DOI: 10.18727/0722-6691/5339

Telluric Correction of VLT Spectra: The New Graphical Interface to Molecfit

John Pritchard[1]
Lodovico Coccato[1]
Wolfram Freudling[1]
Alain Smette[1]

[1] ESO

The removal of absorption features due to Earth's atmosphere is a fundamental and delicate process in the reduction of spectroscopic observations, in particular in the near- and mid-infrared. In this paper we present the new graphical user interface of Molecfit, a package that aims to model the full atmospheric transmission by fitting key absorption features in spectra.

Some of the light from astronomical sources is absorbed by Earth's atmosphere. The atmosphere is completely opaque in some regions of the spectrum, where the signal from the source is therefore unavailable to ground-based telescopes. In other regions, however, the absorption occurs only at specific wavelengths and a series of absorption lines, called 'telluric absorption lines', contaminate the spectra of the observed sources. The correction of these telluric absorption features is a crucial step in the reduction of spectroscopic data. This is particularly relevant for near- and mid-infrared observations, where the depth, number and density of telluric absorption features are high and significantly contaminate the spectrum, blending with the intrinsic spectroscopic features in the spectrum of the object. Figure 1 shows the atmospheric transmission from 0.3 mm to 2.6 mm.

Telluric correction

There are two main strategies to remove telluric absorptions from a spectrum. The first is to observe a source (a telluric standard star) with no intrinsic features. The spectrum of the telluric standard star, normalised to its continuum level, can be used to remove the atmospheric signatures from other spectra taken under the same conditions and with the same instrument and instrument setup. The advantage of this method is that it delivers a telluric transmission convolved with the same spectral resolution as the scientific target(s). The main disadvantages are that it requires taking dedicated observations close in time to the scientific target(s) and that the telluric standards are not observed at the same time as the science exposures, so any changes in the atmosphere will introduce artifacts in the corrected source spectrum.

The second strategy is to generate a model of the atmospheric transmission starting from measurements of humidity and pressure and the column densities of the molecules that shape the telluric features. The last of those can be obtained by measuring specific absorption features on a reference spectrum, which could be either a telluric standard star or the science target itself if it is bright enough. The advantage of this strategy is that, in principle, dedicated telluric standard star observations can be avoided, or at least minimised. The disadvantage is that the method relies on the goodness of the underlying physical ingredients (such as correct treatment of the molecules and how they interact with each other, and how the pressure, temperature and humidity vary with altitude) and instrument-related components such as the line spread function and the goodness of the wavelength calibration.

Molecfit

ESO provides a general tool, named Molecfit (Smette et al., 2015; Kausch et

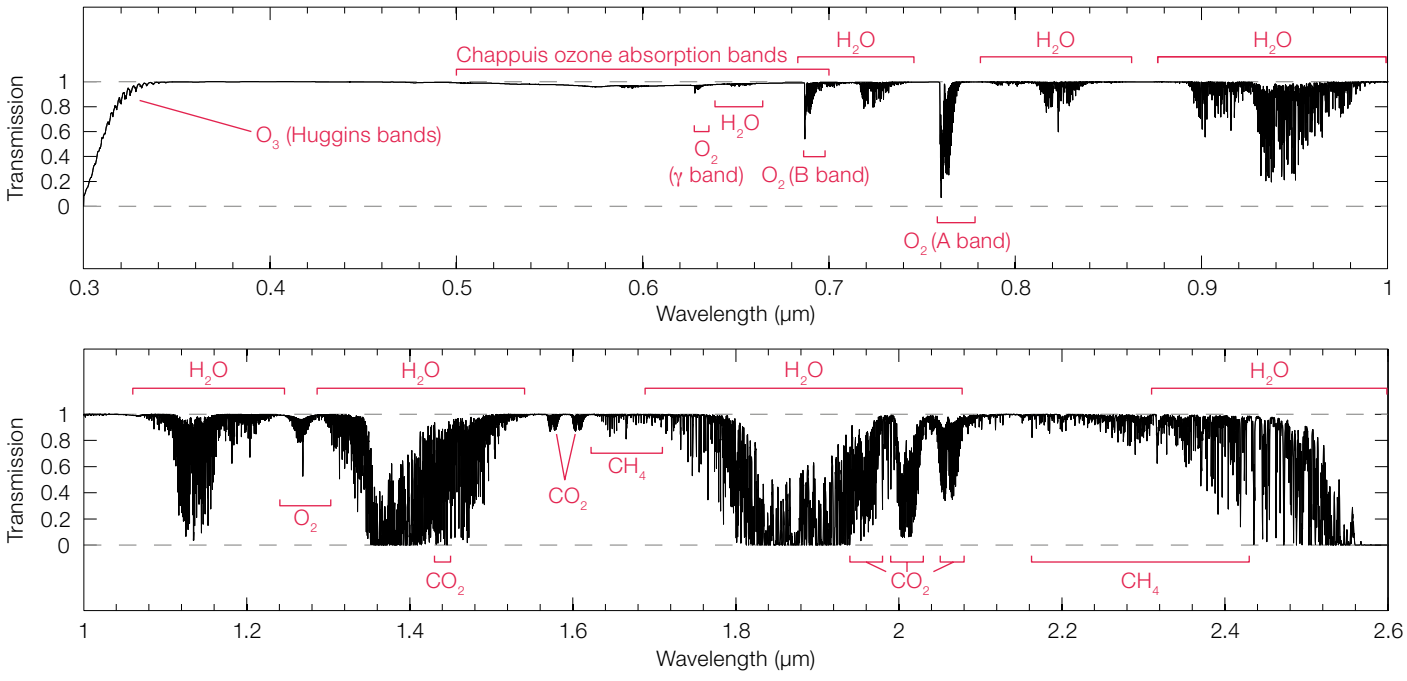

Figure 1. Atmospheric transmission in the optical and near-infrared (from Smette et al., 2015).

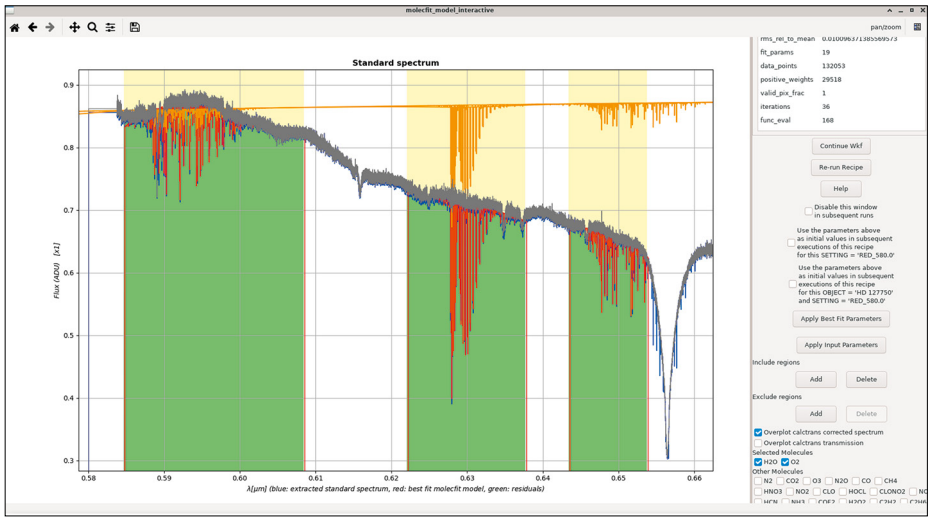

Figure 2. Interactive window of the Molecfit model. The left-hand panel shows the input reference spectrum (blue), the typical transmission curve for H_2O and O_2 (orange), the best fit model (red), the telluric corrected spectrum (grey), and the wavelength regions used in the fit (green). The right-hand panel allows the user to change the recipe parameters.

al., 2015), which aims to remove telluric absorptions using the modelling approach. Molecfit was released on 1 April 2014 as three stand-alone 'executables' and a graphical user interface (GUI) that guides the user through the process of removing telluric features.

As Molecfit was created to be used with most spectrographs, it includes a large number of user parameters. However, although well-tuned to the underlying executables, the way the original GUI was coded made it difficult to maintain and to integrate with the ESO pipeline environment.

Therefore, to facilitate future developments and maintenance and to improve compatibility with existing ESO data and instrument pipelines, Molecfit has been integrated into the ESO data processing infrastructure as a pipeline package[1]. The original stand-alone code is still distributed, but is not supported anymore[2].

Like the original suite, the new version of Molecfit consists of three 'recipes': molecfit_model fits — possibly small — regions of a spectrum, accounting for the shape of the continuum in these regions, spectral resolution and systematics in the wavelength scale, and derives the column densities of the molecules included in the atmosphere; molecfit_calctrans constructs the atmospheric transmission over the whole spectral range of the input spectrum taking account of the atmospheric composition determined by the previous fit, adapting it to the spectrum to be corrected by taking account of any difference in airmass between the spectrum used to derive the model and the spectrum to be corrected; and molecfit_correct applies the above mentioned correction to a scientific spectrum. These recipes can be executed, like any other ESO recipe, from the command line with the esorex command or via an EsoReflex workflow[a] (Freudling et al., 2013).

The first version of Molecfit to be released as a pipeline package and EsoReflex workflow (version 3.0.0) was released in 2020. As the focus of that release was the implementation of the underlying modelling engine, many of the more user-friendly aspects of the GUI of the original version were not implemented in the first version of the workflow.

Since then the underlying engine has been updated and improved and the Molecfit workflow has been overhauled, so that it now includes advanced features that enhance the user's experience of making an efficient telluric correction; this is the topic of this paper.

The most critical aspect of Molecfit is to determine the various parameters that accurately reproduce the transmission spectrum of the atmosphere as seen by the spectrograph: the column densities of the various molecules contributing to the telluric features, the parameters of the line spread function of the spectrograph, the coefficients of the polynomial representing correction of the wavelength calibration, and a good representation of the continuum in the selected regions to be modelled. The workflow overhaul therefore concentrated on the GUI associated with the molecfit_model recipe.

Before starting the workflow, the user must set some basic parameters, such as:

– the directories where the data are located and where the final products will be stored. As for all EsoReflex workflows, the input directories are scanned and files in them are classified. For each science spectrum to be corrected the 'closest-in-time' telluric standard (if present) observed with the same instrumental setup is associated.
– the reference spectrum for the model. The user can decide to fit the atmospheric model on the science file to correct itself (this strategy works best for spectra of high signal-to-noise), or on the associated telluric standard (if present).
– the instrument the data were taken with. The workflow currently recognises data from five instruments (ESPRESSO, GIRAFFE, UVES, VISIR, and X-shooter) and automatically adapts the output files of the ESO pipelines of these instruments into Molecfit-compatible formats (if necessary). It sets robust recipe parameters for these instruments and their configurations, such as molecules and wavelength regions to consider in the fit. The user can change them through the interactive windows that will pop up during the analysis. Data from other instruments, including non-ESO instruments, can also be corrected. However, in such cases adapting the input files to Molecfit-compatible formats (if necessary) and the setup of the recipe parameters are left to the user, either interactively when running the workflow, or by implementing a set of Python methods specific to the instrument in question. Support for more (ESO) instruments is under development[3].

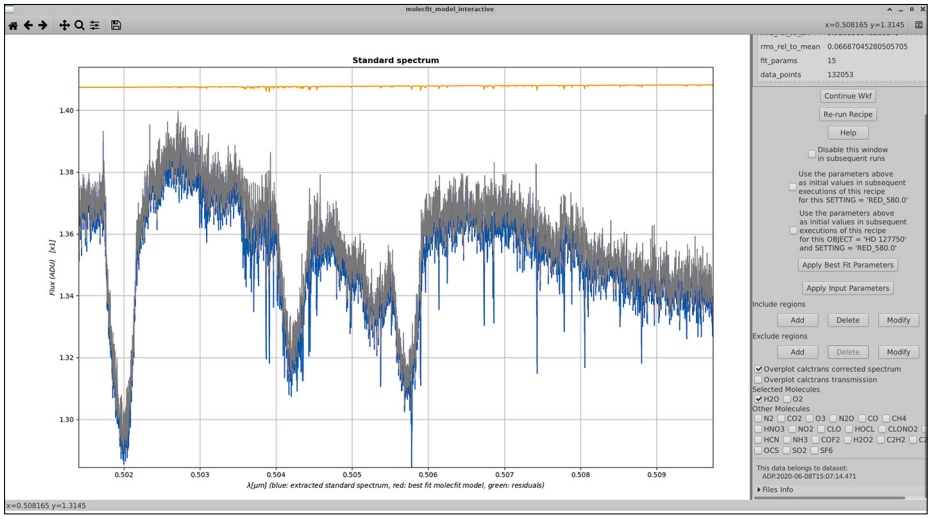

Figure 3. Zoom-in of Figure 2. Note that the corrected spectrum (grey) has the telluric lines removed (blue) even in this wavelength region that was not included in the fit. The power of the method is that one can consider only strong telluric features to determine the model for the entire wavelength range of the data, minimising the contamination from noise or the intrinsic features of the source.

To correct each dataset, the workflow first presents the molecfit_model GUI, with which the user can fine tune the parameters and their initial guesses to use in the first execution of the molecfit_model recipe. The GUI shows the reference spectrum together with pre- or auto-defined wavelength regions and pre- or auto-defined molecules to fit. The user can display a typical transmission curve for each molecule to evaluate whether it has an impact on the telluric absorption in the reference spectrum and therefore to include or exclude it from the model. The wavelength regions can be defined and edited with the mouse. Although there are still more than 100 parameters that control every aspect of the model, they have been grouped into several tabs by experience level to guide users from novice to expert.

Once happy with the initial recipe parameters, the user can run the molecfit_model recipe to compute the fit. Upon completion of the recipe, the GUI is presented again, this time also displaying the fitted model and residuals. It displays the computed corrected spectrum over the full wavelength range of the input spectrum (Figures 2 and 3), allowing the user to further fine tune parameters and rerun the recipe as many times as necessary to obtain an optimum model. The parameter setup can be stored and re-used for other datasets from the same instrument configuration.

Once an optimal model has been computed, the workflow uses the model to construct the telluric correction for the target spectrum. If the reference spectrum used for the model was a telluric standard, Molecfit accounts for the airmass and Precipitate Water Vapour difference between the two spectra. Optionally, the user can provide a function describing the instrumental line spread function at each wavelength, which will be considered when constructing the transmission curve. Finally, the spectrum is corrected. The products of the workflow reflect the format of the input data: if the input spectra comply with the format of the ESO archival standard (known as the phase3 standard), so do the products.

References

Freudling, W. et al. 2013, A&A, 559, A96
Kausch, W. et al. 2015, A&A, 576, A78
Smette, A. et al. 2015, A&A, 576, A77

Links

[1] ESO Pipelines: https://www.eso.org/sci/software/pipelines/
[2] Molecfit: http://www.eso.org/sci/software/pipelines/skytools/molecfit
[3] Molecfit Experimental Version: https://support.eso.org/kb/articles/molecfit-experimental-version

Notes

[a] Integration with the GASGANO GUI, however, has not been implemented, neither is it foreseen.

ESO/P. Horálek

The bright light in the centre of this picture, shining below the Milky Way's dark, pinkish belt, is the planet Jupiter. It is flanked by two hills hosting ESO's Very Large Telescope (left) and VISTA (right) in the Atacama Desert in Chile.