper II), we will investigate the quality of molecfit as a telluric absorption correction tool for VLT/X-shooter spectra.

This paper is organised as follows. Section 2 describes the most important aspects regarding the absorption lines formed in the Earth’s atmosphere. Section 3 provides a description of the molecfit package. The availability of a general tool for telluric absorption correction can impact an observing strategy. A few characteristic cases are described in Sect. 4. Limitations to the use of the tool are summarised in Sect. 5. Examples of successful applications of molecfit on spectra obtained with several ESO instruments are given in Sect. 6. The most important aspects of molecfit are summarised in the conclusion.

2. Absorption arising in the Earth’s atmosphere

The Earth’s atmosphere consists of about 78% of N2, 21% of O2, 1% of Ar, several trace gases and aerosols. Each of the molecules and aerosols affects the light travelling through in different wavelength regimes by absorption and scattering. Figure 1 shows a model transmission curve derived with the sky model developed in a parallel project (Noll et al. 2012). The main absorption regions of the eight major contributing molecular species O2, O3, H2O, CO, CO2, CH4, OCS, and NO are marked. Due to the complexity of the molecules several ro-vibrational bands are clearly visible.

The optical regime is dominated by broad absorption bands from ozone (Huggins & Huggins (1890); Chappuis bands at ~ 0.5 μm < λ/μm < 0.7; Chappuis (1880)), narrow oxygen bands (the prominent A, B and the weaker γ bands at ~ 0.759 < λ/μm < 0.772, 0.686 < λ/μm < 0.695, and 0.628 < λ/μm < 0.634, respectively), and some comparably weak water vapour features. The latter become dominant in the entire infrared regime longwards of the J band. In addition in the HJIR regime the transmission is significantly affected by CO2, CH4, and O2. Between the K band and ~ 18 μm absorption are mainly caused by H2O and CO2, with some contribution from N2O, CH4, and minor absorption features by CO and OCS. In the regime from 18 to 30 μm only water vapour is dominant. Over the whole wavelength range the gases listed in Table 1 lead to absorption features with optical depth reaching up to 5% at the given spectra resolving power (R ~ 10000).

The Earth’s atmosphere is highly variable on several time scales in temperature, pressure, and chemical composition. The

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1 RTM is part of the SCITRAN 2.2 software package, developed by the Institute of Remote Sensing/Institute of Environmental Physics of the University of Bremen, Germany
2 http://www.atm.ox.ac.uk/RPF/
4 The Common Pipeline Library http://www.eso.org/sci/software/cpl/documentation.html based on ANSI C.
Table 1. Species with minor line absorption contribution. The specific spectra are calculated with the radiative transfer code LBLRTM (resolution $R \sim 10000$) without continua to extract the line contribution only. The wavelength ranges are also shown in Fig. 1.

<table>
<thead>
<tr>
<th>species</th>
<th>number in Fig. 1</th>
<th>wavelength range [µm]</th>
<th>optical depth [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>NO</td>
<td>1</td>
<td>5.153–5.556</td>
<td>≤0.3</td>
</tr>
<tr>
<td>HNO$_2$</td>
<td>2</td>
<td>5.743–5.983</td>
<td>≤1</td>
</tr>
<tr>
<td>COF$_2$</td>
<td>3</td>
<td>7.404–7.825</td>
<td>≥2</td>
</tr>
<tr>
<td>H$_2$O</td>
<td>4</td>
<td>10.890–11.694</td>
<td>≤1</td>
</tr>
<tr>
<td>HCN</td>
<td>5</td>
<td>20.452–23.478</td>
<td>≤1</td>
</tr>
<tr>
<td>H$_2$S</td>
<td>6</td>
<td>5.103–5.187</td>
<td>≤0.01</td>
</tr>
<tr>
<td>NH$_3$</td>
<td>7</td>
<td>7.935–8.157</td>
<td>≤0.01</td>
</tr>
<tr>
<td>N$_2$</td>
<td>8</td>
<td>&gt; 19.705</td>
<td>≤0.3</td>
</tr>
<tr>
<td>C$_2$H$_2$</td>
<td>9</td>
<td>12.957–14.523</td>
<td>≤0.5</td>
</tr>
<tr>
<td>C$_2$H$_6$</td>
<td>10</td>
<td>3.332–3.364</td>
<td>≤0.2</td>
</tr>
<tr>
<td>SO$_2$</td>
<td>11</td>
<td>7.243–7.455</td>
<td>≤0.01</td>
</tr>
</tbody>
</table>

The molecfit executable includes the following components:

1. A tool for automatic retrieval of two atmospheric Global Data Assimilation System (GDAS) profiles from a meteorological web site. These profiles bracket the date and time of the observation and can be retrieved for any observatory in the world, although the distributed version has the GDAS profiles available for Cerro Paranal. The profiles are then linearly interpolated to match the time of the observations and merged with a standard profile and local meteorological data to create an input profile for the radiative transfer code;

2. A radiative transfer code to simulate atmospheric emission and transmission spectra;

3. A molecular spectroscopic database;

4. A simple grey body calculator used to simulate the contribution of the continuum from the instrument and telescope;

5. A choice of possible line spread functions (also referred to as kernels);

6. An automated fitting algorithm to adjust the continuum spectrum, wavelength calibration, spectral resolution, and column density of each of the relevant molecules, with the possibility to exclude spectral regions either expressed in pixels or in wavelength regions. Regarding the wavelength calibration and continuum adjustment, only the degree of the polynomials as well as the constant terms for these polynomials can be set by the user in the normal mode. The fitting process is then very robust. However, an expert mode provides additional flexibility in controlling the parameters defining the continuum adjustment and wavelength calibration, at the risk of less robustness in the fitting process.

In the following, we will discuss these components in more details.

3.1. Atmospheric profile

An atmospheric profile typically describes the temperature, pressure, and volume mixing ratio of several molecular species as a function of altitude for a given location. These parameters have a direct impact on the shape and strength of all the telluric lines. For molecfit we use a merged profile based on a reference atmospheric profile, modelled 3-D data, and on-site meteorological measurements.

The reference atmosphere is by default the equatorial standard profile derived by J. Remedios$_6$ and contains abundances of several molecular species up to a height of 120 km, divided into 121 height levels. Due to the low latitude of Cerro Paranal (Lat: -24.6°) the equatorial profile is better suited (Anu Dudhia, priv. comm.) than the other ones available on this web site. We note here that, as it was created in 2001, the molecular composition has changed. In particular, the content of the greenhouse gas carbon dioxide content has increased by ~ 6% (World Meteorological Organization 2012). Molecfit allows the user to either fit or manually adjust the molecular content to take this increase into account. Alternatively, the reference atmosphere used by molecfit can be easily modified to another existing or manually created profile.

The reference atmosphere is then merged with modelled GDAS$_7$ 3-D data provided by the National Oceanic and Atmospheric Administration$_8$ (NOAA). This model contains time-de-

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The most variable relevant molecule is water vapour, which is directly related to the actual weather conditions at the time of observations. However, seasonal, daily and sometimes hourly variations in the volume mixing ratio of various gases have been measured, in particular, for CO$_2$ (Thoning et al. 1989), CH$_4$ (Schneising et al. 2009) and O$_3$ (Ramanathan & Ramana Murthy 1953). In addition, following the World Meteorological Organization (2012) leading to global warming. Daily columns for several molecular species can be obtained from http://www.temis.nl/.

### 3. Description of the molecfit package

The molecfit package mainly consists of three executables:

- **molecfit** either simulates or fits tropospheric and stratospheric emission or absorption telluric lines to an observed (usually, science) spectrum based on a configuration file and/or information provided in the FITS header of the science target file;
- **calctrans** calculates the transmission spectrum over the whole wavelength range of the input spectrum corresponding to the best fit model; optionally, the transmission spectrum can be calculated for a different airmass than the original spectrum;
- **corrfilelist** applies the resulting transmission spectrum to a list of science spectra.

In addition, a Graphical User Interface (GUI) allows one to deal with the data interactively, in particular for the definition of the inclusion and exclusion regions (see Sect. 3.5), although with a slightly reduced flexibility.

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1. http://www.wmo.int/gaw

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6. [http://www.atm.ox.ac.uk/RFM/atm/](http://www.atm.ox.ac.uk/RFM/atm/)


8. [https://ready.arl.noaa.gov/gdas1.php](https://ready.arl.noaa.gov/gdas1.php)
Fig. 1. Synthetic absorption spectrum of the sky between 0.3 and 30 µm calculated with LBLRTM (resolution $R \sim 10000$) using the annual mean profile for Cerro Paranal (Noll et al. 2012). The 8 main molecules $O_2$, $O_3$, $H_2O$, CO, CO$_2$, CH$_4$, OCS, and N$_2$O contribute more than 5% to the absorption in some wavelength regimes. The red regions mark the ranges where they mainly affect the transmission, minor contributions of these molecules are not shown. The green regions denote minor contributions (see Table 1) from the following molecules: (1) NO, (2) HNO$_3$, (3) COF$_2$, (4) H$_2$O$_2$, (5) HCN, (6) NH$_3$, (7) NO$_2$, (8) N$_2$, (9) C$_2$H$_2$, (10), C$_2$H$_6$, and (11) SO$_2$. 
dependent information on the temperature, pressure, relative humidity, wind speed and direction up to a height of ~26 km on a 3 h basis. Due to the geographical 1° × 1° grid we created a set of profiles by means of an interpolation of the four grid points closest to Cerro Paranal to obtain local information. The GDAS profile selected for a specific observation is then by default a linear interpolation of the two resulting profiles closest in time to the observation. The molecfit package contains all the available GDAS profiles for Cerro Paranal since December 1, 2004 at 00:00 UT and the release date of the package. In addition, ESO will regularly maintain such a database for Paranal. For observations obtained later or from another site, molecfit automatically retrieves the appropriate GDAS files.

It may still be possible that no GDAS profiles are available for the time of observations. In the case of Cerro Paranal, molecfit then use the best matching two-months average (Noll et al. 2012). Alternatively, an ASCII profile with the same format as a GDAS profile can also be provided manually.

A further optional refinement of the final profile is achieved by incorporating on-site measurements of the ESO MeteoMonitor (EMM) data, as provided in the FITS header or through the parameter file. The influence of the measured values at the observatory altitude is gradually decreased up to an upper mixing height set by default to ~5 km, where, for Paranal, the wind direction usually changes by ~180°, as revealed by an analysis of the GDAS wind data. Thus, it can be assumed that at this altitude the influence of the local environment (as determined from the EMM data) has diminished. More information on the merging procedure can be found in the molecfit User Manual (Noll et al. 2013).

Water vapour is the most variable molecule as its altitude distribution can change significantly and on a short-time scale. In particular, the largest amount of PWV may not be located in the lowest layers of the atmosphere. Figure 2 illustrate the importance of having a decent profile for water vapour.

The total amount of PWV can optionally be set, if the value can be retrieved independently (for example, from the radiometer; see Kerber et al. 2012). In this case, the merged profile composed by the reference atmosphere, the GDAS data and the local meteo information will be scaled to the requested PWV. In Paper II we examine the impact of this option in detail for X-shooter spectra.

**Fig. 2.** Top: two examples of distribution of water vapour volume mixing ratio as a function of altitude. The black solid line corresponds to a volume mixing ratio of 0 ppmv up to 3.1 km (Paranal altitude is 2.6 km), while the red dashed line corresponds to a constant relative humidity until 3.1 km. The total amount of precipitable water vapour, 2 mm, is identical for both profiles. Bottom: sample of the corresponding transmission spectra at R = 100,000. The higher amount of water vapour in the lower atmospheric layers above the observatory leads to both deeper cores and stronger continuum absorption.

**Fig. 3.** Effect of ground temperature or pressure variation on the H₂O telluric spectrum for two different spectral ranges. Each graph shows the ratio between telluric spectra computed with the indicated ground temperature or pressure. (Top:) variation of 1°C and 10°C. Note that the region close to 3.68 µm shows opposite behaviours. (Bottom:) variation of 1 mb and 10 mb.

Figures 3 illustrates the effect resulting from variation of the ground temperature and pressure, respectively, on the H₂O telluric spectrum. Depending on line parameters, different lines will behave differently with temperature or pressure.

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3.2. Radiative transfer code

The resulting merged atmospheric profile is used as input in the radiative transfer code LNFL/LBLRTM (Clough et al. 2005) in its latest version V12.2. This code package is widely used in atmospheric sciences and is publicly available. It calculates radiance and transmission spectra with a spectral resolving power of about 4 million. More information can be found at the web site.

3.3. Database of molecular parameters

In addition to the profile, the radiative transfer code requires a line database as input. We use the database aer_v_3.2, which is delivered with the LNFL/LBLRTM code package: it is based on an updated version of the HITRAN 2008 database (Rothman et al. 2009) and contains information on more than 2.7 million spectral lines of 42 molecular species (see Table 2). The molecfit line database can be easily updated when a new version becomes available.

Only molecules for which an atmospheric volume mixing ratio profile is available in the standard atmosphere included in molecfit can be used by default. These molecules are identified in Table 2.

3.4. Fitting algorithm

The tool makes use of the C version of the least-squares fitting library mpfit (Markwardt 2009) based on the FORTRAN fitting routine MINPACK-1 (Moré 1978).

3.5. Inclusion and exclusion regions

A spectrum shows a number of features which can be characterised in the following way:

$- \text{intrinsic features from the science object,}$
$- \text{telluric features,}$
$- \text{intrinsic features from the instrument, either caused by the}$
$\text{spectrograph or the detector.}$

Intrinsic features either from the star or from the instrument can interfere with the fitting process. Therefore, molecfit allows one to:

$- \text{select inclusion regions, also called fitting ranges, whose}$
$\text{main purpose is to allow molecfit to determine the}$
$\text{column density of the relevant molecules and to determine}$
$\text{the line spread function (or kernel);}$
$- \text{select exclusion regions within the inclusion regions which}$
$\text{are affected by the presence of intrinsic features from}$
$\text{the science objects;}$
$- \text{mask pixels in the inclusion regions which are affected}$
$\text{purely by instrumental or detector effects.}$

Details can be found in the User Manual (Noll et al. 2013) provided with the code.

3.6. Continuum contribution

The model spectrum, $F_{\text{mod}}(\lambda)$, is scaled by a polynomial of degree $n_c$.

$$F_{\text{mod}}(\lambda) = F_{\text{obs}}(\lambda) \sum_{j=0}^{n_c} a_j \lambda^j.$$  \hspace{1cm} (1)

http://rtweb.aer.com/lblrtm_frame.html

Table 2. List of molecules as provided by the aer line parameter database.

<table>
<thead>
<tr>
<th>#</th>
<th>Molecule</th>
<th>Chemical name</th>
<th>In standard profile?</th>
<th>GUI</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>H$_2$O</td>
<td>Water</td>
<td>X</td>
<td>f</td>
</tr>
<tr>
<td>2</td>
<td>CO$_2$</td>
<td>Carbon dioxide</td>
<td>X</td>
<td>f</td>
</tr>
<tr>
<td>3</td>
<td>O$_3$</td>
<td>Ozonide</td>
<td>X</td>
<td>f</td>
</tr>
<tr>
<td>4</td>
<td>N$_2$O</td>
<td>Nitrous oxide</td>
<td>X</td>
<td>f</td>
</tr>
<tr>
<td>5</td>
<td>CO</td>
<td>Carbon monoxide</td>
<td>X</td>
<td>f</td>
</tr>
<tr>
<td>6</td>
<td>CH$_4$</td>
<td>Methane</td>
<td>X</td>
<td>f</td>
</tr>
<tr>
<td>7</td>
<td>O$_2$</td>
<td>Oxygen</td>
<td>X</td>
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</tr>
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<td>NO</td>
<td>Nitric oxide</td>
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<td>Sulfur dioxide</td>
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<td>c</td>
</tr>
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<td>Nitrogen dioxide</td>
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<td>HCN</td>
<td>Hydrogen cyanide</td>
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<td>c</td>
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<td>25</td>
<td>H$_2$O$_2$</td>
<td>Hydrogen peroxide</td>
<td>X</td>
<td>c</td>
</tr>
<tr>
<td>26</td>
<td>CH$_3$H$_2$</td>
<td>Acetylene</td>
<td>X</td>
<td>c</td>
</tr>
<tr>
<td>27</td>
<td>C$_2$H$_4$</td>
<td>Ethane</td>
<td>X</td>
<td>c</td>
</tr>
<tr>
<td>28</td>
<td>PH$_3$</td>
<td>Phosphine</td>
<td>X</td>
<td>c</td>
</tr>
<tr>
<td>29</td>
<td>CO$_2$F$_2$</td>
<td>Carbonyl fluoride</td>
<td>X</td>
<td>c</td>
</tr>
<tr>
<td>30</td>
<td>SF$_6$</td>
<td>Sulfur hexafluoride</td>
<td>X</td>
<td>c</td>
</tr>
<tr>
<td>31</td>
<td>H$_2$S</td>
<td>Hydrogen sulfide</td>
<td>X</td>
<td>c</td>
</tr>
<tr>
<td>32</td>
<td>HCOOH</td>
<td>Formic acid</td>
<td>X</td>
<td>c</td>
</tr>
<tr>
<td>33</td>
<td>HO$_2$</td>
<td>Hydroperoxyl</td>
<td>X</td>
<td>c</td>
</tr>
<tr>
<td>34</td>
<td>O</td>
<td>Oxygen</td>
<td>X</td>
<td>c</td>
</tr>
<tr>
<td>35</td>
<td>ClONO$_2$</td>
<td>Chlorine nitrate</td>
<td>X</td>
<td>c</td>
</tr>
<tr>
<td>36</td>
<td>NO$_2$</td>
<td>Nitrosourea</td>
<td>X</td>
<td>c</td>
</tr>
<tr>
<td>37</td>
<td>HBrO</td>
<td>Hypobromous acid</td>
<td>X</td>
<td>c</td>
</tr>
<tr>
<td>38</td>
<td>C$_2$H$_4$</td>
<td>Ethylene</td>
<td>X</td>
<td>c</td>
</tr>
<tr>
<td>39</td>
<td>CH$_3$OH</td>
<td>Methanol</td>
<td>X</td>
<td>c</td>
</tr>
<tr>
<td>40</td>
<td>BrO</td>
<td>Bromine oxide</td>
<td>X</td>
<td>c</td>
</tr>
<tr>
<td>41</td>
<td>C$_2$H$_6$</td>
<td>Propane</td>
<td>X</td>
<td>c</td>
</tr>
<tr>
<td>42</td>
<td>C$_2$N$_2$</td>
<td>Acrylonitrile</td>
<td>X</td>
<td>c</td>
</tr>
</tbody>
</table>

Notes. The first column provides the reference number of the molecule as defined in the HITRAN 2008 database; the second column its chemical formula, followed by its chemical name. The fourth column indicates if an atmospheric profile of the molecular volume mixing ratio is available in the equatorial standard profile as included in molecfit. The last column indicates the functionality available through the GUI: f the corresponding column density can be fitted, c the corresponding transmission spectrum is only calculated using the user provided abundance, relative to the one fixed in the reference atmosphere.

For deriving the $n_c + 1$ coefficients $a_j$, the zero point of the wavelength grid is shifted to the centre of the fit range. For $a_0 = 1$ and all other $a_i = 0$, the model spectrum remains unchanged. This is the default configuration for the initial coefficients. In the param-
3.8. Wavelength calibration

Before correcting the continuum, an optional flux conversion can be carried out. Further details are available in the User Manual.

3.7. Telescope background

For sky emission modelling, the telescope background is assumed to be a grey body (black body times emissivity). The parameters of this grey body correspond to the telescope main mirror temperature and an effective emissivity of the telescope and instrument.

3.8. Wavelength calibration

The science spectra to analyse are expected to have an accurate wavelength calibration. However, in each inclusion region, the wavelength calibration can be adjusted based on the telluric lines; this is particularly useful for spectra obtained with in-rate wavelength calibration. However, in each inclusion region, this way, with the understanding that it is only relevant in the case that the inclusion region covers the whole spectrum reasonably well and is well sampled by telluric lines.

Molecfit provides the wavelength calibration obtained in this way, with the understanding that it is only relevant in the case that the inclusion region covers the whole spectrum reasonably well and is well sampled by telluric lines.

3.9. Line spread function

The model spectrum is convolved with up to three different profiles in order to determine the shape of the line spread function. They are:

1. a simple boxcar

\[ F_{\text{box}}(\lambda) = \begin{cases} 1 & \text{for } -w_{\text{box}}/2 \leq \lambda \leq w_{\text{box}}/2 \\ 0 & \text{for } \lambda < -w_{\text{box}}/2 \text{ or } \lambda > w_{\text{box}}/2 \end{cases} \] (4)

which is adapted to the pixel scale and normalised to an integral of 1. This kernel is particularly useful for objects fully covering the entrance slit.

2. a Gaussian

\[ F_{\text{gauss}}(\lambda) = \frac{1}{\sigma \sqrt{2\pi}} \exp \left( -\frac{\lambda^2}{2\sigma^2} \right) \] (5)

centred on 0, where

\[ \sigma = \frac{w_{\text{gauss}}}{2 \sqrt{2\ln 2}} \] (6)

The Full Width at Half Maximum (FWHM), \( w_{\text{gauss}} \), is given in pixels.

3. a Lorentzian

\[ F_{\text{lorentz}}(\lambda) = \frac{1}{\pi} \frac{a}{\lambda^2 + (w_{\text{lorentz}/2})^2} \] (7)

centred on 0, where \( w_{\text{lorentz}} \) is the FWHM, in pixels. Compared to a Gaussian, the Lorentzian approaches the 0-level flux significantly slower, at much larger distances from the maximum.

Note that zero-width components can occur in typical conditions, e.g., the line profile is very close to a pure Lorentzian shape. If this is not intended, the user should reduce the number of degrees of freedom by fixing individual fit components. A zero here identifies a unity convolution (i.e., no change of the input spectrum).

The convolution of a Gaussian and a Lorentzian is called a Voigt profile. A flag (parameter ) allows the user to apply only a single Voigt profile kernel, which is then calculated by an approximate formula that takes the FWHM of Gaussian and Lorentzian as input. For the fit results, the selection should be less important than the relative contributions of boxcar, Gaussian, and Lorentzian to the fitted line profile. Significant changes in the line profile can cause deviations in the water vapour column of more than 10%.

Another flag ( ) allows the user to fit a kernel whose size linearly increases with wavelength. It is suitable for an instrumental setup with nearly constant resolving power, fixed wavelength step size and a wide wavelength range, such as cross-dispersed echelle spectrographs. In this case, the initial FWHM parameters are given for the central wavelength of the full wavelength range (considering the data of all chips).

Finally, a kernel can also be provided by the user in the form of an ASCII table, which then overrules all other options.

3.10. Molecular volume mixing ratio

The volume mixing ratio \( X \) of a molecule for a column of air from the observer at a height \( h_0 \) to the top of atmosphere can be derived by

\[ X = \int_{h_0}^{\infty} \frac{\text{alb}(\text{P}(h))}{T(h)} \frac{\text{d}h}{\text{d}T} \text{d}h \] (8)

if the mixing ratio (or mole fraction) \( x \), air pressure \( P \), and temperature \( T \) are given depending on altitude \( h \) by an atmospheric profile. Volume mixing ratios are usually given in part per million in volume (ppmv).

For \( \text{H}_2\text{O} \), it is also common to provide the column height of PWV in mm (also referred to as amount of PWV). It can be calculated by

\[ \text{PWV} = \frac{m_{\text{tot,H}_2\text{O}}}{\rho_{\text{H}_2\text{O}} R} \int_{h_0}^{\infty} \frac{\text{alb}(h) \text{P}(h)}{T(h)} \text{d}h \] (9)

where

\[ PWV = \int_{h_0}^{\infty} \frac{m_{\text{H}_2\text{O}}(h) \text{P}(h)}{T(h)} \text{d}h \] (9)
where the mole mass of water $m_{\text{mol}, \text{H}_2\text{O}} = 0.0182$ kg, the density of liquid water $\rho_{\text{H}_2\text{O}} = 10^3$ kg m$^{-3}$, and the gas constant $R = 8.31446$ J mol$^{-1}$ K$^{-1}$. The required units of $x$, $P$, $T$, and $h$ are ppmv, Pa, K, and km, respectively. Molecfit outputs the column height for other gases using similar formula.

Since the GDAS profiles and the ESO MeteoMonitor data provide H$_2$O volume mixing ratio as relative humidity $RH$ in percent, it has to be converted to $x$. For this purpose, we have implemented the approximations for vapour pressures of ice and supercooled water as function of temperature as described by (Murphy & Koop 2005). The minimum of both then corresponds to the saturated vapour pressure $P_{\text{sat}}$, which is used to estimate the height-dependent $x$ in ppmv by

$$x(h) = 10^6 \frac{P_{\text{sat}}(T(h)) \cdot RH(h)}{P(h)} \cdot 100. \quad (10)$$

Molecfit allows the user to adjust this quantity based on the observed telluric lines; note that the GUI only allows one to fit the column density for the molecules indicated in the last column of Table 2. This adjustment is done by multiplying the overall atmospheric profile by a single constant. For most molecules, the impact is actually limited to the lowest atmospheric layers.

### 3.11. Supported instruments

One-dimensionnal (1-D) spectra of any visible, near- or mid-infrared instrument could in principle be used by molecfit. Details on the required information can be obtained in the User Manual (Noll et al. 2013). Although the tool has been tailored to ESO-Paranal instruments – in particular, the GDAS profiles are available as a tarball file only for this site – there are no specific limitations neither in terms of format nor geographical location for a ground-based observatory.

### 3.12. Inputs and outputs

Molecfit accepts 1-D spectra provided as ASCII tables, FITS tables and images. The FITS tables can have several extensions corresponding to different chips (e.g. CRlRES). Required keywords are either taken from the FITS header or directly from the parameter file. Finally, ASCII or FITS files for inclusion and exclusion regions can be provided.

The executable molecfit performs the model fit only in the inclusion regions which can cover just a small fraction of the whole wavelength range (e.g. X-shooter, see Paper II). It returns the best-fit models only for the inclusion regions in both an ASCII and a FITS tables, and the best-fit parameters and molecular column densities (including the PWV) in a results ASCII file.

The fitting is separated from the telluric absorption correction performed by the executable calctrans which performs the model calculation for the full spectrum. This separation significantly speeds up the code execution. Running calctrans results in the telluric absorption corrected spectrum in the file format of the input spectrum. Moreover, the best-fit model transmission curve for the full wavelength range is provided by an ASCII or FITS table. These files also contain the best-fit wavelength calibration based on the telluric lines, which is particularly well suited for spectra with unreliable wavelength calibration. Such a calibration works especially well if the inclusion regions, covering the full spectral range, comprise enough and well distributed telluric lines. Finally, the executable corrfilelist allows one to correct a list of files by means of the best-fit model transmission function for telluric absorption. In this case, also 2-D spectra can be provided.

### 4. Impact on observing strategy

Although powerful molecfit is not necessarily suited for telluric corrections in all cases. In this section, we briefly discuss a few situations to consider while deciding on the details of the observing strategy regarding the absorption telluric correction.

#### 4.1. Main cases

Two main cases for the use molecfit can be considered, depending on whether the wavelength calibration of the spectrum is reliable and accurate (residual RMS $\leq 0.1$ pixel or better) or not.

In the case of accurate wavelength calibration, the main requirement is that the spectrum to be corrected has at least one spectral region which includes medium-strength molecular lines of the most variable relevant species isolated enough so that their column density and the line spread function can be determined. Paper II provides more details on the definition and characteristics of the inclusion regions for X-shooter spectra.

If the wavelength calibration is not reliable but needs to be corrected by molecfit based on the telluric line themselves, a – possibly delicate – selection of inclusion and exclusion regions must be carried out, such that only telluric lines appear in the inclusion regions, any intrinsic feature of the object is masked out in the exclusion regions, and with sufficient coverage to be able to determine either an overall continuum or local continua.

#### 4.2. Simple continuum shape and small number of intrinsic features

The easiest spectra which can be modelled by the tool are the ones for objects with a well-defined and simple continuum and with limited confusion between telluric and intrinsic features. In such conditions, the tool can properly model the continuum spectrum of the object and the parameters of the telluric features can be well constrained.

#### 4.3. Large number of intrinsic features

If the number of intrinsic features is large in the spectral domain of interest, several options are possible. The choice of the best option depends on the line crowding: a first constraint is the number of points which can be used to determine the spectral continuum; a second constraint is the number of spectral ranges where telluric lines can be used to determine the column density of the molecules contributing in this spectral domain. An additional constraint arises if the wavelength calibration is not reliable.

Therefore a possible strategy is first to observe a telluric star with the same-setup – or retrieve corresponding data from the archive – and use molecfit on its reduced spectrum to determine which molecules are relevant, the wavelength calibration and continuum determination. Then, molecfit can be applied on the science target using the derived wavelength calibration (if relevant), changing the airmass or fitting the continuum and/or the column densities of the molecules involved. An example of such a strategy is shown below in Sect. 6.6 and is illustrated in particular Fig. 11. Another possible strategy is to ensure that
the spectral setup includes spectral regions which contains representative telluric lines but are free of intrinsic lines.

4.4. Emission line spectra

The telluric transmission spectrum cannot be fitted on the spectrum of an object showing little or no continuum, such as a faint cometary spectrum or an emission line object. A suggested strategy in this case is either to retrieve a spectrum of a telluric star from the archive or observe a telluric star in the spectral set-up of interest. Its spectrum can be modelled by molecfit. The model can then be modified easily by changing the airmass such that it corresponds to the airmass of the science target. If the water vapour at the site is monitored, the model can also be modified accordingly. The number of times telluric stars need to be observed is therefore reduced significantly.

4.5. Fitting sky emission spectra

The tool is able to fit sky emission spectra for molecules and physical processes handled by the radiative transfer code, with the exclusion of lines produced by chemiluminescence (such as OH). Thus, it is possible to determine the wavelength calibration and molecular column density of the relevant molecules using the sky emission spectrum if the spectral range is located in the thermal infrared.

In principle, these parameters can then be used to determine the transmission spectrum. In practice, the accuracy of the transmission spectrum strongly depends on the precision with which the retrieved atmospheric profiles actually represent the true ones. In addition, the line spread function is likely to be different if the source FWHM is smaller than the slit width. Finally, if the source is not properly centred in the slit, a small wavelength offset may need to be determined and applied.

5. Limitations

In this section, we briefly discuss the various factors which limit the accuracy of the molecfit correction of telluric spectra. Such factors can be external to molecfit, related to the accuracy with which instrumental parameters are taken into account or are internal to the method itself.

5.1. External

Molecular parameters accuracy and completeness A first limitation arises due to the completeness of the incorporated line database and on the accuracy of the contained molecular parameters. Currently, the AER line database delivered together with the LBLRTM code is included by default with molecfit. It is usually more frequently updated than the underlying main HITRAN\textsuperscript{10}, and is therefore recommended. However, although molecfit a priori allows one to use the original HITRAN database, this functionality is subject to stability of the database structure.

Molecules in atmospheric profile Molecfit only offers the possibility to fit the overall volume mixing ratio along the line-of-sight in the atmosphere: the overall shape of the profile is not adjusted. If the actual profile differs from the modelled one in some atmospheric layers, systematic errors can occur. In particular such a situation can be caused by specific, temporary volume mixing ratios of a molecule and is relatively frequent for water vapour. Fig. 2 illustrates the possible impact in an extreme case.

Atmospheric profile stability Any correction of telluric absorption requires a relatively stable atmospheric. The arrival of an atmospheric front is a clear case where the atmospheric profile changes suddenly. Even if the GDAS profiles would show such a front, its precise timing and characteristics are usually uncertain and surely depend on the pointing direction. Fortunately, few optical or infra-red astronomical observations are executed in such conditions.

Radiative transfer code accuracy The reader is referred to the publications list available on the LBLRTM web page\textsuperscript{11} for references regarding the validation of the radiative transfer code. In particular, it is worth to report here that “the algorithmic accuracy of LBLRTM is approximately 0.5% and the errors associated with the computational procedures are of the order of five times less than those associated with the line parameters so that the limiting error is that attributable to the line parameters and the line shape”.

5.2. Instrumental

Grating scattering Internal diffusion strongly limits the achievable accuracy of the modelling. Villanueva et al. (2009, internal communication) found that the CRIRES line spread function is best reproduced by a Voigt profile which needs to be calculated over ≈ 1000 pixels in order to account for the grating scattered light within the instrument. As a consequence, it often appears that the core of heavily saturated absorption lines does not reach zero intensity. The amount of flux in the core actually depends on the spectral energy distribution of the light reaching the grating and cannot be modelled accurately by molecfit, as molecfit only applies the convolution of the line spread function to the transmission spectrum and not to the science target one. In addition, later investigation (Uttenthaler 2010, private communication) indicates that the spatial profile of the grating scattered light is different than the one of the direct light.

The observed spectrum therefore combines different effects which cannot be easily modelled by molecfit and therefore limits possible to the accuracy of the correction such that residuals can reach an estimated 1% of the continuum depending on the significance of the grating scattering.

Instrumental background In the case of modelling sky emission spectra, molecfit uses a background defined by a grey body at the temperature of the main mirror of the telescope. It assumes that the thermal background from the instrument is negligible.

Instrumental response curve shape Molecfit fits a low-order polynomial to each inclusion region to the observed continuum of the input (object spectrum). However, it does not make a difference between the intrinsic continuum shape and the effect of the response curve of the instrument. Good results are obtained if the observed continuum of each inclusion region can

\textsuperscript{10} http://www.cfa.harvard.edu/HITRAN/

\textsuperscript{11} In particular, http://rtweb.aer.com/lblrtm_ref_pub.html
be well modelled by such polynomials. Alternatively, the user may provide a normalised spectrum as input.

5.3. Internal

Good initial guess values. By essence of the Levenberg-Marquardt fitting approach, molecfit needs and is sensitive to the initial guess solution. In particular, molecfit is designed to refine the wavelength calibration and continuum determination but it is not designed to measure these values from an uncalibrated spectrum. Adequate initial estimates improve the robustness of the fit and the speed of the convergence process. Knowledge of the line spread function and spectral resolving power are also important albeit the latter can be adjusted by molecfit.

Finite pixel size. Molecfit results are best when the spectral resolution is at least Nyquist sampled by the instrument. In any case, molecfit takes into account the finite pixel size of the spectrum: molecfit estimates the highest pixel resolution in a spectrum by evaluating the wavelength grid. An oversampling factor of 5 is then applied on the input to the radiative transfer code.

6. Examples

In the following, we illustrate some potential uses of molecfit with various ESO instruments.

6.1. UVES

The prototype version of molecfit was used to determine the location and strength of telluric absorption lines in Very Large Telescope-UV-Visual Échelle Spectrograph (UVES, Dekker et al. 2000) Rapid Response Mode or Target of Opportunity programmes of γ-ray bursts: indeed, some H2O lines mimic lines associated with high-redshift Damped Ly-α (DLA) lines. For example, in the spectrum of GRB050730 (Ledoux et al. 2009), H2O lines appear coincident in wavelength with the Si 3P1/2 - 3P1/2 \( \lambda \) 1816 line, and affect the Fe 6D7/2 - 6P7/2 and 6P5/2 - 4D5/2 lines, all associated with the \( \lambda \) = 3.69857 DLA. Similarly, as shown in Fig. 4, the use of molecfit was allowed to determine the location and strength of the H2O lines affecting the Fe 4D7/2, \( \lambda \) 2382, \( \lambda \) 2374, Fe 4D7/2, \( \lambda \) 2382 and \( \lambda \) 2389 lines (amongst others) associated with the \( \lambda \) = 3.42743 DLA in the spectrum of GRB080310 (De Cia et al. 2012).

6.2. FLAMES

Figure 5 presents a Fibre Large Array Multi Element Spectrograph (FLAMES)/Giraffe spectrum of the O4 V star NGC 3603-117 observed with the LR8 setting and the ARGUS integral field unit (data courtesy: M. Gieles; Prog. ID: 079-D-0374(A)), providing a spectral resolving power of 10400. The presented spectrum corresponds to the brightest spaxel on the object.

The presence of water vapour telluric absorption lines impedes a precise determination of the width and centroid of the Paschen hydrogen lines at 901 and 923 nm. However, there is usually no observation of telluric star for FLAMES. Molecfit can be used to determine the PWV and correct the science spectrum by the transmission spectrum. As a result, a precise determination of the width and position of the lines was obtained, multiplying by three the number of lines available for, e.g., radial velocity measurements in that spectral region.

Fig. 5. Spectrum of NGC 3603-117. (Black:) Original spectrum. (Red:) Telluric line corrected spectrum. The spectral range covered by the shaded area was used to determine the amount of PWV.

6.3. SINFONI

Archival data of the field of the binary star 2MASS J01033563-5515561 obtained with the Spectrograph for Integral Field Observations in the Near Infrared (SINFONI, Eisenhauer et al. 2003) for programme ID 290.C-5022(A) were retrieved and reduced with the SINFONI pipeline and default parameters. Only 20 s Detector Integration Time (DIT) J-band exposures obtained at a median airmass of 1.28 are shown here. The telluric star Hip 024337 was observed at an airmass of 1.33, approximately 66 min after the start of the first science exposure. The spectrum of B and of the telluric star were extracted using a 3-pixels radius centred on the photocenter of each source. Hot pixels or cosmics in the reduced spectrum affected were manually edited out.

Inclusion regions were selected to cover telluric lines caused by H2O and O2. Exclusion regions were defined for the pixels affected by cosmics. Figure 6 shows the original spectrum and compares its correction by the transmission spectrum calculated by molecfit and by the telluric star. The spectrum corrected by the transmission spectrum calculated by molecfit is slightly less noisy than the one corrected by the telluric star spectrum and does not show the effect of the H Paschen β line. On the other hand, the correction of the lines in the ~ 1.13 μm water vapour band is slightly less good probably because of a small change in the line spread function.

6.4. X-shooter

A reduced X-shooter (Vernet et al. 2011) spectrum of the Luminous Blue Variable star R71 was kindly provided to us by Andrea Mehner. The data were obtained on February 1, 2014 as part of the programme ID 092.D-0024(A). The slit width used was 5 × 11″; the exposure time was 20 s. Figure 7 shows the original spectrum together with the spectrum corrected by the transmission spectrum calculated by molecfit, based on the fitting made in the regions marked in shadow.

A reduced spectrum of the γ-ray burst GRB 130606A (Ukwatta et al. 2013) at redshift \( z = 5.9 \) (Castro-Tirado et al. 2013; Xu et al. 2013) was kindly provided to us by Thomas Kruehler. The data were obtained under programme ID 091.C-0934(C) (P. J. Fynbo). The exposure time totalled 2400 s using nodding (4 × 600 s). The 0.9x11/H slit was used (i.e., includes the K-band blocking filter). Figure 8 shows the near-infrared GRB spectrum and a small region affected by both telluric and intervening absorption lines.
Fig. 4. H$_2$O telluric absorption lines affecting absorption lines associated with the $z = 2.42743$ DLA in the UVES spectrum of GRB080310. The telluric lines - modelled by molecfit - are shaded in yellow; the models for the different components ($a$, $b$, $c$, $d$) of the absorption system are represented with different colours (blue, cyan, green, orange), while the combined model is in red. See De Cia et al. (2012) for details.

Fig. 6. SINFONI J band spectrum of 2MASS J01033563-5515561 B. (Bottom:) Pipeline reduced spectrum. The yellow shaded areas show the spectral ranges of the inclusion regions. Exclusion regions appear in blue. (Medium:) Spectrum divided by the spectrum of the telluric star. (Top:) Spectrum divided by the transmission spectrum calculated by molecfit.

6.5. VISIR

Archival data of MCG-3-34-064 obtained with the VLT Imager and Spectrometer for mid Infra Red (VISIR) for the programme 280.B-5068(A) were retrieved and reduced with the VISIR 2.0.0 pipeline and default parameters. Only the 12.4 $\mu$m LR spectrum obtained at a median airmass of 1.01 is shown here.

Inclusion regions were selected to cover telluric lines caused by H$_2$O. An exclusion region was defined covering the redshifted [Ne I] line.

Figure 9 shows the original spectrum and compares its correction by the transmission spectrum calculated by molecfit and by the telluric star.

Fig. 7. Visible arm X-shooter spectrum of R71 LBV star. The pipeline reduced spectrum is shown in black. The shaded areas show the inclusion regions used to model the line spread function and determine the column densities of H$_2$O and O$_2$. The spectrum corrected by derived transmission spectrum is shown in red.

6.6. CRIRES

Spectra obtained with the Cryogenic high-resolution IR Échelle Spectrograph (CRIRES, Kaeufl et al. 2004) before mid-July
it (Villanueva et al. 2009, internal communication), in particular Lorentzian. Therefore a Voigt profile is usually best to represent although the line spread function is usually well modelled by VISIR low-resolution inclusion regions. The two bottom graphs show the spectral range Fig. 8. Near-infrared arm X-shooter spectrum of GRB 130606A. The top graph shows the complete spectrum. The shaded areas show the inclusion regions. The two bottom graphs show the spectral range 1.150 < \( \lambda / \mu \text{m} \) < 1.160 affected by both telluric and intervening absorption lines. Middle: molecfit corrected spectrum. Bottom: the red spectrum shows the transmission spectrum multiplied by \( 2.8 \times 10^{-17} \) for comparison plotted over the original spectrum (in black).

Fig. 9. VISIR low-resolution \( \lambda 1.24 \mu \text{m} \) spectrum of MCG-3-34-064. (Bottom:) pipeline reduced spectrum. The yellow shaded areas show the spectral ranges of the inclusion regions. Exclusion region, centred on the redshifted [Ne I], appear in blue shade. (Medium bottom:) derived transmission spectrum. (Medium top:) Spectrum divided by the telluric star and an additional first degree polynomial for display purpose. (Top:) Spectrum divided by the transmission spectrum calculated by molecfit.

2014 – when the instrument is removed from operations to undergo an upgrade – covered a small spectral range \( \Delta \lambda = \lambda / 700 \). Although the line spread function is usually well modelled by a Gaussian function (Seifahrt et al. 2010), its wings are more Lorentzian. Therefore a Voigt profile is usually best to represent it (Villanueva et al. 2009, internal communication), in particular, to attempt to model the light scattered on the grating which causes even heavily saturated line to appear with residual light in their core. The kernel width on the other hand depends on the quality of the Adaptive Optics (AO) correction – when the AO is used –, which in turns depends on the ‘AO star’ magnitude and on the turbulence profile of the atmosphere. On the other hand, for non-AO observation, it may also depend on the actual slit width; one should note here that the slit mechanism lacked reliability before the installation of fixed slit widths in September 2011 (Smoker 2014).

As mentioned in the CRIRES User Manual (Smoker 2014), CRIRES spectra are often affected by unprecise wavelength calibration, due to a lack of calibration lines. Molecfit can solve this problem in a number of situations using the telluric lines themselves when they are well distributed over the spectral range and not too mixed with lines intrinsic to the science target.

Figure 10 shows an extract (detector #2 only) of the 4889.5 nm setting spectra for three stars obtained as part of the CRIRES-POP programme (Lebzelter et al. 2012): the A0 IV star \( \gamma \) Gem, observed on October 20, 2010; the F8 V star \( \alpha \) For, observed on October 31, 2009 and the M4 V Barnard’s star, observed on July 7, 2010. No telluric stars were observed for this programme. The number of intrinsic lines increases for late type stars therefore requiring an increase in the number and size of exclusion regions; consequently, an F8V star is approximately the latest type star for which molecfit can be used in a non-expert mode.

For later type stars, the expert mode is required. The variable carbon star \( \chi \) TrA was observed on September 22, 2010 as part of the same programme. Regarding the molecular content of the atmosphere molecfit was configured to fit only the column density for H2O and CO2, while the O1 and OCS column densities were fixed. The polynomial coefficients for the continuum and wavelength calibration were copied from the results of the fit to the \( \gamma \) Gem spectrum. The wavelength solution found for \( \gamma \) Gem was kept fixed. This method allowed one to obtain a very good results for the telluric line correction, as shown in Fig. 11.

7. Conclusion

Molecfit is a versatile tool to model and correct telluric absorption lines. Compared to previous similar tools, molecfit takes into account the best knowledge of temperature, pressure and humidity in the atmosphere above the observatory. This approach allows one to regularly reach an accuracy of the order of 2% of the continuum or better in correcting optically thin telluric absorption lines.

Best results are obtained if the following conditions are met: (1) the input spectrum already has an accurate wavelength calibration, (2) the continuum in the inclusion regions is already corrected or can be well modelled by low-degree polynomials, (3) the inclusion regions cover optically thin lines of the relevant molecules whose column density varies significantly with time (mostly water vapour, but also, CO2, O1) and whose shapes allow one to determine the line spread function with sufficient precision. On the other hand, molecfit can use the telluric lines themselves to provide an improved wavelength calibration, provided that they are well spread over the spectral range of interest and are reasonably unaffected by intrinsic spectral lines of the science target.

Finally, it is important to remember that any correction method cannot recover with accuracy any science target feature coincident in wavelength with \( r \geq 2 \) telluric absorption lines. Such optically thick lines can be easily identified in high-resolution spectra (such as obtained by CRIRES) where these lines are often spectrally resolved; however, in low to medium
resolution spectra (such as X-shooter), their shape is mainly determined by the instrument spectral resolution. In other words, even apparently weak telluric absorption lines can be caused by optically thick lines.

Acknowledgements. A prototype version of molecfit was built around the Reference Forward Model, a GENLN2-based line-by-line radiative transfer model originally developed at the Atmospheric, Oceanic and Planetary Physics Laboratory, Oxford University, to provide reference spectral calculations for the MIPAS launched on the ENVISAT satellite in 2002. We warmly thank Amu Duthia for his help in various phases of the prototype development. We also thank Andreas Seifahrt for his help in the usage of LNFL/LBLRTM. This study was carried out in the framework of the Austrian ESO In-Kind project funded by BM:wf under contracts BMWF-10-490(0009-II/10)2009 and BMWF-10-490(0008-II/3)2011. This publication is also supported by the Austrian Science Fund (FWF): P26130. A.G. acknowledges support from FONDECYT grant 3130361. We would like to thank the participants to an internal ESO mini-workshop who provided us with sample spectra from various instruments obtained for various scientific purposes: their help allowed us to identify a number of problems in a previous version of the molecfit package. We are also grateful to Andrea Mehlner, Thomas Knüll, and Patrick Lee for providing spectra ahead of publications and to Annalisa De Cia for providing Fig. 4.

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Fig. 10. Extract (detector #2) of CRIRES 4889.5 nm setting spectra of γ Gem (top), α For (middle) and Barnard's star (bottom). In each case, the bottom graph shows the original, reduced spectrum and the blue-shaded exclusion regions; the red spectrum shows the molecfit derived transmission spectrum scaled by a constant factor. The top graph shows the molecfit corrected spectrum.

Fig. 11. Extract (detector #2) of CRIRES 4889.5 nm setting spectra of X TrA; the red spectrum shows the molecfit derived transmission spectrum scaled by a constant factor. The top graph shows the corrected spectrum. Molecfit was used in expert mode in this case.
Article F:
Molecfit: A general tool for telluric absorption correction

II. Quantitative evaluation on ESO-VLT/X-Shooter spectra

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II. Quantitative evaluation on ESO-VLT/X-Shooter spectra

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ABSTRACT

Context. Absorption by molecules in the Earth’s atmosphere strongly affects ground-based astronomical observations. The resulting absorption line strength and shape depend on the highly variable physical state of the atmosphere. Usually, supplementary observations of so-called telluric standard stars are needed to correct for this effect, which is telescope time expensive. We have developed the software package molecfit to fit synthetic transmission spectra to observations. The transmission spectra are calculated by means of the radiative transfer code LBLRTM and atmospheric profiles created by merging a static standard atmosphere, direct on-site measurements, and a 3D world wide atmospheric model containing water vapour, temperature, and pressure profiles.

Aims. We evaluate the quality of the telluric absorption correction using molecfit with a set of archival ESO-VLT/X-Shooter visible and near-IR spectra.

Methods. Due to the wavelength coverage from the $U$ to the $K$ band X-Shooter is well suited to investigate the quality of the telluric absorption correction with respect to the observing conditions, the instrumental set-up, input parameters of the code, the signal-to-noise of the input spectrum, and the atmospheric profiles. These investigations are based on two figures of merit $I_a$ and $I_{res}$, describing the systematic offsets and the remaining small-scale residuals of the corrections. The results are compared with the standard method for the telluric absorption correction performed with the IRAF task telluric.

Results. The evaluation of the telluric correction with molecfit reveals a convincing removal of atmospheric absorption features. The comparison with the IRAF task telluric shows significantly weaker small-scale residuals and offsets for molecfit.

Conclusions. Fitted synthetic transmission spectra are an excellent alternative to the correction based on telluric standard stars. In addition, molecfit offers wide flexibility for adaption to various instruments and observing sites.

Key words. Radiative transfer – Atmospheric effects – Instrumentation: spectrographs – Methods: data analysis – Methods: numerical – Techniques: spectroscopic

1. Introduction

Ground-based observations are naturally affected by various physical processes in the Earth’s atmosphere, in particular scattering and absorption. The dynamics of the weather conditions, seasonal effects, or climate change lead to variabilities in temperature, pressure, and the chemical composition on time scales from seconds to decades making the absorption correction a demanding matter. Thus, any data calibration usually needs supplementary calibration frames. However, this approach is very expensive in terms of telescope time, as these data should be taken directly before or after the science target.

This particularly applies to the correction arising from molecular absorption in the Earth’s atmosphere. The required supplementary calibration frames are observations of telluric standard stars (hereafter TSS). The TSS are usually bright hot stars, e.g. B-type, showing only few, well known intrinsic spectral features. The TSS have to be observed at a similar airmass, time, and line of sight as the science target to probe the same atmospheric column.

Within the framework of the in-kind contribution of Austria’s accession to the European Southern Observatory (ESO), we developed a comprehensive sky background model\textsuperscript{3} covering a wavelength range from 0.3 to 30 $\mu$m (Noll et al. 2012). It was originally designed for the ESO Exposure Time Calculator\textsuperscript{2} and incorporates several components, e.g. airglow, scattered moonlight (Jones et al. 2013), zodiacal light (Leinert et al. 1998), scattered starlight, and the telescope emission modelled as grey body. It also contains a spectral model of the Earth’s lower atmosphere in local thermal equilibrium calculated by means of the

\textsuperscript{1}http://www.eso.org/observing/etc/skycalc/skycalc.htm
\textsuperscript{2}http://www.eso.org/observing/etc/
radiative transfer code LNFL/LBLRTM\textsuperscript{3} (Clough et al. 2005). This code is used with the spectral line parameter database aer\textsubscript{v}3.2, which is based on HITRAN\textsuperscript{4} (Rothman et al. 2009) and delivered together with the code. Averaged atmospheric profiles for Cerro Paranal describing the chemical composition as a function of height (combination of the ESO MeteoMonitor\textsuperscript{5}, a standard atmosphere\textsuperscript{6} and the 3D Global Data Assimilation System (GDAS) model\textsuperscript{7}) are also used as input. The GDAS model is provided by the National Oceanic and Atmospheric Administration (NOAA)\textsuperscript{8} and contains time-dependent profiles of the temperature, pressure, and humidity.

The ESO In-Kind software also includes tools for removing the atmospheric signature in spectra\textsuperscript{9}. The package molecfit\textsuperscript{10} is an alternative approach for performing the telluric absorption correction by means of theoretically calculated transmission spectra based on the atmospheric model. We use the previously mentioned radiative transfer code and line database to achieve synthetic transmission curves. The required atmospheric input profile is created in the same way as for the sky model, but for a given time and not averaged. The algorithm and package functionalities are described in more detail in Smette et al. (2014) (hereafter Paper I). Here, we evaluate the quality of molecfit as a telluric absorption correction tool for ESO Very Large Telescope (VLT) instruments. The focus lies on observations taken with the X-Shooter instrument (Vernet et al. 2011), an echelle spectrograph covering simultaneously the wavelength regime from the $U$ to the $K$ band at medium resolution. We use two methods: (a) a statistical study of the quality of the correction by means of figures of merit, and (b) a comparison of the molecfit correction with that obtained using the traditional method based on observations of TSS.

We first briefly describe the method of the telluric absorption correction incorporated in molecfit (Sect. 2). A description of the test data set is given in Sect. 3. The results on the quality of the telluric absorption correction based on molecfit and a comprehensive investigation on various influences are discussed in Sect. 4. In Sect. 5, we give a detailed comparison with the classical method based on TSS. Section 6 provides a summary of our findings.

2. Telluric correction with molecfit

The correction with the molecfit package is performed in two steps:

- Determination of the best-fit atmospheric and instrumental parameters (programme molecfit): they are related to the total column densities of the input atmosphere profile and the instrumental parameters (spectral line profile, wavelength calibration, continuum position) are optimised by means of a $\chi^2$-Levenberg-Marquardt minimisation algorithm (see Paper I for a comprehensive description of the underlying algorithms) to best reproduce the observed telluric spectrum in selected wavelength regions. By varying the scaling factor of the molecular profiles of the initial input atmospheric profile, the programme iteratively calculates transmission curves, which are fitted to the input science spectrum. To minimise the calculation time and/or to avoid regions affected by stellar spectral features or instrument defects, the fitting is restricted to user-defined spectral ranges.

- Correction of the telluric spectrum (programmes calctrans/corrfilelist): the best-fit atmospheric and instrumental parameters are used to calculate the atmospheric transmission spectrum over the entire wavelength range of the scientific observation; de facto extrapolating the adjusted telluric spectrum outside the adopted fitted regions. The science spectrum is then divided by this transmission curve to produce telluric corrected data. The supplementary programme corrfilelist allows the correction of a set of science spectra obtained under the same conditions.

3. The data set

In order to evaluate the performance of molecfit, we have used archival data obtained with the X-Shooter instrument mounted at the ESO VLT (Vernet et al. 2011). This instrument covers the entire wavelength range from $\lambda = 0.3$ to $2.5 \mu$m in three spectral arms (UVB, VIS, and NIR) at medium resolution ($R \approx 3300$ to 18200, depending on the slit width) simultaneously. This broad wavelength regime gives the opportunity to study the several absorption bands of different species simultaneously (e.g. H$_2$O, O$_2$, CO$_2$).

We have reduced the entire publicly available ESO archive data from October 2009 to March 2013, leading to a comprehensive data set taken under various observing conditions, since X-Shooter is frequently used. We used the ESO standard pipeline in version V2.0.0 under Reflex V2.3 on our cluster\textsuperscript{10}.\n
\begin{table}[h]
\centering
\caption{Table of object types used for the method comparison}
\begin{tabular}{llll}
\hline
\# & object type & counts [ADU] & slit ["\!"] \\
\hline
1 & B[e] star & 7684 & 0.4x11 \\
2 & E0 galaxy & 5236 & 0.9x11 \\
3 & galaxy & 384 & 1.2x11 \\
4 & Carbon star & 143250 & 0.9x11 \\
5 & cE galaxy & 804 & 1.5x11 \\
6 & Carbon star & 50587 & 0.9x11 \\
7 & Sc galaxy & 269 & 0.9x11 \\
8 & star (unknown type) & 4198 & 0.4x11 \\
9 & O star & 3427 & 0.4x11 \\
10 & Blazar & 320 & 1.2x11 \\
11 & white dwarf & 3163 & 0.9x11 \\
12 & SB0-a galaxy & 2592 & 0.9x11 \\
13 & FOV star & 650 & 0.4x11 \\
14 & variable low mass star & 5545 & 0.4x11 \\
15 & variable low mass star & 2675 & 0.4x11 \\
16 & Type I SN candidate & 364 & 0.9x11 \\
17 & PN & 6214 & 0.4x11 \\
18 & variable star & 9001 & 0.4x11 \\
19 & Seyfert 2 Galaxy & 462 & 1.5x11 \\
20 & Seyfert 2 Galaxy & 1833 & 1.5x11 \\
21 & S0 galaxy & 95281 & 1.2x11 \\
22 & S0/a galaxy & 1589 & 1.2x11 \\
23 & SB0 galaxy & 8336 & 0.6x11 \\
24 & ultracool WD & 1136 & 0.9x11 \\
\hline
\end{tabular}
\end{table}
For studying the influence of the atmospheric conditions and instrumental set-ups on the quality of telluric absorption correction (see Sect. 4), we have taken all 1D spectra of TSS without flux calibration until March 2013. In total, there are 4218 NIR- and 3823 VIS-arm spectra. UVB-arm spectra were not considered due to the lack of molecular absorption features\(^{11}\). Due to occasional failures of the automatic X-Shooter pipeline, the number of obtained spectra is lower than the number of exposures in the archive. Since the obtained set of reduced data was large enough for our purpose, we did not attempt to re-run the pipeline manually (possibly using tuned reduction parameters) for the cases for which the automatic approach failed.

For the comparison with the classical method described in Sect. 5, we have selected 24 science observations in conjunction with their corresponding TSS observations manually from our X-Shooter test data set in order to perform a comparison between the telluric absorption correction achieved with molecfit and the classical method related to TSS. The science test data sets were selected to cover a wide range of astrophysical objects, observation periods, slit width, and counts (in ADU, see Table 1) to also estimate the limits of the application of both methods. The TSS spectra were selected to coincide best with the airmass and the date of the corresponding science observation (see Table 2) and were usually reduced with the same flat field. As the majority of the telluric absorption features arise in the infrared regime, we restrict this investigation to NIR-arm data.

### 4. Quality of telluric absorption correction

In the following, we evaluate the quality of telluric absorption correction with molecfit. For this purpose, we investigate a large sample of TSS spectra taken with the X-Shooter spectrograph (see Sect. 3). We mainly focus on the NIR arm, where the telluric absorption correction is most crucial. We also complement the discussion with results from the VIS arm. The molecfit test set-up for the data set and the quality indicators used are discussed in Sect. 4.1. The results are shown in Sects. 4.2 to 4.4. The effect of changing the fitting ranges and molecfit input parameters is discussed for an example spectrum in Sects. 4.5 and 4.6, respectively. Finally, the influence of differences in the input water vapour profile is described in Sect. 4.7.

#### 4.1. Test set-up and figures of merit

The performance of molecfit was tested with a fixed input parameter set. This approach is appropriate to estimate statistically the quality of the correction on a large set of data. Nevertheless, further quality improvements could be obtained by adjusting the fitting parameters for each individual spectrum.

For the NIR arm, the applied set-up is shown in Table 3 (see also Paper I). For the wavelength range from 1 to 2.5\(\mu\)m, the model-relevant molecules are \(\text{O}_2\), \(\text{CO}_2\), \(\text{H}_2\text{O}\), \(\text{CH}_4\), and \(\text{CO}\). For the VIS arm, it is sufficient to consider \(\text{O}_2\) and \(\text{H}_2\text{O}\). Only water vapour is fitted in spectra of both arms, since the concentration variations and the impact on the X-Shooter data of the other species are expected to be small. The equatorial standard atmosphere profile that we use is already more than a decade old (prepared by J. J. Remedios 2001; see Seifarth et al. 2010). As the global \(\text{CO}_2\) concentration increases with time (World Meteorological Organization 2012), the input \(\text{CO}_2\) column was multiplied by 1.05 to be representative of the X-Shooter archival data.

A linear fit \(\chi^2 = 1\) was performed to correct the continua of the spectra in each of the fitting ranges (see below). The initial continuum factor \(\chi^2 = 0\) was set to \(10^3\) to be in the order of the typical counts level in ADU of X-Shooter data without flux calibration. For the wavelength grid correction, only a constant shift was allowed \(\chi^2 = 0\) (see Sect. 4.6 for a discussion). For the instrumental profile, a combination of a boxcar and Gaussian was assumed. A possible Lorentzian was not considered, since a study of the shape of the line profiles did not reveal significant Lorentzian wings. The width of the initial boxcar was chosen to be 75% of the slit width, which should be close to the real value for the different slits (as tests indicate). An exception is the 5” slit, which is, however, rarely used for observations of science targets. For the Gaussian, a reasonable initial FWHM of 1 pixel \(\chi^2 = 0\) and a kernel size of 3 FWHM \(\chi^2 = 0\) were given. Since echelle spectra are fitted, the kernel was selected to be proportional to the wavelength \(\chi^2 = 0\). The profile-related input parameters refer to the central wavelengths of 1.74\(\mu\)m and 0.78\(\mu\)m for the NIR and VIS

#### Table 4. Wavelength ranges (vacuum) for fitting NIR- and VIS-arm X-Shooter TSS spectra

<table>
<thead>
<tr>
<th>Arm</th>
<th>No.</th>
<th>(\lambda_{\text{min}}) [(\mu)m]</th>
<th>(\lambda_{\text{max}}) [(\mu)m]</th>
<th>Main molecule</th>
</tr>
</thead>
<tbody>
<tr>
<td>NIR</td>
<td>1</td>
<td>1.120</td>
<td>1.130</td>
<td>(\text{H}_2\text{O})</td>
</tr>
<tr>
<td>NIR</td>
<td>2</td>
<td>1.470</td>
<td>1.480</td>
<td>(\text{H}_2\text{O})</td>
</tr>
<tr>
<td>NIR</td>
<td>3</td>
<td>1.800</td>
<td>1.810</td>
<td>(\text{H}_2\text{O})</td>
</tr>
<tr>
<td>NIR</td>
<td>4</td>
<td>2.060</td>
<td>2.070</td>
<td>(\text{CO}_2)</td>
</tr>
<tr>
<td>NIR</td>
<td>5</td>
<td>2.350</td>
<td>2.360</td>
<td>(\text{CH}_4)</td>
</tr>
<tr>
<td>VIS</td>
<td>1</td>
<td>0.686</td>
<td>0.694</td>
<td>(\text{O}_2)</td>
</tr>
<tr>
<td>VIS</td>
<td>2</td>
<td>0.759</td>
<td>0.770</td>
<td>(\text{O}_2)</td>
</tr>
<tr>
<td>VIS</td>
<td>3</td>
<td>0.930</td>
<td>0.945</td>
<td>(\text{H}_2\text{O})</td>
</tr>
</tbody>
</table>

11Note that the ozone absorption by the Huggins and Chappuis bands (see Paper I) is usually taken into account by the extinction correction (see e.g. Patat et al. 2011).

![Fig. 1. Binned reference X-Shooter NIR-arm model transmission spectrum for a mean amount of precipitable water vapour (PWV) of 3.1 mm and an airmass of 1. The 1 nm wide bins marked by red symbols are indicated as well. The figure also shows the fitting ranges (yellow bars) that were used by molecfit (see also Table 4).](image-url)
Table 2. X-Shooter NIR-arm data set used for the method comparison.

<table>
<thead>
<tr>
<th>#</th>
<th>object</th>
<th>Science observations</th>
<th></th>
<th>star</th>
<th>Telluric standards</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>airmass</td>
<td>obs. date $t_{\text{GET}}$</td>
<td></td>
<td>airmass</td>
<td>obs. date $t_{\text{RES}}$</td>
</tr>
<tr>
<td>1</td>
<td>V921-Sco</td>
<td>1.109</td>
<td>2010-03-10T09:01:02</td>
<td></td>
<td>Hip084409</td>
<td>1.058</td>
</tr>
<tr>
<td>2</td>
<td>NGC5812</td>
<td>1.06</td>
<td>2010-03-13T08:57:03</td>
<td></td>
<td>Hip073345</td>
<td>1.128</td>
</tr>
<tr>
<td>3</td>
<td>SDSS 1057-0629</td>
<td>1.45</td>
<td>2010-03-19T01:32:02</td>
<td></td>
<td>Hip068124</td>
<td>1.72</td>
</tr>
<tr>
<td>4</td>
<td>HE 1011-0942</td>
<td>1.201</td>
<td>2010-03-22T00:51:05</td>
<td></td>
<td>Hip037963</td>
<td>1.214</td>
</tr>
<tr>
<td>5</td>
<td>CM07-1214</td>
<td>1.424</td>
<td>2010-03-24T01:59:55</td>
<td></td>
<td>Hip063541</td>
<td>1.225</td>
</tr>
<tr>
<td>7</td>
<td>ESO-206</td>
<td>1.096</td>
<td>2009-12-22T05:02:34</td>
<td></td>
<td>Hip024811</td>
<td>1.097</td>
</tr>
<tr>
<td>11</td>
<td>LTT3218</td>
<td>1.04</td>
<td>2010-03-28T02:04:02</td>
<td></td>
<td>Hip043763</td>
<td>1.201</td>
</tr>
<tr>
<td>13</td>
<td>PDS415</td>
<td>1.011</td>
<td>2010-03-31T09:03:42</td>
<td></td>
<td>Hip077900</td>
<td>1.026</td>
</tr>
<tr>
<td>14</td>
<td>G1S88</td>
<td>1.113</td>
<td>2010-07-19T02:04:00</td>
<td></td>
<td>Hip094986</td>
<td>1.132</td>
</tr>
<tr>
<td>15</td>
<td>G1S88</td>
<td>1.086</td>
<td>2010-07-19T01:43:43</td>
<td></td>
<td>Hip094986</td>
<td>1.132</td>
</tr>
<tr>
<td>17</td>
<td>IC1266</td>
<td>1.222</td>
<td>2010-07-05T05:54:38</td>
<td></td>
<td>Hip085885</td>
<td>1.248</td>
</tr>
<tr>
<td>18</td>
<td>HD 165222</td>
<td>1.748</td>
<td>2010-06-28T07:53:24</td>
<td></td>
<td>Hip088795</td>
<td>1.693</td>
</tr>
<tr>
<td>23</td>
<td>NGC5206</td>
<td>1.094</td>
<td>2011-02-18T08:02:23</td>
<td></td>
<td>HD130163</td>
<td>1.124</td>
</tr>
</tbody>
</table>

Notes.

1 The set is selected to cover a wide range of astrophysical objects, the airmass, the time/date of the observation, and the median of the flux (in ADU) as approximate value to estimate the overall flux level. 2 $\Delta t_{\text{RES}}$ = $t_{\text{GET}}$ − $t_{\text{RES}}$ (approximate values)

Running molecfit for the input parameters listed in Table 3 and the fitting ranges shown in Table 4 results in the best-fit parameters for each sample exposure (see Sect. 3). These are then used by calctrans (see Sect. 2) to provide a telluric absorption corrected spectrum for the full wavelength range (see Fig. 2). The quality of the fitting in the pre-defined windows can be evaluated by considering the RMS from the molecfit results file. However, the quality of the telluric absorption correction must be studied over the whole spectral range with respect to the quality of the resulting object spectrum and therefore requires a different analysis. For this purpose, we have defined the figures of merit $I_{\text{ff}}$ and $I_{\text{res}}$. The former measures the continuum-normalised difference between the original and telluric absorption corrected spectrum, relative to the telluric line strength. The latter traces the continuum-normalised standard deviation of the residuals of the correction, relative to the telluric line strength. Therefore, $I_{\text{ff}}$ and $I_{\text{res}}$ are indicators of large-scale systematic offsets in the telluric absorption corrected spectra and small-scale (or high-frequency) variations of the residuals, respectively. The calculation of these quality indicators is described in the following steps:

- First, each telluric absorption corrected NIR- and VIS-arm spectrum was divided into 1 nm and 0.5 nm wide bins, respectively (corresponding to about 17 and 25 pixels, i.e. a few resolution elements; cf. Sect. 4.4).
- The mean and the standard deviation were calculated for each of these bins (see Fig. 2).
The interpolated continuum intensity for each bin was then to be independent of the absolute flux, the offsets and standard deviations of each bin were divided by the interpolated continuum mean values.

To provide the resulting values relative to the absorption line strengths (see Fig. 3), the relative offsets and standard deviations were divided by 1 minus the average transmission $T$ for each bin.

Five transmission ranges were defined for a detailed analysis of the telluric absorption correction. Apart from a wide range from 0.1 to 0.95, ranges centred around 0.9, 0.8, 0.5, and 0.2 were defined (see Figs. 1 to 3).

The bins that belong to each of the five ranges were determined by using the best-fit transmission spectra of the individual sample spectra. Thus, the bin assignment depends on the airmass, amount of atmospheric water vapour, and spectral resolution.

Finally, to obtain the figures of merit and to reduce the effect of outliers, we took the median of the relative offset and standard deviation of the bins for each transmission range as shown in Fig. 3. The resulting quality indicators $I_{\text{off}}$ and $I_{\text{res}}$ are used in the subsequent analysis. If the transmission range is not specified explicitly, the results for the wide range are given. Note that the systematic offsets of the correction and the intra-bin standard deviations of the residuals are given relative to the telluric line strength. For providing them relative to the object continuum, $I_{\text{off}}$ and $I_{\text{res}}$ have to be multiplied by $1 - T$. More details on the interpretation of our figures of merit can be found in Sect. 4.3.

### 4.2. Outliers

The indicator $I_{\text{res}}$ measures variations in the counts level within each of the narrow bins of a telluric absorption corrected spectrum. Primarily, this traces the small-scale quality of the telluric absorption correction. However, random noise, defects in the spectra, sky subtraction residuals, and spectral features of the observed object can also cause an increase of $I_{\text{res}}$. This is demonstrated for random noise in Fig. 4, which shows a clear increase of the scatter for lower mean counts, i.e., decreasing S/N. In order to avoid difficulties in interpreting the $I_{\text{res}}$ sample statistics, spectra with counts less than $10^5$ ADU are excluded from further analysis. This threshold concerns 120 spectra of the NIR arm (i.e. 2.8% of the sample) and 36 spectra of the VIS arm (0.9%).

Excluding these data does not mean that their corrected spectra

---

**Table 3. Molecfit parameter set-up for the telluric absorption correction evaluation of NIR-arm X-Shooter TSS spectra**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Short description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^{-3}$</td>
<td></td>
<td>factor to convert the input wavelength units into $\mu$m</td>
</tr>
<tr>
<td>air</td>
<td></td>
<td>wavelengths in vacuum or air</td>
</tr>
<tr>
<td>$10^{-2}$</td>
<td></td>
<td>relative $\chi^2$ convergence criterion</td>
</tr>
<tr>
<td>$10^{-2}$</td>
<td></td>
<td>relative parameter convergence criterion</td>
</tr>
<tr>
<td>O2 CO2 H2O CH4 CO</td>
<td>list of molecules to be included in the model</td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>0.0 1 0.0</td>
<td>flags for if each molecule is to be fit ($1=$yes, $0=$no)</td>
</tr>
<tr>
<td>1</td>
<td>1.05 1.1 1.1</td>
<td>relative molecular column densities ($1=$ input profile)</td>
</tr>
<tr>
<td>1</td>
<td></td>
<td>flag for polynomial fit of the continuum ($1=$yes, $0=$no)</td>
</tr>
<tr>
<td>1</td>
<td></td>
<td>degree of polynomial for the continuum fit</td>
</tr>
<tr>
<td>10$^3$</td>
<td></td>
<td>initial constant term for the continuum fit</td>
</tr>
<tr>
<td>1</td>
<td></td>
<td>flag for refinement of wavelength solution ($1=$yes, $0=$no)</td>
</tr>
<tr>
<td>0</td>
<td></td>
<td>degree of Chebyshev polynomial for refined wavelength solution</td>
</tr>
<tr>
<td>0</td>
<td></td>
<td>initial constant term of the Chebyshev polynomial</td>
</tr>
<tr>
<td>1</td>
<td></td>
<td>flag for resolution fit using a boxcar filter ($1=$yes, $0=$no)</td>
</tr>
<tr>
<td>0.75</td>
<td></td>
<td>initial value for FWHM of boxcar relative to slit width ($\geq 0$ and $\leq 2$)</td>
</tr>
<tr>
<td>1</td>
<td></td>
<td>kernel mode ($0=$independent Gaussian and Lorentzian, $1=$Voigt profile)</td>
</tr>
<tr>
<td>1</td>
<td></td>
<td>flag for resolution fit using a Gaussian filter ($1=$yes, $0=$no)</td>
</tr>
<tr>
<td>1</td>
<td></td>
<td>initial value for FWHM of Gaussian (in pixels)</td>
</tr>
<tr>
<td>0</td>
<td></td>
<td>flag for resolution fit using a Lorentzian filter ($1=$yes, $0=$no)</td>
</tr>
<tr>
<td>0</td>
<td></td>
<td>initial value for FWHM of Lorentzian (in pixels)</td>
</tr>
<tr>
<td>1.0</td>
<td></td>
<td>kernel size in units of FWHM</td>
</tr>
<tr>
<td>$20^{-2}$</td>
<td></td>
<td>flag for selecting a constant ($=0$) or a variable kernel ($=1$)</td>
</tr>
</tbody>
</table>

$^*$ Input/output parameters, parameters taken from FITS keywords, and parameters with standard values are not listed (see the Molecfit User Manual for more details).
Fig. 2. Quality of telluric absorption correction for an example TSS spectrum taken with the NIR arm of the X-Shooter spectrograph. The star was observed with a 1.2" slit at an airmass of 1.32. The seeing was 0.76" and the PWV (as derived from the fitting) was 1.46 mm. **Upper panel:** The telluric absorption corrected spectrum (red) is shown in comparison with the original spectrum (black). **Middle and lower panels:** Mean counts and standard deviation in ADU for a grid of 1 nm bins for the telluric absorption corrected example spectrum. The two subfigures also highlight the pixels for the continuum interpolation (red) and the different transmission ranges for the quality analysis of the telluric absorption correction. For more details, see Fig. 1.

have a bad quality. For example, the mean $I_{\text{off}}$ for NIR-arm spectra with counts between $10^3$ and $10^4$ ADU is 0.000 ($\sigma = 0.053$), i.e. there are no systematic continuum offsets on average. For a more profound discussion of the quality of the telluric absorption correction for low-$S/N$ spectra, see Sect. 5.

The X-Shooter pipeline produces output files which also contain errors and bad pixel masks. With the latter, the marked pixels are not considered for the molecfit fitting procedure. Sometimes in the NIR arm, it seems that more pixels were rejected by the pipeline than required. In the case of a very small number of available pixels, the fit becomes unreliable. While the standard deviation might even decrease, systematic offsets are expected to become more significant. In addition, crucial continuum pixels for the interpolation of ranges with strong absorption bands could be missing, which makes the derivation of $I_{\text{off}}$ less reliable. For this reason, we excluded 247 NIR-arm spectra (5.9%) with less than half the maximum number of pixels in the fitting ranges.

So far, we have mainly rejected spectra where a proper calculation of the quality indicators $I_{\text{off}}$ and $I_{\text{res}}$ could not be guaranteed. However, for evaluating the quality of the telluric absorption correction, it is important to know the fraction of obviously failed fits. For this purpose, we studied the best-fit FWHM of the instrumental profile (combined boxcar and Gaussian) and the best-fit shift of the wavelength grid. Interestingly, only a small number of NIR-arm spectra (no VIS-arm spectra) showed values which were clearly separated from the general distribution. 28 best-fit model spectra with a FWHM above 10 pixels (or below 1.5 pixels) or wavelength shifts of more than 2.5 pixels relative to the sample mean could be identified as clear outliers. 14
Table 5. Sample averages and standard deviations for the transmission-dependent indicators $I_{\text{off}}$ and $I_{\text{res}}$ of the quality of the telluric absorption correction of NIR-arm X-Shooter spectra

<table>
<thead>
<tr>
<th>Ref. $T$</th>
<th>$T$ range</th>
<th>$I_{\text{off}}$ mean</th>
<th>$I_{\text{off}}$ σ</th>
<th>$I_{\text{res}}$ mean</th>
<th>$I_{\text{res}}$ σ</th>
</tr>
</thead>
<tbody>
<tr>
<td>—</td>
<td>0.10−0.95</td>
<td>−0.009</td>
<td>0.032</td>
<td>0.196</td>
<td>0.063</td>
</tr>
<tr>
<td>0.9</td>
<td>0.88−0.92</td>
<td>−0.008</td>
<td>0.044</td>
<td>0.209</td>
<td>0.071</td>
</tr>
<tr>
<td>0.8</td>
<td>0.75−0.85</td>
<td>−0.024</td>
<td>0.046</td>
<td>0.184</td>
<td>0.068</td>
</tr>
<tr>
<td>0.5</td>
<td>0.45−0.55</td>
<td>−0.004</td>
<td>0.038</td>
<td>0.150</td>
<td>0.059</td>
</tr>
<tr>
<td>0.2</td>
<td>0.15−0.25</td>
<td>+0.035</td>
<td>0.063</td>
<td>0.237</td>
<td>0.136</td>
</tr>
</tbody>
</table>

4.3. Influence of line transmission and observing conditions

For the filtered NIR-arm sample (see Sect. 4.2), Table 5 shows the mean values and standard deviations of the quality indicators $I_{\text{off}}$ and $I_{\text{res}}$ for the five transmission ranges listed. In addition, the individual values for the wide transmission range from 0.1 to 0.95 are plotted in Fig. 5. The latter does not indicate significant features in the distribution of the data points. $I_{\text{off}}$ clusters around a value of 0, which means that the telluric absorption correction does not appear to be affected by systematic offsets. The scatter is only about 3% of the line strengths. The mean $I_{\text{res}}$ is about 0.20 with a scatter of 0.06, i.e. the relative standard deviation of the residuals of the corrected telluric absorption lines is about 20%. This translates into typical flux errors of 2% and 10% for spectral ranges with $T = 0.9$ and 0.5, respectively. The mean $I_{\text{off}}$ and $I_{\text{res}}$ values for the X-Shooter VIS arm −0.002 ($\sigma = 0.048$) and 0.184 ($\sigma = 0.059$) are very similar to the NIR-arm results. This implies that the telluric absorption correction is of good quality in both X-Shooter arms.

Table 5 lists $I_{\text{off}}$ and $I_{\text{res}}$ depending on the four narrow transmission ranges centred at $T = 0.9, 0.8, 0.5$, and 0.2. The distributions agree quite well with the results for the wide transmission range. Consequently, the mixing of transmissions is not crucial for the resulting quality indicators, at least if $T$ very close to 1 and 0 are not considered (as for our wide $T$ range). In the case of very high $T$, random noise, systematic errors in the reduced spectra, and features of the observed object can have a strong effect on the figures of merit due to the normalisation by $1 − T$ (see Fig. 3). However, the quality of the telluric absorption correction is not affected by this issue, because of the negligible line strength. In the case of very low $T$, the relatively low S/N, possible zeropoint errors, and the strong variation in $T$ over narrow wavelength ranges can also cause high $I_{\text{off}}$ and $I_{\text{res}}$. Wavelengths with very low atmospheric transmission are hard to correct (see
Fig. 2). However, this is usually not an issue due to the very low S/N and the corresponding lack of information. The \( I_{\text{res}} \) values in Table 5 illustrate the described effects. The minimum of 0.15 is obtained for intermediate transmissions \( (T = 0.5) \), whereas the values for \( T = 0.9 \) and 0.2 are above 0.2.

The rough proportionality of the telluric absorption correction errors and \( 1 - T \) implies that the overall correction quality of a spectrum depends on the airmass of the observation and the column density of the molecular species concerned. This can be understood by considering that the transmission \( T \) is related to the optical depth along the line of sight \( \tau \) for each wavelength \( \lambda \) by

\[
T(\lambda) = e^{-\tau(\lambda)},
\]

where \( \tau \) can be approximated by the product of the optical depth at zenith \( \tau_0 \) and the airmass \( X \):

\[
\tau(\lambda) \approx \tau_0(\lambda) X.
\]

This works best if the geometrical distributions of the given molecule and air are similar. Finally, the optical depth \( \tau_0 \) for molecular absorption by a single species can be calculated by

\[
\tau_0(\lambda) = \sigma_{ab}(\lambda) \int_{0}^{\infty} n(h) dh,
\]

where \( \sigma_{ab} \) is the wavelength-dependent absorption cross section and the integral corresponds to the column density of the molecule, which is derived from the density \( n \) at heights \( h \) above the observer at \( h_0 \). Consequently, telluric absorption correction is most difficult if a target is observed at a large zenith distance and with a high atmospheric water vapour content. The amount of water vapour is critical, since most prominent bands in the X-Shooter wavelength range are caused by this molecule and the concentration and distribution is highly variable. Figure 6 shows the amount of precipitable water vapour (PWV) in mm as derived by molecfit from the discussed NIR-arm sample spectra. The fitted PWV range from 0.2 to 18.2 mm with a mean value of 5.2 mm. Therefore, the quality of the correction of atmospheric water vapour abundance. In winter, the PWV is relatively low (mean of 1.9 mm for meteorological winter), whereas the highest amounts and a large scatter are found in summer (mean of 5.2 mm). Therefore, the quality of the correction of water vapour bands may roughly depend on the time of the year. This is not the case for molecular oxygen and carbon dioxide water vapour bands may roughly depend on the time of the year.

The fitted PWV range from 0.2 to 18.2 mm with a mean value of 5.2 mm. Therefore, the quality of the correction of atmospheric water vapour abundance. In winter, the PWV is relatively low (mean of 1.9 mm for meteorological winter), whereas the highest amounts and a large scatter are found in summer (mean of 5.2 mm). Therefore, the quality of the correction of water vapour bands may roughly depend on the time of the year. This is not the case for molecular oxygen and carbon dioxide water vapour bands may roughly depend on the time of the year.

4.4. Influence of resolution

Since the echelle gratings of the X-Shooter spectrographs are fixed, the slit width is the only instrumental parameter that affects the line-spread functions of the resulting spectra. For the NIR and VIS arms, seven different widths from 0.4” to 5.0” can be selected as displayed in Table 6.** Apart from the slit selection, the FWHM of a line is also influenced by the seeing at the time of the observation of a point-like standard star. Wider slits are more affected by the atmospheric conditions than narrower ones. For this reason, Table 6 shows an increase of the FWHM (as derived from the combined best-fit boxcar and Gaussian kernels, see Sect. 4.1) as well as its scatter with increasing slit width for the NIR arm.

The slit-dependent results for the quality indicators \( I_{\text{ds}} \) and \( I_{\text{res}} \) for the wide transmission range are also provided by Table 6. The systematic offsets appear to indicate a weak trend from slight overcorrection for the 0.4” slit to moderate under-

<table>
<thead>
<tr>
<th>Slit [&quot;]</th>
<th>( N )</th>
<th>FWHM ( [\text{pixels}] )</th>
<th>( I_{\text{ds}} )</th>
<th>( I_{\text{res}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.4</td>
<td>437</td>
<td>2.49 0.20</td>
<td>+0.008</td>
<td>0.059</td>
</tr>
<tr>
<td>0.6</td>
<td>711</td>
<td>3.07 0.31</td>
<td>−0.002</td>
<td>0.020</td>
</tr>
<tr>
<td>0.9</td>
<td>1927</td>
<td>3.95 0.74</td>
<td>−0.012</td>
<td>0.027</td>
</tr>
<tr>
<td>1.2</td>
<td>566</td>
<td>4.44 1.01</td>
<td>−0.015</td>
<td>0.024</td>
</tr>
<tr>
<td>1.5</td>
<td>148</td>
<td>5.03 1.62</td>
<td>−0.020</td>
<td>0.020</td>
</tr>
<tr>
<td>5.0</td>
<td>48</td>
<td>5.41 1.37</td>
<td>−0.037</td>
<td>0.025</td>
</tr>
</tbody>
</table>

**Since the FWHM depends on the wavelength due to the wavelength-dependent contribution of the different orders of the echelle spectrum, the FWHM is given for the centre of the full NIR-arm wavelength range, i.e. 1.74 \( \mu \text{m} \) (see also Sect. 4.1). For spectra taken with a X-blocking filter, which only extend up to 2.1 \( \mu \text{m} \), the FWHM was corrected to be also representative of 1.74 \( \mu \text{m} \).
decreasing slit width or FWHM. The mean and Table 5).

In the following, we focus on broadening of the slit width seems to contribute to a correction for the 5.0" slit. However, except for the value for the rarely used 5.0" slit, the mean offsets can be considered as negligible. Nevertheless, the slit width seems to contribute to a broadening of the distribution of the entire data set (see Fig. 5 and Table 5).

As indicated by Fig. 8 and Table 6, the intra-bin variations of the residuals of the telluric absorption correction increase with decreasing slit width or FWHM. The mean values range from 0.153 and 0.219. This clear dependence broadens the distribution of the entire data set (see Fig. 5 and Table 5). The trend could be explained by the steepness of the line profiles if a line comprises only a few pixels (about 25 pixels for the 0.4" slit of the NIR arm). In this case, small discrepancies between the modelled and the true profile can cause significant residuals. On the other hand, the scatter in the NIR/VIS arm is calculated for bins of a width of 1 mm/0.5 mm (about 17/25 pixels). If the FWHM is low, more (probably uncorrelated) resolution elements fit into the bin range. This effect could also augment the telluric absorption correction when these ranges are changed. For this purpose, we tested the NIR-arm example spectrum shown in Fig. 2, which is characterised by an airmass of 1.32 and a best-fit PWV of 1.46 mm. We took different subsets of the five standard NIR-arm windows (which had to include at least one water vapour band) and ran molecfit and calctrans to obtain the telluric absorption correction.

Table 7 shows the results of the seven test runs we performed. The table indicates the selected fitting ranges (see Table 4 for the numbers), the relative RMS of the fit, the best-fit FWHM, the best-fit PWV, and the two quality indicators \( I_{\text{dist}} \) and \( I_{\text{res}} \) (see Sect. 4.1). The table entries for the different parameters show a clear difference in the quality of the fit and the telluric absorption correction depending on the fitting ranges considered. As expected, the RMS of the fit is reduced if the number of the fitting ranges is decreased. The resulting FWHM range from 69% to 101% of the value of the standard run. For the PWV, we obtained values from 90% to 115%. The largest deviations are found for runs that were based on only one fitting range. For the quality of the telluric absorption correction as measured by \( I_{\text{dist}} \) and \( I_{\text{res}} \), there is a similar trend. However, the quality of the correction also strongly depends on the ranges involved. While the fit only depending on Range 1 (1.12−1.13 \( \mu m \)) is by far the worst (Run 2), the result for Run 4, which is only based on Range 3 (1.80−1.81 \( \mu m \)), is remarkably good. This is also illustrated by Fig. 9, which shows the mean values and relative standard deviations for 1 mm bins of the resulting spectra of Run 2 and 4 in comparison with the standard Run 1. Run 2 only indicates a good telluric absorption correction in the fitted range. Run 4 shows a reasonable correction over the entire wavelength range.

Since the results for the molecfit runs with single fitting ranges differ significantly, we performed the model fitting and telluric absorption correction for single ranges that cover telluric lines in the same bands such as Runs 2 and 3, but with different wavelength limits. Only ranges were selected where lines of intermediate strength dominate (see Table 1). For ranges of the same

4.5. Influence of fitting ranges

So far, the discussion has been based on a fixed set of fitting ranges (see Table 4 and Sect. 4.1). In the following, we focus on changes in the quality of the telluric absorption correction when different subsets of the five standard NIR-arm windows (which had to include at least one water vapour band) and ran molecfit and calctrans to obtain the telluric absorption correction.

Table 7 shows the results of the seven test runs we performed. The table indicates the selected fitting ranges (see Table 4 for the numbers), the relative RMS of the fit, the best-fit FWHM, the best-fit PWV, and the two quality indicators \( I_{\text{dist}} \) and \( I_{\text{res}} \) (see Sect. 4.1). The table entries for the different parameters show a clear difference in the quality of the fit and the telluric absorption correction depending on the fitting ranges considered. As expected, the RMS of the fit is reduced if the number of the fitting ranges is decreased. The resulting FWHM range from 69% to 101% of the value of the standard run. For the PWV, we obtained values from 90% to 115%. The largest deviations are found for runs that were based on only one fitting range. For the quality of the telluric absorption correction as measured by \( I_{\text{dist}} \) and \( I_{\text{res}} \), there is a similar trend. However, the quality of the correction also strongly depends on the ranges involved. While the fit only depending on Range 1 (1.12−1.13 \( \mu m \)) is by far the worst (Run 2), the result for Run 4, which is only based on Range 3 (1.80−1.81 \( \mu m \)), is remarkably good. This is also illustrated by Fig. 9, which shows the mean values and relative standard deviations for 1 mm bins of the resulting spectra of Run 2 and 4 in comparison with the standard Run 1. Run 2 only indicates a good telluric absorption correction in the fitted range. Run 4 shows a reasonable correction over the entire wavelength range.

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\[ \text{Table 7. Influence of fitting ranges on the telluric absorption correction of the NIR-arm spectrum displayed in Fig. 2} \]

<table>
<thead>
<tr>
<th>Run</th>
<th>Ranges</th>
<th>Rel. RMS</th>
<th>FWHM [pixels]</th>
<th>PWV [mm]</th>
<th>( I_{\text{dist}} )</th>
<th>( I_{\text{res}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1 2 3 4 5</td>
<td>0.054</td>
<td>3.76</td>
<td>1.46</td>
<td>-0.008 0.235</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>1−−−−−−</td>
<td>0.030</td>
<td>3.19</td>
<td>1.19</td>
<td>+0.085 0.349</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>2−−−−−−</td>
<td>0.022</td>
<td>2.60</td>
<td>1.32</td>
<td>-0.063 0.246</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>−−3−−−−</td>
<td>0.028</td>
<td>3.08</td>
<td>1.40</td>
<td>-0.041 0.222</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>1 2 3−−−</td>
<td>0.066</td>
<td>3.79</td>
<td>1.48</td>
<td>-0.004 0.238</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>1−−−−−5</td>
<td>0.035</td>
<td>3.29</td>
<td>1.56</td>
<td>+0.039 0.315</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>−−2−−4</td>
<td>0.034</td>
<td>3.28</td>
<td>1.36</td>
<td>-0.036 0.235</td>
<td></td>
</tr>
</tbody>
</table>

\* For the wavelength limits of the different ranges with the indicated numbers, see Table 4.

\[ \text{Table 8. Influence of changing fitting ranges in a molecular band on the telluric absorption correction of the NIR-arm spectrum displayed in Fig. 2} \]

<table>
<thead>
<tr>
<th>Run</th>
<th>Range [( \mu m )]</th>
<th>Rel. RMS</th>
<th>FWHM [pixels]</th>
<th>PWV [mm]</th>
<th>( I_{\text{dist}} )</th>
<th>( I_{\text{res}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2a</td>
<td>1.12−1.13</td>
<td>0.030</td>
<td>3.19</td>
<td>1.68</td>
<td>+0.085 0.349</td>
<td></td>
</tr>
<tr>
<td>2b</td>
<td>1.13−1.14</td>
<td>0.033</td>
<td>3.21</td>
<td>1.72</td>
<td>+0.101 0.399</td>
<td></td>
</tr>
<tr>
<td>2c</td>
<td>1.14−1.15</td>
<td>0.039</td>
<td>3.03</td>
<td>1.42</td>
<td>+0.061 0.502</td>
<td></td>
</tr>
<tr>
<td>3a</td>
<td>1.47−1.48</td>
<td>0.022</td>
<td>2.60</td>
<td>1.32</td>
<td>-0.063 0.246</td>
<td></td>
</tr>
<tr>
<td>3b</td>
<td>1.46−1.47</td>
<td>0.021</td>
<td>2.78</td>
<td>1.37</td>
<td>-0.044 0.237</td>
<td></td>
</tr>
<tr>
<td>3c</td>
<td>1.45−1.46</td>
<td>0.023</td>
<td>2.97</td>
<td>1.35</td>
<td>-0.067 0.256</td>
<td></td>
</tr>
<tr>
<td>4a</td>
<td>1.44−1.45</td>
<td>0.023</td>
<td>2.97</td>
<td>1.35</td>
<td>-0.067 0.256</td>
<td></td>
</tr>
<tr>
<td>4b</td>
<td>1.44−1.46</td>
<td>0.036</td>
<td>2.82</td>
<td>1.37</td>
<td>-0.045 0.242</td>
<td></td>
</tr>
</tbody>
</table>

\* same runs as in Table 7

\[ \text{Fig. 9. Mean counts in ADU and standard deviation relative to mean counts for a grid of 1 mm bins of the telluric absorption corrected example spectrum shown in Fig. 2 for three different sets of fitting ranges. The black spectrum equals the one in Fig. 2 and corresponds to the standard set-up of windows described in Table 4. The red and the green spectra were calculated by only using a single fitting range (see legand and Table 7).} \]
Table 9. Influence of wavelength grid correction by a Chebyshev polynomial of order $n$ on the telluric absorption correction of the spectrum displayed in Fig. 2.

<table>
<thead>
<tr>
<th>$n$</th>
<th>Rel. RMS [pixels]</th>
<th>FWHM [mm]</th>
<th>PWV</th>
<th>$I_{\text{diff}}$</th>
<th>$I_{\text{res}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.054</td>
<td>3.76</td>
<td>1.46</td>
<td>-0.008</td>
<td>0.235</td>
</tr>
<tr>
<td>1</td>
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<td>7.25</td>
<td>1.51</td>
<td>-0.046</td>
<td>0.456</td>
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<tr>
<td>3</td>
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<td>7.05</td>
<td>1.51</td>
<td>-0.053</td>
<td>0.459</td>
</tr>
<tr>
<td>5</td>
<td>0.120</td>
<td>6.98</td>
<td>1.51</td>
<td>-0.050</td>
<td>0.453</td>
</tr>
</tbody>
</table>

Table 10. Influence of wavelength grid correction by a Chebyshev polynomial of order $n$ on the telluric absorption correction of the spectrum displayed in Fig. 2 for the fixed best-fit line profile ($n = 0.560$ and $n = 1.671$) as derived from the standard test run.

<table>
<thead>
<tr>
<th>$n$</th>
<th>Rel. RMS [pixels]</th>
<th>FWHM [mm]</th>
<th>PWV</th>
<th>$I_{\text{diff}}$</th>
<th>$I_{\text{res}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.054</td>
<td>3.75</td>
<td>1.47</td>
<td>-0.007</td>
<td>0.235</td>
</tr>
<tr>
<td>1</td>
<td>0.031</td>
<td>3.75</td>
<td>1.44</td>
<td>-0.028</td>
<td>0.195</td>
</tr>
<tr>
<td>3</td>
<td>0.040</td>
<td>3.75</td>
<td>1.39</td>
<td>-0.042</td>
<td>0.262</td>
</tr>
<tr>
<td>5</td>
<td>0.031</td>
<td>3.75</td>
<td>1.42</td>
<td>-0.021</td>
<td>0.343</td>
</tr>
</tbody>
</table>

H$_2$O band, Table 8 reveals similar values for the listed parameters. This suggests that changing centre and width of a fitting range in a band (in a reasonable way) has a lower impact than changing the band.

These results show that fitting ranges should carefully be selected. Ranges in the H$_2$O band at 1.13 $\mu$m appear to be especially critical. The PWV, $I_{\text{diff}}$, and $I_{\text{res}}$ values are unsatisfying if these ranges are not combined with ranges in other molecular bands. Since the line depths of the different ranges are comparable, this does not seem to explain the discrepancies. The differences in the best-fit line shapes and shifts could imply that the issue is linked to the structure of the X-Shooter composite echelle spectra consisting of many orders. At least, the molecular lines of the 1.13 $\mu$m band cover less pixels than those in bands at longer wavelengths. In view of the uncertainties in the line profile and wavelength calibration, a good telluric absorption correction over the entire wavelength range (see Fig. 9) requires that all critical molecular absorption bands are probed by fitting ranges. Therefore, our standard set of fitting windows (see Table 4) is well defined, even though only low order correction of the different kinds of systematic deviations from the atmospheric transmission model is possible (see Sect. 4.6). The best fit is always the result of a compromise, as indicated by the smaller residuals for individual fitting ranges in the corresponding wavelength regimes (see Fig. 9).

### 4.6. Influence of input parameters

Next, we investigate the influence of the input fit parameters on the quality of the telluric absorption correction. In this respect, our input parameter set (see Table 3) appears to be a reasonable choice (see discussion in Sect. 4.1). However, there could be a critical restriction of the maximum order of the Chebyshev polynomial for the correction of the wavelength grid. The selection $n = 0$ only allows a constant shift of the wavelength grid. As discussed in Sect. 4.5, this is most likely not sufficient to achieve good fits in all the different fitting ranges at the same time. For this reason, we studied the effect of the $n$ parameter on the quality of the fit. Table 9 shows the results of our investigation of the standard NIR-arm example (see Fig. 2) for four different orders of the polynomial. The results columns are the same as in Table 7. The values for the relative RMS, FWHM, $I_{\text{diff}}$, and $I_{\text{res}}$ clearly imply that the fits of the runs with $n = 1, 3$, and 5 failed. The main reason for the failure is indicated by the doubling of the FWHM for these runs. It appears that the increase of the degree of freedom by the additional coefficients of the Chebyshev polynomial caused degeneracies, which led to an erroneous fit of the instrumental profile. In other words, the fitting algorithm was not able to find the global $\chi^2$ minimum.

To make the wavelength correction more robust, we performed a second series of runs with a reduced degree of freedom. For this purpose, we fixed the properties of the line profile. We took the best-fit results of the standard run and set $n = 0.560$, $n = 1.671$, and the corresponding fit flags to 0 (cf. Table 3). The results for the four different degrees of the Chebyshev polynomial are listed in Table 10. For the higher $n$, the fits in the five fitting ranges are now better than for the standard run, as the relative RMS indicate. The PWV values and the related $I_{\text{diff}}$ for systematic offsets are relatively stable. The small-scale residuals indicator $I_{\text{res}}$ is the lowest (0.195) for a linear wavelength correction function, i.e. $n = 1$. Higher order corrections indicate worse $I_{\text{res}}$ (0.343 for $n = 3$, 0.453 for $n = 5$). They tend to deteriorate the telluric absorption correction, despite the fixed line profile. This is also demonstrated by Fig. 10, which shows the mean values and relative standard deviations for 1 nm bins of the telluric absorption corrected spectrum for the different fits of the standard run. For higher degrees of the polynomial, the quality of the correction seems to be highly wavelength dependent.

These findings suggest that very high orders are risky because of fit degeneracies. The situation could improve if there were more and/or broader fitting ranges. However, this approach would have some limitations due to the code run time increasing, continuum modelling by low order polynomials, and the small fraction of wavelengths with suitably strong absorption lines. Ir-
respectively of these issues, the example has shown that a combination of two runs (where the second run benefits from the results of the first run) could significantly improve the quality of the telluric absorption correction. For a successful $\chi^2$ minimisation, the number of free parameters should not be too high. In particular, this concerns parameters related to the wavelength grid correction and the line profile shape, which are prone to $\chi^2$ degeneracies. Note that the line profile parameters are especially critical for low-resolution spectra suffering from line blends, narrow wavelength ranges with only small numbers of telluric absorption lines, and studies of trace gas concentrations requiring a high accuracy (e.g. Kausch et al. 2013). In the latter case, the presence of faint but broad line wings (as modelled by a Lorentzian kernel, see Table 3), which are difficult to fit, could have a significant effect on the retrieved concentrations.

4.7. Influence of the input atmospheric profile

Water vapour is an abundant and very variable component of the Earth’s atmosphere (see Fig. 6). Most telluric absorption in the X-Shooter NIR-arm range is caused by this molecule. Therefore, the quality of the telluric absorption correction strongly depends on a good fit of the water vapour column density.

The PWV fit requires a scaling of the input water vapour profile. The parameter $\text{relcol}$ describes the relative scaling with respect to the input profile. Fig. 11 shows the final PWV value from the best-fit versus the best-fit relcol (see Table 3) for the NIR-arm data set selected in Sect. 4.2. The mean factor is 0.87 with a scatter of 0.26. This is relatively close to 1, i.e. the case that the PWV of the input profile is the best-fit one. However, for low PWV, the merged input profiles tend to have too much water vapour. For PWV below the median value of 2.2, the mean scaling factor is 0.73, whereas for PWV above the median, a mean factor of 1.01 is obtained. The standard deviation is similar in both cases (0.22 versus 0.23). In view of the significant scatter and the systematic offsets at low PWV, a reliable scaling of the input profiles is indispensable. Uncertainties related to this procedure significantly affect the quality of the telluric absorption correction.

To more accurately investigate the effect of the initial atmospheric profiles, we used data of a radiometer, which was installed on Cerro Paranal in October 2011 for water vapour monitoring purposes (Kerber et al. 2012a,b). It is a Low Humidity And Temperature PROfilin microwave radiometer (LHATPRO), manufactured by Radiometer Physics GmbH (RPG13). The instrument uses several channels across the strong water vapour emission line at 183 GHz, necessary for measuring the low levels of PWV that are common on Cerro Paranal. Details of the radiometer are described in Rose et al. (2005). This radiometer provides continuous direct on-site measurements of the temperature, and the water vapour content up to a height of about 12 km, and the integrated water vapour (PWV), identical to the PWV. We created an additional set of initial atmospheric profiles for molecfit in the same way as the default combination of a standard atmosphere, GDAS model, and ESO MeteoMonitor described in Paper I, but replacing the GDAS data by the radiometer profiles and skipped the MeteoMonitor data since the latter profiles already contain this information.

From our X-Shooter data set we selected 549 telluric standard star observations covering the period of the radiometer data (Jan, Feb, Aug-Dec 2012). Every spectrum was fitted with molecfit incorporating both, the GDAS/MeteoMonitor and the LHATPRO based set, respectively. In both cases, we used the closest available data. We finally applied a telluric absorption correction based on both methods.

The telluric corrected spectra differ usually by only a few per cent, with larger deviations in the ranges with strong atmospheric absorption (see Fig. 12 for an example).

For a closer look, we also compared the resulting values and the water vapour content values, PWV and IWV respectively, for the whole data set. Figure 13 gives the comparison of the parameters between the GDAS and the LHATPRO based fits. As expected, the LHATPRO based scaling parameters are closer to unity (median value = 0.95) than the parameter derived with the help of the GDAS model (median value = 0.92). This means that the atmospheric profile based on the radiometer data requires less scaling than the modelled one. In addition, the scatter $\sigma_G = 0.13$ for the LHATPRO method is significantly lower than the GDAS based scatter ($\sigma_G = 0.25$). This is expected, since the LHATPRO profiles are direct on-site measurements providing more accurate estimates of the actual atmospheric conditions than the combined GDAS/MeteoMonitor model.

Although the radiometer based initial profiles lead to less scatter in the relcol parameter, the quality of the final telluric absorption correction is comparable within a few per cent. This means that due to the adaption with the scaling parameter, an inappropriate initial atmospheric profile also leads to a good telluric absorption correction. We therefore conclude that the underlying fitting algorithm incorporated in molecfit is highly efficient. However, it appears that the derived PWV value is over-estimating the real water vapour content in the case of very dry observing conditions. This indicates inadequate input profiles.

5. Comparison with the classical method

The classical way of the telluric absorption correction is done with the help of TSS. A widely used tool for this purpose is the IRAF task telluric14. The IRAF task telluric requires a science spectrum in conjunction with a transmission curve which is derived from the corresponding TSS spectrum. The task also performs a wavelength shift and a scaling of the input spectrum.

---

13 http://www.radiometer-physics.de/
To obtain the transmission spectra, we used the following approach: We fitted a cubic spline to base points selected on positions with or close to transmission = 1 in the TSS spectrum (see Fig. 14). The positions of the base points were individually chosen for every TSS spectrum to obtain a fair comparison. The TSS spectrum is then normalised by this spline fit. As TSS usually show no or only minor intrinsic spectral features, the resulting absorption features mostly arise from the Earth’s atmosphere. This transmission curve was then applied to the science spectrum with the IRAF task telluric. We compared the resulting corrected spectra with the results obtained by molecfit and calctrans. For this purpose, we applied molecfit using directly the science targets instead of the TSS observations, incorporating the parameters listed in Table 3 and the five standard fitting ranges (see Table 4) for the same examples.

Figure 15 shows as example the telluric corrected science spectrum of the galaxy NGC5638 (test data set #12, see Tables 1 and 2) obtained with the IRAF task (red lines) and molecfit (blue lines) in the two most distinct atmospheric absorption bands at about 1.35 to 1.6 \(\mu m\) and 1.8 to 2.0 \(\mu m\). Both methods work reasonably well with this data set, although the ADU value is not very high (median ADU_{TSS} = 2592). However, significantly higher residuals (due to the division values up to about \(10^6\) ADU in the bluer absorption band occur) are visible in the case of the IRAF correction. In addition, some spectral residuals (hydrogen Brackett lines) introduced by the TSS are visible in the range between 1.55 to 1.7 \(\mu m\) (see small panel in Fig. 14). The molecfit transmission curve relies on a radiative transfer model of the Earth’s atmosphere only, therefore such spectral remnants resulting from a telluric standard star can not occur.
For the quantification of the differences in the telluric corrections based on the two different methods, we determined the offset indicator $I_{\text{off}}$ and the small-scale residual indicator $I_{\text{res}}$ for both data sets as described in Sect. 4 (see Table 11). To also investigate the influence of low signals, we skipped the 10$^5$ ADU selection criterion, which was used for the investigation of the TSS (see Sect. 4.2). We divided the data into two subsets, a low-ADU set ($<1000$ ADU, red points in Fig. 16) and a high-ADU set ($\geq 1000$ ADU, blue points). This leads to sample sizes of 7 and 17 spectra, respectively.

The $I_{\text{off}}$ values for both methods cluster around zero, which is in agreement with our findings in Sect. 4.3 (see Fig. 5). We focus on the absolute offsets $|I_{\text{off}}|$ (see Fig. 16(a)) to investigate the overall offset difference. The mean value
\[
\langle |I_{\text{off}}|_{\text{IRAF}} \rangle - \langle |I_{\text{off}}|_{\text{molecfit}} \rangle > 0.075
\]
reveals significantly higher offsets in the case of the IRAF based method. The comparison for the small-scale residual parameter $I_{\text{res}}$ shows a different result (see Fig. 16(b)). The mean $I_{\text{res}}$ difference $\langle |I_{\text{res}}|_{\text{IRAF}} - |I_{\text{res}}|_{\text{molecfit}} \rangle = 0.427$ shows significantly higher residuals in the case of the IRAF based method (cf. Fig. 15 for an example). This is true for all examples, except #4 and #10, which show marginally smaller residuals for the IRAF method.

Both figures of merit show a strong dependency on the signal level. Figure 16(a) reveals that the high-ADU data set processed with the IRAF task tends to show higher offsets than when using molecfit. For the low-ADU subset no clear trend is visible (cf. also Fig. 16(c)), but it has a larger dispersion than the high-ADU subset. The mean of the high-ADU subset $\langle |I_{\text{off}}| \rangle$ processed with molecfit is about 4.2 times higher than the corresponding low-ADU value (see Table 12). This ratio is 2.4 times for the subsets processed with IRAF. However, $\langle |I_{\text{off}}| \rangle$ is smaller for spectra corrected using molecfit. This indicates that molecfit is more dependent on the signal level than the IRAF task. $\langle |I_{\text{off}}| \rangle$ of the high- and the low-ADU for IRAF exceed by about 50% and 20% the corresponding values obtained with molecfit, respectively (see Table 12). molecfit leads to smaller mean values of $|I_{\text{off}}|$ in both subsets taking the entire set into account. We therefore conclude that it results into smaller offsets than the IRAF task in general.

A similar trend is visible with the means of the $I_{\text{res}}$ parameter. Figure 16(b) shows that all low-ADU subset members lead to higher small-scale residuals in both methods due to the low S/N ratio, with a similar difference between the results for the low- and the high-ADU sets (cf. also Fig. 16). The means of the $I_{\text{res}}$ parameter are lower in the case of molecfit (see Table 12), independent of the subset.

6. Summary and conclusion
We have developed the software package molecfit consisting of routines to fit synthetic atmospheric transmission spectra to...
science data (programme molecfit, see Paper I) and to apply this synthetic spectra as telluric absorption correction to science files (programmes calctrans and corrfilelist). We have extensively tested the software with a large X-Shooter data set to evaluate the performance of the package with two figures of merit, the offset and the small-scale residual parameters, $I_{\text{off}}$ and $I_{\text{res}}$, respectively. In the following, we summarise our findings:

- The telluric absorption correction with molecfit of TSS does not introduce systematic offsets in the corrected spectra. The scatter of $I_{\text{off}}$ is about 3% of the line strength. The relative small-scale residual strength is about 20% (see Sect. 4.3 and Fig. 5) for the NIR arm, i.e. the quality of the correction is roughly proportional to the strength of the telluric absorption lines. The VIS arm data show results of similar quality.
- The telluric correction shows a dependency on the number of pixels per FWHM. The small-scale residuals increase with decreasing slit width or FWHM.

### Table 11. Table of the figures of merit $I_{\text{off}}$ and $I_{\text{res}}$ for the test data set shown in Table 1

<table>
<thead>
<tr>
<th>#</th>
<th>molecfit</th>
<th>IRAF</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$I_{\text{off}}$</td>
<td>$I_{\text{res}}$</td>
</tr>
<tr>
<td>1</td>
<td>-0.111</td>
<td>+0.233</td>
</tr>
<tr>
<td>2</td>
<td>+0.012</td>
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</tr>
<tr>
<td>3</td>
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<td>4</td>
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<tr>
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<tr>
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<tr>
<td>22</td>
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<tr>
<td>23</td>
<td>+0.042</td>
<td>+0.388</td>
</tr>
<tr>
<td>24</td>
<td>+0.074</td>
<td>+0.820</td>
</tr>
</tbody>
</table>

### Table 12. Mean values of abs($I_{\text{off}}$) and abs($I_{\text{res}}$) for the entire test data set (all), the high ADU (highADU) and the low ADU (lowADU) subset, derived for both telluric absorption correction methods

<table>
<thead>
<tr>
<th></th>
<th>molecfit</th>
<th>IRAF</th>
</tr>
</thead>
<tbody>
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<td>$&lt;</td>
<td>I_{\text{off}}</td>
<td>&gt;$ all</td>
</tr>
<tr>
<td>$&lt;</td>
<td>I_{\text{off}}</td>
<td>&gt;$ highADU</td>
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<tr>
<td>$</td>
<td>I_{\text{off}}</td>
<td>&gt;$ lowADU</td>
</tr>
<tr>
<td>Factor high-to-low</td>
<td>4.2</td>
<td>2.4</td>
</tr>
<tr>
<td>$&lt;</td>
<td>I_{\text{res}}</td>
<td>&gt;$ all</td>
</tr>
<tr>
<td>$&lt;</td>
<td>I_{\text{res}}</td>
<td>&gt;$ highADU</td>
</tr>
<tr>
<td>$</td>
<td>I_{\text{res}}</td>
<td>&gt;$ lowADU</td>
</tr>
<tr>
<td>Factor low-to-high</td>
<td>5.6</td>
<td>3.3</td>
</tr>
</tbody>
</table>

Fig. 16. Comparison of the figures of merit $|I_{\text{off}}|$ and $|I_{\text{res}}|$ for the two methods (IRAF = IRAF task telluric; MF = molecfit). Examples with a low ADU median (< 1000 ADU) are marked in red. See text for more details.
molecfit tends to be too high in the case of very dry observing conditions. However, this does not affect the quality of the telluric corrections.

- A comparison with the classical method performed with the IRAF task telluric shows that the resulting systematic offsets tend to be smaller for molecfit, at least for the medium and high-ADU data (depending on the S/N). Molecfit also leads to significantly lower small-scale residuals.

- Molecfit is also applicable to low S/N data. However, there may be a loss of quality in the telluric correction leading to more residuals. Data with extremely low S/N cannot be fitted reliably. In this case, a TSS can alternatively be used for the fit instead of the science spectrum.

The incorporation of synthetic atmospheric transmission spectra based on theoretical calculations provides a promising way to perform the telluric absorption correction. The highly efficient underlying algorithm of molecfit offers the opportunity to achieve a reasonable and reliable correction without supplementary observations of TSS which are time expensive. In addition, the applicability of molecfit with standard parameters allows an efficient usage without time-consuming optimisations. We also successfully applied molecfit to several other ESO instruments covering several wavelength and resolution regimes, e.g. CRIRES and VISIR (see Paper I). Only a slight adaption of instrument dependent parameters is necessary. Any required information can be added in the parameter file if the FITS header of the files does not contain ESO compliant keywords, which are read by molecfit. Although the software is delivered with meteorological data for Cerro Paranal, it provides the capability to create atmospheric profiles appropriate also for other observing sites. This flexibility makes molecfit a general tool for the telluric absorption correction adaptable to various instruments and observing sites.

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Article G:
An advanced scattered moonlight model

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An Advanced Scattered Moonlight Model

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Correcting and predicting the flux coming from the background sky is a crucial aspect of observational astronomy. We have developed a sky background model for this purpose, and it is the most complete and universal sky model that we know of to date.

The largest natural source of light at night in the optical is the Moon, and it is a major contributor to the astronomical sky background. An improved spectroscopic scattered moonlight model, which is applicable from 0.3 to 2.5 \(\mu\)m, has been developed and studied with a set of FORS1 spectra and a dedicated X-shooter dataset. To our knowledge, this is the first spectroscopic model extending into the infrared and it has been tested for many lunar phases and geometries of the Moon and target observations.

Introduction

The current trend in astronomy is to build larger and larger telescopes, for example the future European Extremely Large Telescope (E-ELT). The operating costs for running these large telescopes are high and careful planning of observations is crucial since telescope time is expensive and always in demand. Thus, more accurate predictions and estimations of the noise coming from the sky background are needed to better understand how long an exposure is necessary for a given observation to reach a desired signal-to-noise ratio. The brightest natural source of light in the night sky in the optical, is the Moon (when it is above the horizon). Even in the near-infrared (NIR), there is some flux from the Moon that should be considered.

As part of the Austrian contribution to ESO, the University of Innsbruck in-kind group developed a spectroscopic sky background model from 0.3 to 30 \(\mu\)m for the Very Large Telescope (VLT) and the nearby future site of the E-ELT, for the ESO Exposure Time Calculator (ETC). The model is described in Noll et al. (2012). An example of an output emission spectrum from our sky background model is shown in Figure 1, and the model is available\(^1\). Part of this sky background model is an advanced, spectroscopic scattered moonlight model, verified from 0.3 to 2.1 \(\mu\)m. It provides a spectrum of the scattered moonlight, visible at the observer, depending on the atmospheric conditions, the altitude of, and the angular distance between the target and Moon, and the lunar phase and distance.

The long-standing scattered moonlight model used by ESO for the ETC was due to Walker (1987). It provides a table of the magnitudes for five photometric bands of the night sky at five different lunar phases. This model is limited when it comes to producing a scattered moonlight spectrum which is accurate enough for current and future telescope operations.

Another, widely used scattered moonlight model was developed by Krisciunas \\& Schaefer (1991). It again only uses a photometric model based on 33 observations in the V-band taken at Mauna Kea (2800 metres above sea level). This empirical fit was separated into various specific functions, such as initial intensity from the Moon, Rayleigh and Mie scattering. It is simple, convenient, and easy to use with an accuracy between 8 and 23\%, when not near full Moon and for V-band data from Mauna Kea. In a previous paper (Noll et al., 2012), we presented a spectroscopic extension of the Krisciunas \\& Schaefer (1991) model, which was originally used in our sky background model. It was optimised for Cerro Paranal and covered the optical regime. Several scaling factors for the different functions were introduced to better fit data from Cerro Paranal.

We have improved the scattered moonlight model and it has evolved beyond the initial ESO ETC application. In the optical, the model was calibrated and investigated with 141 spectra and has an overall uncertainty of \(\sigma < 0.2\) mag. With some dedicated X-shooter observations, we have verified the model in the optical and extended it to the NIR. It has been split into physically based modules which are given by either physical models or the best current fits. The present version is optimised for Cerro Paranal, but can be modified for any location with information about its atmospheric properties. Since our scattered moonlight model produces a spectrum, it can be used for finding spectral features and trends as well as photometric magnitudes.

We will first present the scattered moonlight model in the optical, then the model from the ultraviolet (UV) to the NIR.

Figure 1. An example of the output from the sky background model of Noll et al. (2012). The output of the sky background model includes an emission spectrum (shown here) and a transmission spectrum. The various components of the sky background model are also shown.
Scattered moonlight model in the optical region

Scattered moonlight is most influential in the optical. The scattered moonlight model was originally developed, tested, and calibrated in the optical regime with a FOcal Reducer/low dispersion Spectrograph (FORS1) dataset from Patat (2008). We used 141 spectra which had moonlight present and decent weather conditions. For a full description of the model, the data and analysis, see Jones et al. (2013).

The moonlight model is divided into several regions. The Solar spectrum from Colina et al. (1996) is the initial source of the scattered moonlight. Then the light is reflected off the lunar surface and for this we use the empirical fit from Kieffer & Stone (2005), which depends on several lunar parameters. This fit was done using narrowband photometry, so we interpolated it as a function of wavelength. We also needed to extrapolate it to a new moon phase. Next the reflected light is scattered and absorbed in the Earth’s atmosphere before reaching the telescope.

We have designed fully 3D single and double scattering calculations with an approximation to higher orders. For the scattering we use the Rayleigh approximation for the molecules and Mie scattering for the aerosols. Rayleigh scattering can be well parametrised and the molecules in the atmosphere are fairly stable. On the other hand, Mie scattering can be complicated and the aerosols can vary on timescales of hours. In the optical, an empirical fit was derived from Patat et al. (2011). We decomposed this fit into reasonable aerosol size distributions for a remote continental area, like Cerro Paranal, from Warmack & Williams (2012), by scaling the column density of the various components. Then we used the scaled distributions to produce the Mie phase function (Grainger et al. 2004; Bohren & Huffman 1983).

Altogether we had developed a scattered moonlight model, which is spectroscopic and tested from 0.4 to 0.9 µm. It depends on the latitude of, and the angular distance between the Moon and target, lunar phase and distance and the atmospheric conditions.

Results for the optical scattered moonlight model

We found that the sky background model with the new scattered moonlight model fitted the FORS1 observations well, with an uncertainty of < 0.2 µm. Figure 2 shows an example of observed data with the scattered moonlight and sky background model overlaid. The model is able to reproduce the observed radiance spectra.

In Figure 3, we show the mean and uncertainty, σ, of the difference between the sky background model and the FORS1 observations. Also shown are the mean and σ for the nights with and without moonlight. The uncertainty increases towards redder wavelengths where the sky emission lines are prominent.

The scattered moonlight model performs better than the previous extrapolated version of Krisciunas & Schaefer (1991), as shown in Figure 4. For this analysis, we took the sky observations and subtracted the other background components using the sky background model. Then we compared these spectra containing only observed scattered moonlight with the scattered moonlight model. The error bars include the errors associated with the other components in the sky background model. This analysis was done for both the new advanced scattered moonlight model and the previous one based on Krisciunas & Schaefer (1991), labelled in the Figure as KS91. The error bars for the new model are consistently smaller, and the mean for all the spectra is closer to zero. For the mean of new scattered moonlight model minus the FORS1 observations to be at zero, we needed to multiply the model by 1.2. We suspect that the uncertainty in the flux calibration of the FORS1 data could significantly contribute to this global scaling factor.

Scattered moonlight model from UV to NIR

We have now extended and verified our scattered moonlight model. With dedicated observations from X-shooter (Vernet et al., 2011), we were able to test the model from 0.3 to 2.1 µm. With the data in the NIR and observations at multiple distances from the Moon, we can better investigate the aerosol scattering and constrain the Mie scattering used in the model.

We have a unique dataset taken with X-shooter for the purpose of verifying and extending our scattered moonlight model (Proposal ID: 491.L-0659) to the NIR. These data include observations of plain sky taken at three different lunar phases (runs a, b, and c) and at six different angular distances (7, 13, 20, 45, 90, 110 degrees) from the Moon. Additionally, the same standard star was observed at two different airmasses for each lunar phase run.

For the analysis we selected certain wavelength ranges, hereafter called inclusion regions. These regions are parts of the spectrum that should be free of sky emission lines and absorption features. The number of pixels per arc are 850, 850, and 653 for the UVB, VIS, and NIR X-shooter

![Figure 2](image-url)
arms, respectively and are non-consecutive. In Figure 5, we show the observed spectrum from run b at 45 degrees; overlaid are the sky background model (without sky emission lines for clarity), the scattered moonlight model, other components (except the sky emission lines) of the sky background model, the inclusion regions and the transmission spectrum.

For the aerosol extinction curve, in the optical, we used a decomposition of the empirical fit found in Patat et al. (2011). With the X-shooter data, we can take a different approach. We use the remote continental tropospheric and stratospheric aerosol size distributions (Warneck & Williams, 2012), and produce a grid of different scalings of the column density for each aerosol type. Then we used these parameters to produce the Mie phase function using an IDL code based on Bohren & Huffman (1983) and Grainger et al. (2004). Each aerosol distribution is approximated as a lognormal distribution described by \( n \) the number density of particles, \( R \) the mean radius of the particles, and a parameter \( s \) which determines the spread in radii of the particles. The default parameters for the various aerosols are listed in Table 1.

<table>
<thead>
<tr>
<th>Type</th>
<th>( n ) (cm(^{-3}))</th>
<th>( R ) (10(^{-1}) (\mu)m)</th>
<th>( \log s ) (10(^{-3}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trop nucleation</td>
<td>( 0.20 \times 10^{2} )</td>
<td>0.58</td>
<td>1.61</td>
</tr>
<tr>
<td>Trop accumulation</td>
<td>( 2.90 \times 10^{2} )</td>
<td>0.58</td>
<td>2.17</td>
</tr>
<tr>
<td>Trop coarse</td>
<td>( 3.00 \times 10^{-1} )</td>
<td>9.00</td>
<td>3.80</td>
</tr>
<tr>
<td>Stratospheric</td>
<td>( 4.49 \times 10^{2} )</td>
<td>9.00</td>
<td>2.48</td>
</tr>
<tr>
<td>Added coarse</td>
<td>( 1.00 \times 10^{3} )</td>
<td>9.00</td>
<td>1.00</td>
</tr>
</tbody>
</table>

Table 1. Aerosol modes. Note: the values used for Mie scattering of remote continental aerosols are from Warneck & Williams (2012), except for the added coarse mode (see text for details).
The grid is logarithmically spaced, varying the column density for each aerosol type, except for the tropospheric nucleation mode which is negligible and left at 100%. The column density is directly related to the number density n, where we assumed a convenient effective aerosol layer width of 1 km. We also linearly varied the atmospheric refractive index, N.

The amount of aerosols can vary each night (e.g., Buton et al. 2013), and so far the full analysis has been done for the one night of run b (23 July 2013). We also performed a similar analysis with the aerosol grid for the spectrophotometric standard star observations taken that night. More details will be given in a future publication (Jones et al., in prep.).

When the sky observation was at close angular distances to the Moon, in particular the 7 and 13 degree offsets, we noticed a significant amount of extra observed flux compared with the modelled flux. We speculate that this could be caused either by some direct moonlight entering the detector or some additional tropospheric coarse mode which would increase the Mie forward scattering. Since we have no control over the first scenario, we explored the likelihood of the second. We added an additional aerosol size distribution for a particle with \( R = 1 \mu m \) and \( \log s = 0.1 \), which is optimal for increasing the flux at small angular distances. We also varied the column density of this new mode in the same way as the others (see Table 1).

Results of UV to NIR scattered moonlight model

After analysing the X-shooter observations with the scattered moonlight model for the various aerosol parameters, we have found the model with the highest likelihood matches the data well. Also shown for comparison is the model which is the least likely from our grid. This model, with different amounts of aerosols, does not fit the observations, especially at smaller angular distances. The two spectra with the largest angular distances (90 and 110°) are not very sensitive to the choice of aerosols. The model here reproduces the data, which leads credence to the other parts (non-aerosol scattering) of the model being accurate. By adding in the additional coarse mode, we were not able to successfully reproduce the extra flux seen at 7 degrees (not shown in Figure). Additionally, the spectrum at 13 degrees seems to behave differently than the other spectra analysed. The possibility of having extra flux coming from direct moonlight entering the dome and hitting the detector cannot be excluded. We would like to caution others about observations close to the Moon. Even in the J-band, some extra flux is detected.

Prospects

From the UV to the NIR, our scattered moonlight model seems to fit the observed data well. With the X-shooter data we can better constrain the aerosol scattering. The optical depth of aerosols \( \tau_{aerosol} \) for the night of run b is quite a bit lower than the one empirically found by Patat et al. (2011). We deduce that the variation in the amount of aerosols present at Cerro Paranal.

Overall, our improved scattered moonlight can well represent the observations. It has now been verified in the optical with FORS1 data and from the UV to NIR with X-shooter data. In addition, we have tested the model for many different lunar phases and at a range of distances between the Moon and target observation. The remaining main source of uncertainty is with the atmospheric conditions.

Acknowledgements

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References

Walker, A. 1987, NOAO Newsletter, 10, 16

Links

1 ESO Exposure Time Calculator sky model: http://www.eso.org/observing/etc/skycalc/skycalc.htm
Contributions

Article A
“An atmospheric radiation model for Cerro Paranal. I. The optical spectral range”

As part of the UIBK in-kind group, I helped test and verify the model in general. Also, I verified the aerosol extinction curve using LBLRTM to confirm what was previously published. I participated in the science and progress meetings at ESO. Additionally, I helped with the editing the paper.

Article B
“An advanced scattered moonlight model for Cerro Paranal”
Jones, A.; Noll, S.; Kausch, W.; Szyszka, C.; Kimeswenger, S.

As first author, I was the major contributor for this paper. I designed and developed the scattered moonlight model completely, except for the scattering codes that were done by S. Noll.

Article C
“Skycorr: A general tool for spectroscopic sky subtraction”

As part of the UIBK in-kind group, I helped test and verify the model in general. I participated in the an ESO workshop to test how easy skycorr is to use. Additionally, I helped with the editing the paper.

Article D
“Investigating the aerosol extinction using an advanced scattered moonlight model”
Jones, A.; Noll, S.; Kausch, W.; Szyszka, C.; Kimeswenger, S.
Astronomy & Astrophysics, submitted 2 May 2014

As first author, I was the major contributor for this paper. I performed the investigation and
created the grid the scattered moonlight models. I also extended the model into the NIR. I was PI on a 9 hour observing proposal for X-Shooter data on the VLT of the plain sky which we used to verify the sky background model and extend it into the NIR.

**Article E**

“Molecfit: a general tool for telluric absorption correction I. Method and application to ESO instruments”
Astronomy & Astrophysics, submitted 2 April 2014

As part of the UIBK in-kind group, I helped test and verify the model in general. I performed some analysis with CRIRES data to compare the amount of water vapor derived from molecfit with those measured at Cerro Paranal. I also participated in an ESO workshop to test the molecfit GUI. Additionally, I helped with the editing the paper.

**Article F**

“Molecfit: A general tool for telluric absorption correction II. Quantitative evaluation on ESO-VLT/X-Shooter spectra”
Astronomy & Astrophysics, submitted 30 March 2014

As part of the UIBK in-kind group, I helped test and verify the model in general. I performed some analysis with CRIRES data to compare the amount of water vapor derived from molecfit with those measured at Cerro Paranal. I also participated in an ESO workshop to test the molecfit GUI. Additionally, I helped with the editing the paper.

**Article G**

“An advanced scattered moonlight model”
Jones, A.; Noll, S.; Kausch, W.; Szyszka, C.; Kimeswenger, S.
The Messenger, ESO, June 2014 (No 156), p. 31-34

As first author, I was the major contributor for this paper. I had designed and developed the scattered moonlight model from 0.3 to 2.1 \( \mu m \). I was the PI for the observing proposal to collect X-Shooter data of the plain sky in order to verify and extend the model into the NIR.
Acknowledgement

There are many people I would like to thank. I would like to thank Stefan Kimeswenger, Stefan Noll, Wolfgang Kausch, and Cezary Szyszka for all their help and supervision; the Austrian Ministry of Science for funding; ESO for the help, collaboration, and data. I would like to especially thank all my friends and family whom over the many years have always given me love and support.

"Snakes, why’d it have to be snakes"
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Datum                             Unterschrift