Precise Modelling of Telluric Features in Astronomical Spectra

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Ground-based astronomical observations suffer from the disturbing effects of the Earth's atmosphere. Oxygen, water vapour and a number of atmospheric trace gases absorb and emit light at discrete frequencies, shaping observing bands in the near- and mid-infrared and leaving their fingerprints — telluric absorption and emission lines — in astronomical spectra. The standard approach of removing the absorption lines is to observe a telluric standard star: a time-consuming and often imperfect solution. Alternatively, the spectral features of the Earth's atmosphere can be modelled using a radiative transfer code, often delivering a satisfying solution that removes these features without additional observations. In addition the model also provides a precise wavelength solution and an instrumental profile.

The Earth's atmosphere consists of a rich gas mixture. While its main constituent, nitrogen (N_2), does not exhibit any rotational–vibrational transitions, most other molecules do. Strong absorption line systems from water vapour (H_2O), carbon dioxide (CO_2) and ozone (O_3) shape the well-known photometric bandpasses in the near- and mid-infrared. In addition, oxygen (O_2) shows strong absorption bands in the red optical; other molecules such as nitrous oxide (N_2O), carbon monoxide (CO), or methane (CH_4) contribute noticeably to the atmospheric transmission losses in the near- and mid-infrared, often hampering the observation of important astrophysical lines.

While the Earth's atmosphere absorbs light from astronomical sources at a large number of frequencies from the ultraviolet to radio wavelengths, it also emits light in the same transitions, radiating its thermal energy into space. At wavelengths longer than about 2300 nm, the emission originating from the Earth's atmosphere competes with the signal from astronomical sources. The break-even point depends on many factors, such as the spatial resolution, slit width, and detector characteristics of the spectrograph, but also on the height of the observing site. Since the atmospheric emission is spatially extended, it affects the spectrum of the astronomical target similarly to the nearby sky and can thus be removed by beam-switching (nodding) techniques or by fitting and subtracting the two-dimensional signal along the slit.

Empirical calibration

Removing the telluric absorption features is more difficult since their exact signature is only imprinted in the source spectrum. Traditionally, telluric absorption features are removed by observing a so-called telluric standard star before or after the observation of the science target at the same airmass, subsequently dividing the spectrum of the science target by that of the telluric standard. Typically, early-type stars with spectral types ranging from early B to late A are used for this purpose, since they exhibit rather featureless spectra, except for strong hydrogen lines. Since these stars are often fast rotators, other weak stellar features, for example helium lines, are further suppressed. Alternatively, early-to-mid G-type stars can serve as telluric standards as well, since high resolution Fourier transform spectra (FTS) of the Sun provide the necessary template to compensate for their intrinsic stellar features. The observation of telluric standard stars is a standard procedure and commonly employed for all spectrographs operating on ESO telescopes. It is often part of the calibration plan for the instrument and, in these cases, is automatically provided for service mode observations. Since telluric lines generally do not scale linearly with airmass and observing conditions are time variable, it is necessary to observe a telluric standard star at the same airmass and close in time to the science target in the same instrumental setup. Special software tools at the telescope allow the efficient selection of an appropriate standard star.

Nevertheless, using standard stars as empirical calibrators has several disadvantages. The observation of standard stars is time-consuming, especially when science targets are bright or high signal-to-noise requirements are to be met. For the brightest standard stars, the time required for telescope and instrument presets ultimately limits the efficiency of this method. Moreover, on instruments like CRIRES, the instrumental profile depends on the performance of an adaptive optics system, and thus, on the observing conditions and source brightness. Changes in the instrumental profile lead to changes in the line shape of unresolved spectral lines. In these cases standard stars rarely provide a perfect match to the science target, effectively limiting the precision with which telluric features can be removed.

Other shortcomings originate from the intrinsic stellar features of the standard stars. Hydrogen and helium lines in early-type standards cannot be perfectly removed and thus affect the line profiles of the same species in the spectrum of the science target. A further complication in removing these lines occurs when the wavelength coverage of the spectrum is shorter than the line widths of broad hydrogen lines, which can easily be the case for CRIRES. Early-type stars can also exhibit other spectral features, such as oxygen or carbon lines in the near-infrared, often as emission features originating under non-local thermodynamic equilibrium (non-LTE) conditions. Similarly, mismatches in the line depths of solar-type standard stars with the solar FTS atlas, attributable to abundance differences or deviating effective temperatures, can leave residuals of the standard star's intrinsic features in the final spectrum.

Modelling telluric features

Alternatively, the telluric absorption spectrum can be synthesised, using a radiative transfer code in combination with a layered model of the Earth's atmosphere and a database containing the transition data for all molecules in consideration. We have successfully used the program LBLRTM (Clough et al., 1992) for this purpose. LBLRTM is a non-commercial layer-by-layer radiative transfer code tailored to produce telluric spectra under various atmospheric geometries. The code is generally available to the community and uses the high resolution transmission molecular absorption database HITRAN (Rothman et al., 2009) as a molecular line database. HITRAN contains energy levels, frequencies, line strengths, pressure-broadening and -shift coefficients, for more than 1.7 million spectral lines of 42 different molecules and their common isotopes from the red optical to the sub-mm.

A layered model of the Earth's atmosphere serves as the primary input for LBLRTM and contains temperature, pressure and molecular abundance information as a function of atmospheric height at the observatory. For a representative, yet accessible model of the atmospheric conditions at the time of the observation, we supplement a static model of the atmosphere with meteorological data for temperature, pressure and humidity of the troposphere and lower stratosphere (surface height ≤ 26 km). LBLRTM converts the atmospheric model into individual isothermal layers and calculates absorption and emission spectra for a given path through the atmosphere, i.e. for a given zenith angle or airmass.

A single model run takes only a few seconds on a standard desktop PC. The resulting spectrum has an intrinsic reso-

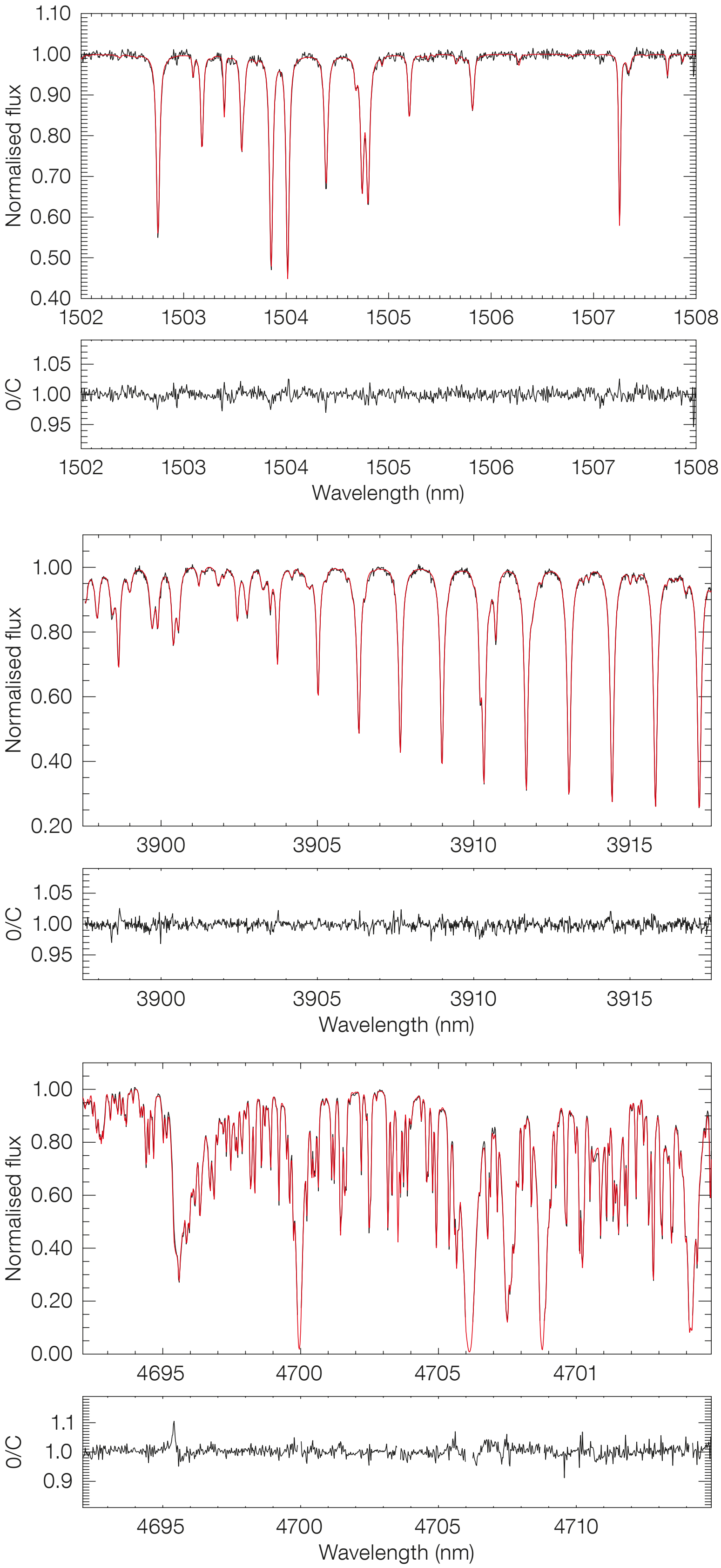

Figure 1. Examples of synthesised telluric spectra fitted to CRIRES observations of standard stars. Each panel shows the measured spectrum in black and the model overplotted in red. We show the residuals after division by the models, i.e., after removal of the telluric absorption lines, at the bottom of each panel. Top panel: Water vapour (H_2O) lines in the *H*-band. Middle panel: Nitrous oxide (N_2O) and water vapour (H_2O) in the *L*-band. Bottom panel: Ozone (O_3), carbon monoxide (CO), carbon dioxide (CO_2), and water vapour (H_2O) lines in the *M*-band.

lution that is set to resolve the narrowest telluric lines in a given spectral region. Resolving powers are thus often of the order of 10^6 and the model spectrum needs to be convolved with the instrumental profile of the spectrograph to match the measured telluric spectrum. To first order, the instrumental profile can be represented by a single Gaussian function. More complex profiles might be used if higher precisions and signal-to-noise ratios need to be achieved. At the same time, the abundance of certain molecules might be over- or underestimated by the atmospheric model, especially for strongly variable species such as water vapour. Given the extreme geographical location of most astronomical observatories, including Cerro Paranal, general meteorological models rarely reproduce the exact water vapour levels on site. Thus, the model data need to be matched to the actual observing conditions. A chi-squared fitting algorithm can be employed to solve for the instrumental profile and to re-adjust the abundance of the molecular species in the atmospheric model while minimising the residuals between the observed spectrum and the spectral model.

We show some example fits to spectra obtained with the CRIRES spectrograph in Figure 1. The resolving power was $R \sim 65\,000$–$80\,000$ as measured from the width of the instrumental profile, which was fitted at the same time as a single Gaussian function. More examples and a detailed discussion of the fitting performance can be found in Seifahrt et al. (2010). In all cases, the abundance of most atmospheric species was slightly modified by a few percent during fitting to achieve an optimal result. The fit process also included the wavelength solution for the CRIRES spectra. This step is critical, since narrow and steep telluric lines are sensitive to small wavelength errors and produce notable residuals for wavelength mismatches as small as ~30 m/s. A typical fit process, including various runs of LBLRTM takes about two minutes to converge over the spectral coverage of a single CRIRES detector. We have also successfully applied the code to optical high resolution spectra from UVES and to low resolution near-infrared spectra from SINFONI.

Wavelength calibration as added value

Fitting telluric lines to empirical spectra not only provides a model of the telluric absorption, it also delivers a precise wavelength solution. This is an important added value of this method, given that the wavelength calibration for high resolution near- and mid-infrared spectra is often challenging. Rare gas emission line lamps used in low resolution near-infrared spectrographs, such as He, Ne, Xe, and Kr lamps, provide only a sparse line density and are only of very limited use at high spectral resolution (see also Aldenius et al., 2008). Even the rich spectra of ThAr emission line lamps, commonly employed by high resolution optical spectrographs, have a much lower line density in the near-infrared than in the red optical. Typical line densities of ~400 lines per 100 nm around $\lambda = 1000$ nm drop quickly to less than ~20 lines per 100 nm at $\lambda = 2500$ nm. Given the typical wavelength coverage of ~λ/200 per CRIRES detector, many spectral settings remain poorly calibrated. Moreover the dynamic range of the ThAr emission spectrum is very high due to the strong contrast between the Th and Ar lines, leaving weaker lines at low signal-to-noise ratios while nearby stronger lines quickly saturate.

Often atmospheric OH* emission lines (commonly referred to as airglow emission) are used for wavelength calibration in the near-infrared, especially for low- and mid-resolution spectrographs. OH* is a chemical radical and its transitions originate from non-LTE processes in high atmospheric layers. They appear in emission but not in absorption in astronomical spectra and constitute the dominant background source in the near-infrared *J*- and *H*-bands. However, neither the line density nor the line strength of individual OH* lines is high enough to make this species useful for the wavelength calibration of high-resolution spectrographs. For example, the small spatial pixel scale of CRIRES (86 milliarcseconds/pix) makes the use of OH* lines especially challenging, given that each pixel covers less than 10^{-2} arcsecond^2 on the sky.

In contrast, the atmospheric features of other regular molecules in LTE, as we model them with LBLRTM, show a high density of strong absorption lines and thus provide a natural *in situ* wavelength calibration. Since they are imprinted in the source spectrum before the light reaches the spectrograph, these lines suffer the same instrumental effects as the intrinsic lines in the stellar spectrum. Hence, in contrast to all emission line sources used to wavelength calibrate long-slit spectra, telluric absorption lines provide an intrinsically more precise calibration source, especially since lamp emission lines are recorded in separate exposures, often hours after the science spectra and thus after potential changes in the spectrograph setup.

Performance and limitations

As can be seen in the examples presented in Figure 1, the modelling of telluric absorption lines is not perfect, but leaves residuals at the 2% level for most lines when observed at high spectral resolution. A few lines exhibit even stronger residuals. The main reasons for these mismatches are imprecise line data in the HITRAN database and insufficient treatment of line coupling (also known as line mixing) in the radiative transfer code. The latter is, for example, responsible for the strong residuals of the CO_2 Q-branch at 4695 nm (see the lower panel of Figure 1). Other limitations may arise from uncertainties in the determination of the instrumental profile and the atmospheric model.

Line data in HITRAN have strongly varying accuracy levels. Typical uncertainties of line positions range from a few to several hundred m/s, but can be as high as several km/s in extreme cases. Line strengths are rarely precise to the 1% level. However, the HITRAN database is constantly updated and the data quality will further improve in the future. Also, individual line data can be re-fitted when comparing synthesised spectra with high resolution spectra of standard stars before applying the code to spectra of science targets.

Despite these limitations, synthesised telluric spectra can provide the same or even better telluric correction than empirical spectra. The question of when to use empirical spectra or a telluric model depends on a number of factors and should be decided on a case-by-case basis. However, the use of a telluric model should be strongly considered for regions where standard stars have spectral features, when instrumental setups (including the instrumental profile) cannot be reproduced, or when observations encompass a wide range in airmass.

Some recent and ongoing science programmes entirely rely on telluric models for calibration. One example is the CIRES–POP project, dedicated to providing the community with a high resolution, high signal-to-noise near-infrared spectral atlas of several stars across the Hertzsprung–Russell diagram (Lebzelter et al., 2010). Data reduction for this project employs telluric models to wavelength calibrate settings that lack coverage by ThAr lines or gas cells. CRIRES–POP concentrates on very bright stars and uses a large number of CRIRES settings. Obtaining spectra of telluric standard stars for each science target would be very time consuming, at least doubling the total observing time. Most importantly, the programme includes observations of early-type stars to map their spectra to search for unaccounted lines. This process would prove impossible if a standard star of similar spectral type was used as an atmospheric calibrator.

Another project utilising telluric models is the CRIRES radial velocity campaign to search for extrasolar planets around mid-to-late M-type stars (Bean et al., 2010a,b). The wavelength calibration for this project relies on a custom-built ammonia gas cell, given the need to determine radial velocities to the m/s level. The telluric features present in all observations obtained by this programme need to be corrected to a high level of precision. Obtaining high signal-to-noise standard star spectra for all science observations would have made the project less time-effective. Also, the instrumental profile between the science observation and the standard star must match; a challenging requirement for CRIRES. Given the sensitivity of the radial velocity method to small changes in the instrumental profile, the use of standard star observations would have compromised the achievable long-term radial velocity precision, strongly favouring the telluric modelling approach.

Last but not least, telluric models are not only used to wavelength calibrate and to correct for the telluric features in observed spectra, but also to plan observations and predict the atmospheric throughput based on meteorological forecasts. For example, the exposure time calculator for CRIRES employs a telluric model to allow the user to check spectral settings for the impact of telluric absorption under different water vapour levels.

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NGC 3603, shown here in a VLT FORS three-colour composite (from *V*-, *R*- and *I*-band images), is a young Galactic starburst cluster situated at a distance of 6.8 kiloparsecs. With many dozens of massive young hot stars and an age of a few Myr, it is the focus of many studies as a nearby template for extragalactic starburst environments.