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# Telluric Correction of IRTF Spectra with Atmospheric Models

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# 1 Preamble

Accurate model spectra of the Earth's transmission will reduce the need for taking spectra of telluric standard stars at the IRTF. This document describes the program xtellcor_model, an adaptation of xtellcor (Vacca et al. 2003), that uses atmospheric models to divide out telluric absorption in iSHELL spectra. Other instruments are not addressed yet. The code is still under development, but a test version is available. In Section 2 we give a very brief summary of how to use the program. Section 5 gives detailed background information, and Sections 6 and onward give more detailed usage instructions, examples, and summaries of known issues and future work.

# 2 Cookbook

This is a brief summary of how to run xtellcor_model. For more detailed information, see Section 6.

I. reduce the iSHELL data using Spextool, but do not correct for telluric absorption and do not merge the orders

II. this step is optional. If one wants to correct for the order blaze shape, then one needs to reduce the flat fields in Spextool and extract spectra using an extended source aperture.

III. download the xtellcor_model package (http://irtfweb.ifa.hawaii.edu/research/dr_resources/) and unpack it in a directory that is in Spextool's IDL path (for a typical Spextool installation this is a called Spextool/ and contains subdirectories data/, helpfiles/, pro/, etc.)

IV. start Spextool (the version for iSHELL)

V. on IDL prompt, enter xtellcor_model

VI. step 1: load reduced iSHELL spectrum

VII. step 2: retrieve the atmospheric model.

a. The molecules that contribute the most to a given mode are preceded by '*'. Scaling their column densities to the observations can be done automatically by entering -1 in the box. This is typically always needed for $H_2O$ and $CH_4$.

b. Click 'Retrieve Atmospheric Model'. The fitting and download typically takes 1-2 minutes.

VIII. step 3: inspect the quality of the model spectrum. Different molecules can be plotted using the 'atmosphere' button. Apply small wavelength shifts for optimal division. If it does not look satisfactory, go back to step 2 and adjust the column density scaling factor of the molecule(s) of interest.

IX. step 4: this step is optional. Divide out the order blaze shape by using flat fields, by loading the extracted flat field spectrum produced at instruction II above.

X. step 5: plot and save the telluric and blaze function corrected spectra to fits file.

# 3 Do's and Don'ts

In its current state Xtellcor_model works well if these four conditions are true:

- if the science lines of interest are narrower than ~20% of an echelle order
- if the science can be done using line-to-continuum ratios
- if flux calibration is not important
- if the target spectrum is not densely packed with spectral features (i.e., if there are no isolated telluric lines to optimize the atmospheric model to)

In these particular, though fairly common, science cases the observer may consider not observing telluric standard stars.

Conversely, most likely Xtellcor_model is currently insufficient in the following science cases, and telluric standards must still be observed:

- if the emission or absorption width of the astronomical lines of interest is broader than ~20% of an echelle order
- if the broad spectral shape (across many orders, e.g., continuum emission or solid state features) is of scientific interest
- if flux calibration is of science interest, i.e., if line-to-continuum ratio's are insufficient for the science goals
- targets with little 'free' continuum emission, e.g., late M-giants.

# 4 Sample Data

The xtellcor_model distribution includes a sample iSHELL observation ("extractedstandard.fits") in the K3 mode with the 0.375 arcsec slit. It has been reduced with Spextool version 5.0.1, but not divided over a standard star and not order-merged. The corresponding extracted flat field for the optional order blaze correction is also provided ("spectraflat_k3_6-10.fits").

# 5 Background

A telluric absorption correction technique that uses weather models in combination with high spectral resolution transmission models was thoroughly tested on ESO/CRIRES (R=50,000-100,000) infrared spectra, yielding a correction accuracy of 2% or better, even near strong telluric lines (Seifahrt et al. 2010). The atmospheric radiative transfer code LBLRTM (Line-By-Line Radiative Transfer Model; Clough et al. 2005; http://rtweb.aer.com/lblrtm.html) was favored by Seifahrt et al. They recommend to use it with weather information (vertical profiles of pressure, temperature, and $H_2O$ abundance) from GDAS (Global Data Assimilation System) models, and with MIPAS (http://www-

atm.physics.ox.ac.uk/RFM/atm/) model atmospheres for other molecules and at the highest altitudes. This method was subsequently adopted by a number of other groups:

- Molecfit: a C-based fitting code, developed by ESO for their UV, optical, and infrared spectrometers (Smette et al. 2015) and included in their Common Pipeline Library.
- Telfit: a Python-based fitting code tested on optical high resolution spectra (R=80,000; Gullikson et al. 2014). In contrast to the other codes, Telfit adjusts the vertical temperature and pressure profiles to measurements at the telescope at the time of the observations.
- Telrem: an IDL-based fitting code developed for the ESO instrument X-Shooter (Rudolf et al. 2016).

All these fitting programs, Molecfit, Telfit, and Telrem require the LBLRTM atmospheric model code (FORTRAN) and the line list code LNLF (FORTRAN) along with the large LBLRTM-formatted line list (1.8 GB) to be installed by the users on their local machines. The same is true for the GDAS data files, which are ~0.5 GB in size for every week of data.

Installing the code and weather data will be big hurdles for many IRTF users, and therefore we decided to use an online server that generates these models. As we were building such server at the IRTF, we were made aware of the Planetary Spectrum Generator (PSG; https://psg.gsfc.nasa.gov/; Villanueva et al. 2018) that does mostly what is needed. We thus converted the much used Spextool program xtellcor (Vacca et al. 2003) to use PSG models rather than standard stars to correct for telluric lines in iSHELL spectra. We named it “xtellcor_model”. The rest of this document is about using the program “xtellcor_model” on iSHELL spectra. Its use on SpeX spectra has not been implemented yet. We note that in xtellcor, the telluric calibrators are also used to divide out the instrument’s order blaze shapes, and with the modeling approach we rely on flat fields for this, which is done within “xtellcor_model”.

# 6 Using “xtellcor_model”

Xtellcor_model is not integrated in the Spextool distribution yet; it can be run by unpacking the tar file in a directory that’s in Spextool’s IDL path. Then on the IDL command enter xtellcor_model and the GUI (Figure 1) appears. The steps on the GUI labeled 1-5 are fairly self-explanatory but are further described below.

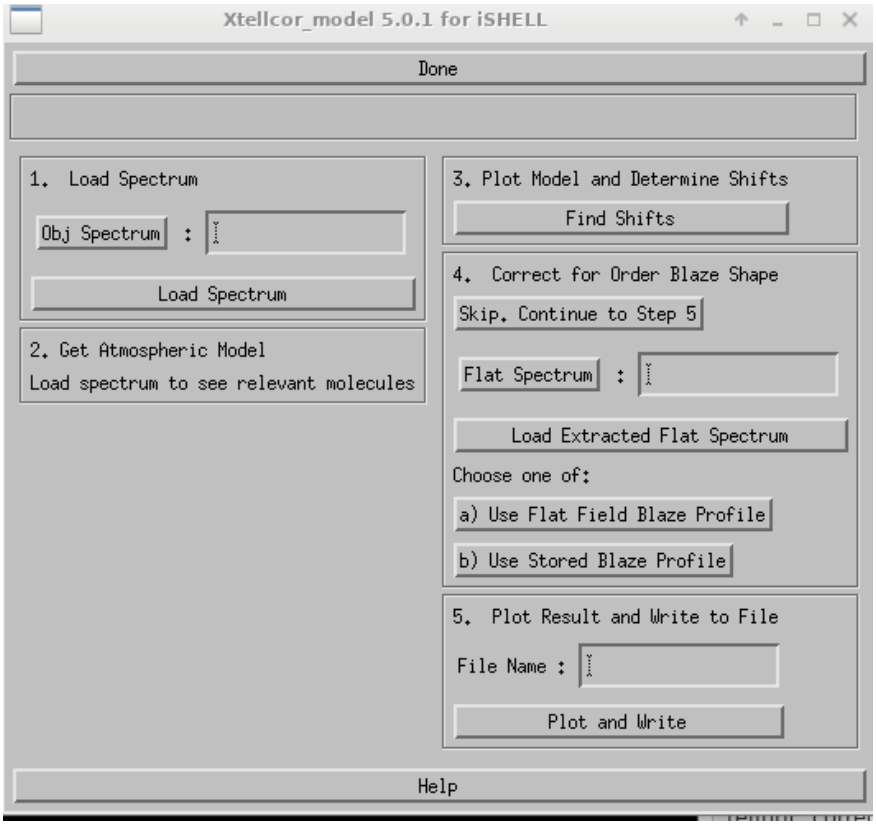


*Figure 1: GUI for xtellcor_model.*

## Step 1: Load Spectrum

This loads a FITS file of an observation that has been fully reduced in Spextool, except for telluric line correction and order merging. The header keywords are used to determine essential parameters, such as the instrument configuration, slit width, date of observation, and airmass. After clicking ‘Load Spectrum’, the step 2 information is updated such that only the atmospheric molecules relevant for this configuration’s wavelength range are displayed (Figure 2).

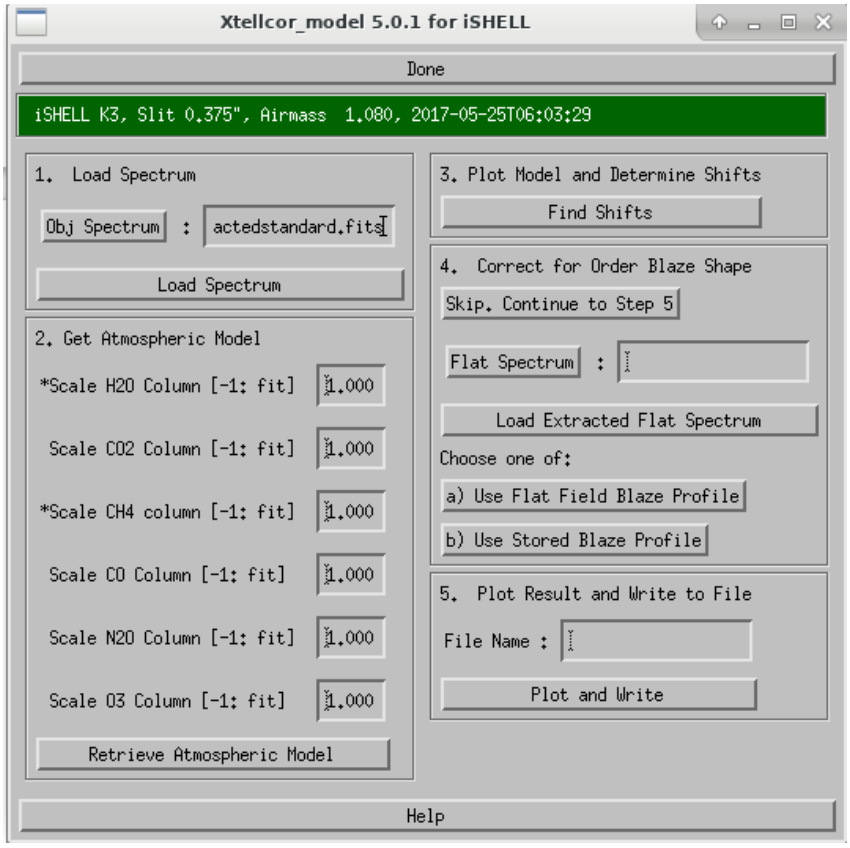


*Figure 2: After loading the data, step 2 only displays molecules relevant to the atmospheric transmission in this iSHELL configuration. Species preceded by '*' are most important: they have lines stronger than 10% absorption.*

## Step 2: Get Atmospheric Model

Clicking 'Retrieve Atmospheric Model' will get the model spectrum from the server using the weather conditions at the time of the observations. This usually takes 1-2 minutes. The IDL prompt shows the progress. Subsequent comparison of this model with the data at step 3 will in most cases reveal that the $H_2O$ lines do not fit well and often other major species (preceded by '*' in the list) need adjustment as well. This can be done by re-doing step 2 and adjusting the relative scaling factors by hand (educated guess) or by automated fitting. In the latter case, enter -1 in the scaling boxes. The fitting is done to a couple of individual telluric lines, defined in the file "teltool_lines.dat", and then the median across the best-fit scaling factors is taken. If one wants to inspect the fits, they are plotted in a postscript file ("xtellcor_model_fittedlines…..ps"; Figure 3). The fitting is done by $\chi^2$ minimization to the line profile by varying the molecular column and peak wavelength. Experience so far has shown typical scaling factors of 0.1-2 for $H_2O$ and up to 1.4 for other species. A few iterations between step 2 and 3 to get the best scaling factors are typically needed. The wavelength shift is presently not applied to the data,

however, because it is found to not be a constant across echelle orders and instead must be done in step 3.

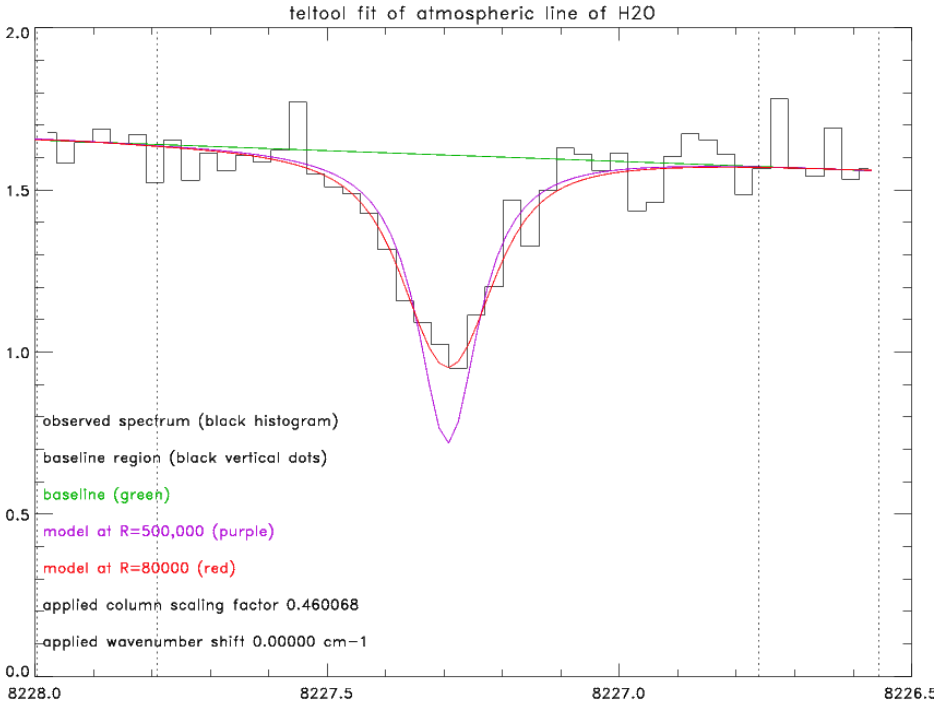


*Figure 3: Example fit to an individual atmospheric line to get the best column scaling factor. These plots are saved in files named "xtellcor_model_fittedlines....ps".*

## Step 3: Plot Model and Determine Shifts

This step can be used to inspect the fitting result and if needed, one can go back to step 2 and adjust the column scaling factors. Under the button ‘atmosphere’ (Figure 4) one can overplot (in yellow) the total transmission model or that for individual molecules. The main function here, however, is to correct for small wavelength calibration errors. Residuals can be greatly reduced by applying sub-pixel shifts. We find that currently, shifts can vary within orders and across orders, and the user needs to decide what’s best. To help with that, one can do an automated determination by clicking ‘s’ on the command line and then define a line to fit to with the left mouse button. The ‘apply to all button’ is useful. When satisfactory shifts are determined, click ‘accept’.

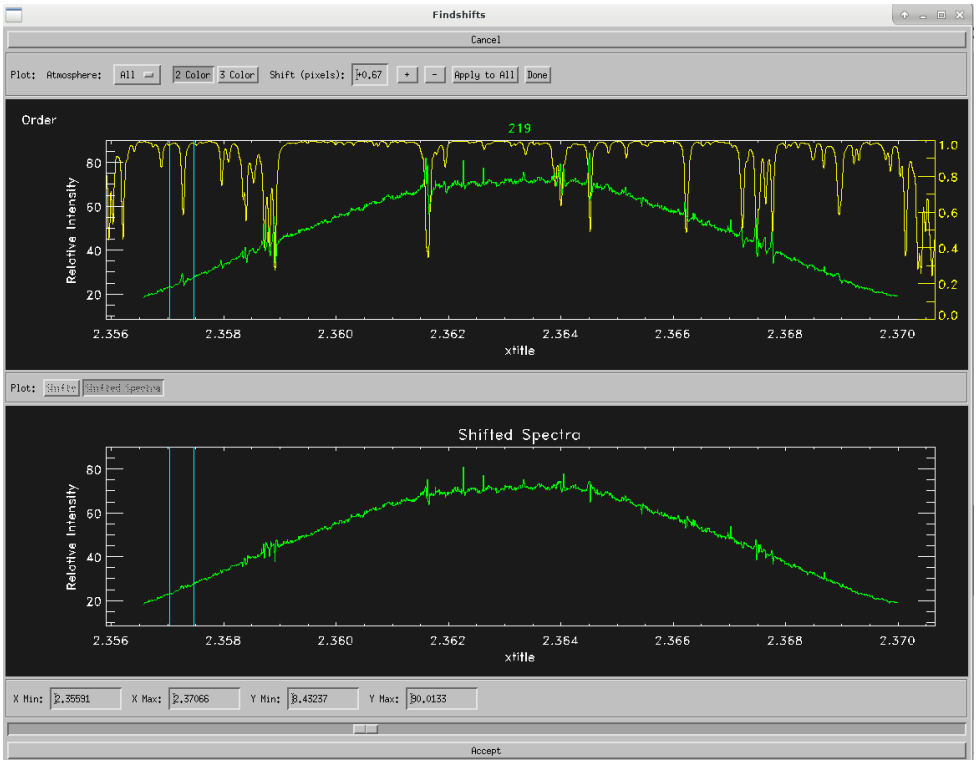


*Figure 4: tool to inspect the telluric correction and determine sub-pixel wavelength shifts. The top panel shows the division before the shift is applied. Note that the curvature of the order is because no blaze correction has been applied yet (see step 4).*

## Step 4: Correct for Order Blaze Shape

At this stage, the telluric correction is done, but the spectral orders are still strongly curved due to the grating blaze (Figure 4). In xtellcor, the standard star is used to correct for that, but xtellcor_model relies on the flat fields. However, if this order blaze is not affecting the science analysis (e.g., for the study of individual narrow lines), this step can be skipped. If not skipped, the user will need to use Spextool to reduce the flat fields, i.e., use the extended source method to extract a section along the slit. This extracted flat field spectrum is then loaded in this step 4 and subsequently divided over the data (step 4a). Step 4b also offers the possibility to divide over a pre-defined median blaze function in case there are problems with the observed flat field spectrum.

Here we describe the process in which the blaze shape is divided out. This should be considered background information, and most users can skip it and continue with section 6. A plain division of the data over the extracted flat is not always possible, because some orders contain molecular absorption lines (due to the air between the flat field lamp and the instrument window). Instead, all orders are divided over the same flat spectrum, determined by medianing over orders not affected by molecular lines. The file ishell_good_flat_blaze_orders.dat defines those orders and typically does not need to be adjusted. For this to work, the medianing and division cannot be done on a wavelength scale, because

the blaze shape depends on echelle order number (*m*). Instead a scale *X* that is common to all orders is used:

$$X = m\left(1 - \left(\lambda_c(m)/\lambda\right)\right)$$

where $\lambda_c$ is the wavelength of the peak of the blaze function. The theoretical value of $\lambda_c$ is calculated from the grating equation, which for an immersion grating instrument in pseudo-Littrow configuration like iSHELL is defined as

$$m\lambda_c(m) = n.\sigma.\cos(\gamma).2\sin(\delta)$$

where *n* is the refractive index of the immersion grating material silicon, σ the grating groove width in micron, γ the out of plane angle of the echelle, and δ the blaze angle. If the correct $\lambda_c$ is found for order *m*, then the observed intensity *R(X)* should match the theoretical blaze function

$$R(X) = [\sin(\pi\alpha X)/(\pi\alpha X)]^2$$

with

$$\alpha = \cos^2(\delta)$$

a grating constant. But we find that $\lambda_c$ deviates from the observed flat spectrum by a small amount, possibly due to an inaccuracy in *n*. To mitigate this, we determine the peak intensity of each observed flat that is not compromised by molecular absorption (Figure 5) and determine the correction factor to $\lambda_c$ as a function of *m* (Figure 6). The next step is then to median all ‘good’ orders on the *X* scale and it is this median flat spectrum (Figure 7) that is divided over each spectral order observed for the science target.

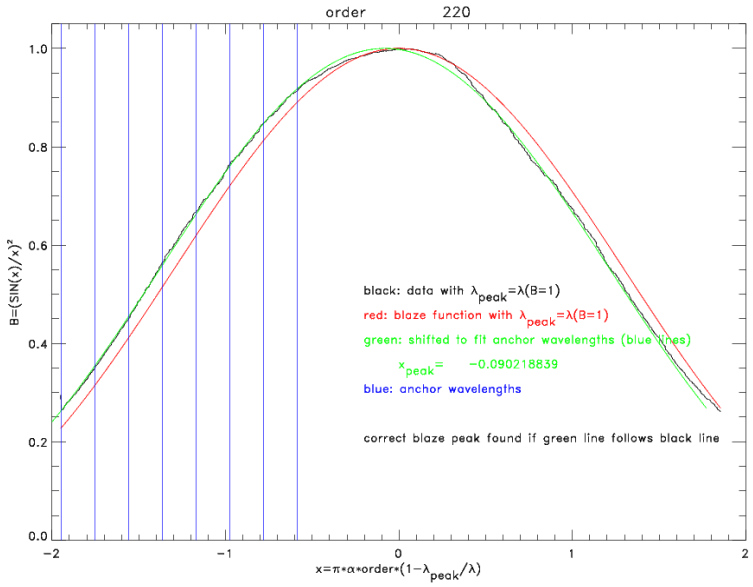


*Figure 5: One iSHELL spectral order (black) extracted from the flat field compared to the theoretical blaze function (red) and after a shift to the observed peak wavelength $\lambda_c$ (green) following normalization at the wavelengths indicated in vertical blue lines. This plot can be found in xtellcor_model_blazepeaks...ps*

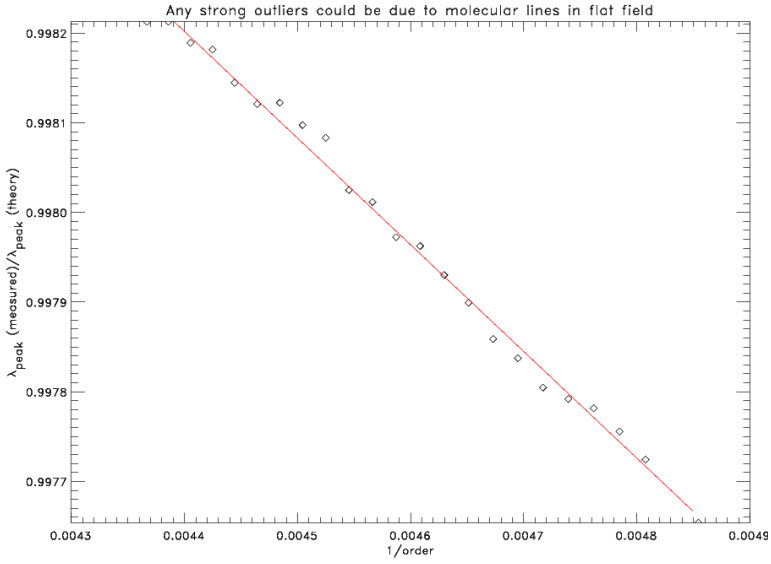


*Figure 6: Blaze peak wavelength correction factor (y-axis) versus the inverse of the echlle order (x-axis). The red line is a linear fit that is used in the blaze correction. This plot is produced as part of xtellcor_model_blazepeaks...ps*

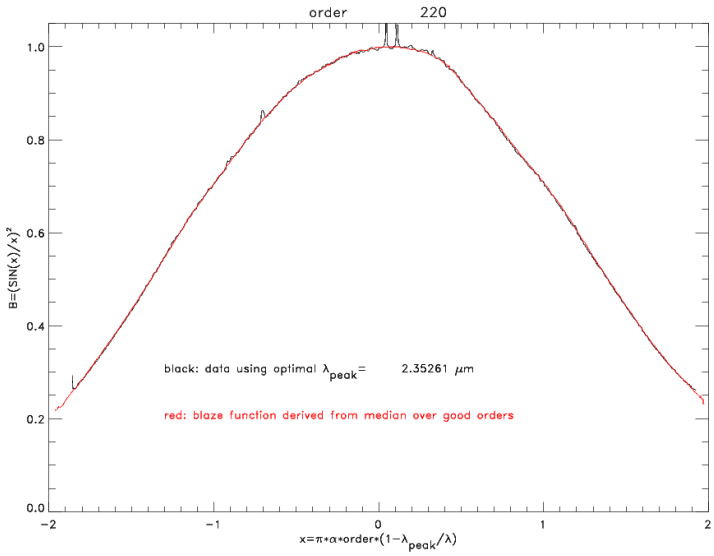


*Figure 7: Signal from a single echelle order derived from the flat field (black) compared to the blaze function medianed over all orders (red). All orders will be divided over this median function. This plot can be found in xtellcor_model_blazemedian_....ps*

## Step 5: Plot Result and Write to File

Finally, the atmospheric absorption and (optionally) blaze shape corrected spectra can be written to fits file. Two files are written to disk: file.fits and file_tellspec.fits. The latter contains both the complete atmospheric model and the transmission for each molecule. At the same time the spectrum is plotted, which is particularly useful to see how well the blaze shapes were corrected for (Figure 8). Note that in this case, the plotted atmospheric transmission spectrum is a generic ATRAN model, not the one optimized to the observations.

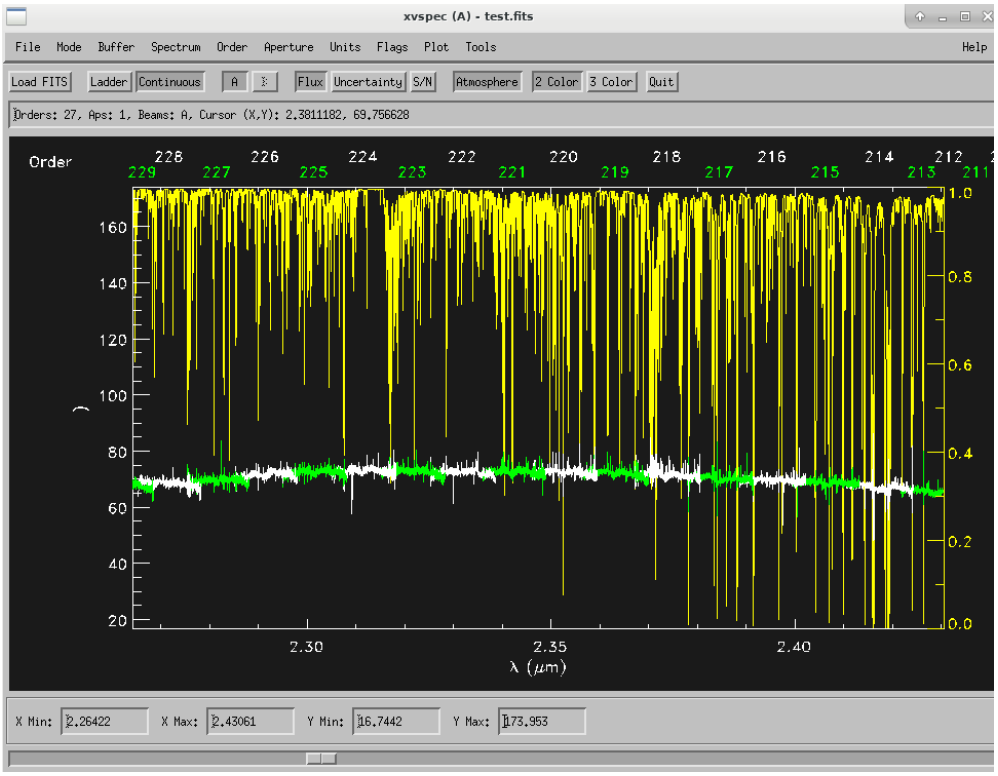


*Figure 8: Fully atmosphere and (optional) blaze-shape corrected spectrum. Yellow is an atmospheric transmission model (a generic ATRAN model, not the one optimized to the observation) and white and green the echelle orders.*

# 7 Examples

Figures 9-11 show a few examples of atmospheric correction of observed iSHELL spectra, comparing the use of models (xtellcor_model) versus standard stars (xtellcor).

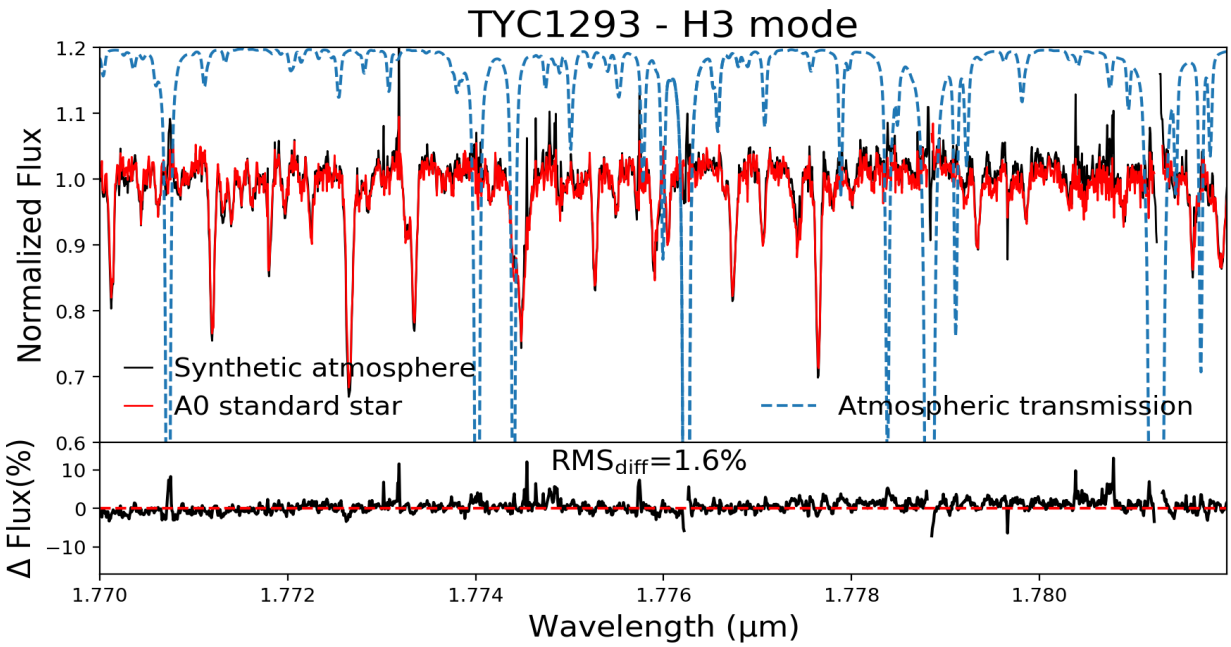


*Figure 9: Example of using xtellcor_model on an iSHELL H3 spectrum with the 0.75 arcsec slit. Top panel: science target divided over telluric standard (red) compared to science target divided over atmospheric model (black). The blue dashed line is the atmospheric model. Bottom panel: difference between the two in percentage. Note that many of the narrow black spikes are not caused by the atmospheric correction. They are likely artifacts due the nonlinearity correction. That problem is still under investigation.*

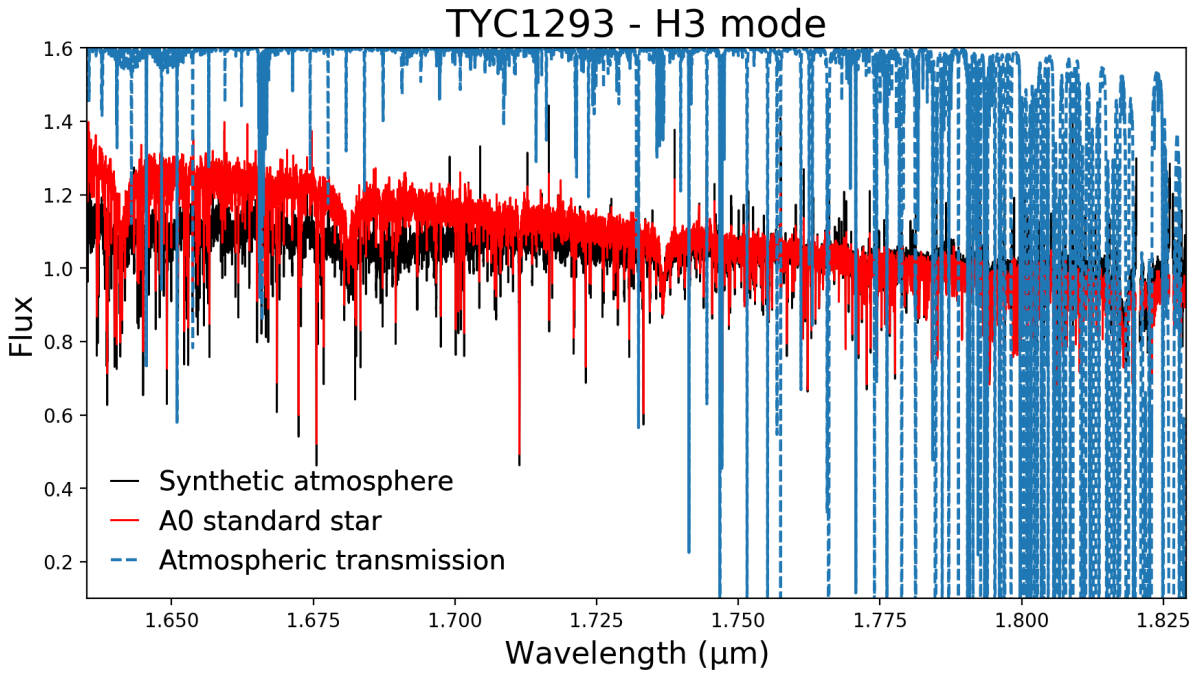


*Figure 10: iSHELL H3 spectrum (0.75" slit) corrected for telluric absorption using a standard star (red) and an atmospheric model (black). The atmospheric model is the blue dashed line. The difference in overall slope is an artifact of the blaze shape correction.*

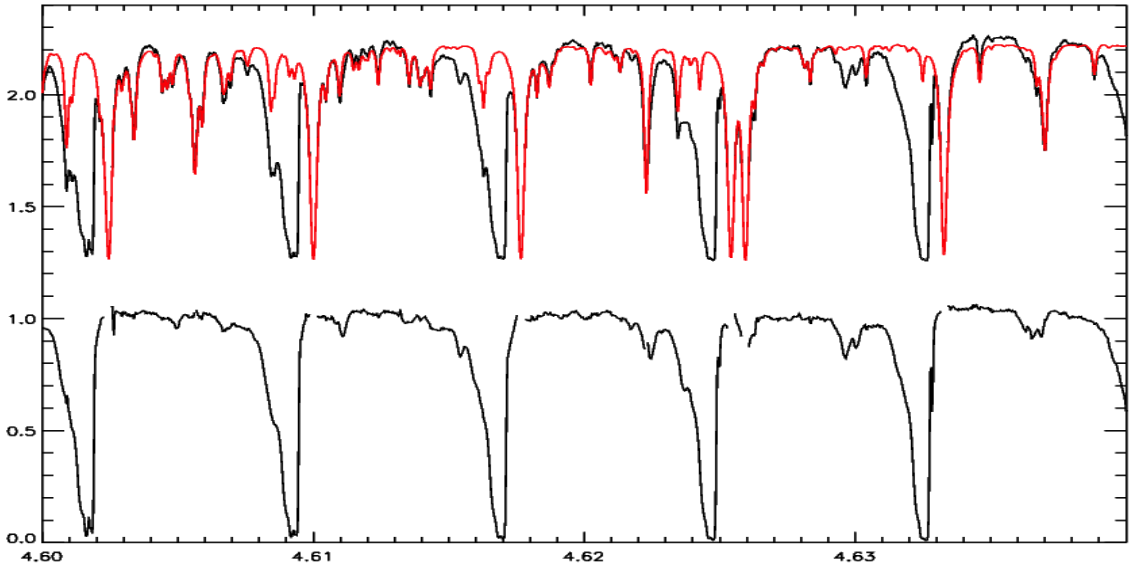


*Figure 11: iSHELL M-band spectrum of a massive protostar. This target has an M-band magnitude of around 1 and no telluric standard stars of comparable brightness could be found. The top black spectrum is the data before telluric correction and the red line is the atmospheric model. The bottom spectrum is after telluric correction. Most structure seen in this spectrum is real (Barr et al., subm. to ApJL).*

# 8 Known Issues and Troubleshooting

The use of xtellcor_model is limited depending on the target being observed, the science being done, or yet unresolved calibration or software issues. Many of these issues will be addressed in future releases. Here we provide a summary.

## Residual Telluric Features

The automatic determination of the molecular scaling factors not seldomly leaves atmospheric residuals that the user will have to improve on by manually adjusting the scaling factors. Future developments are planned to reduce the need for user intervention:

- Presently, one scaling factor per molecule is determined from the median of the factors across the pre-defined lines. Simultaneous fitting over multiple lines or entire or multiple orders would give better results, but is currently not done as it requires baseline fitting that is difficult to generalize for the many different kinds of targets that iSHELL observers study (e.g., targets with many or few lines, with emission or absorption lines, with weak or strong continua, with broad dust emission or absorption lines).

In addition, poor fits to the telluric spectrum may occur for data obtained less than 2 months ago. This is because the database with weather information that PSG uses (MERRA2) is updated only after 2 months. For more recent data, atmospheric conditions of exactly one year earlier are used by PSG.

## Residual Order Curvature

The blaze shape correction (section ) sometimes leaves residual curvature in the orders (Figure 12). We tentatively find that this can be solved by small adjustments (~1%) of the grating constant α (section 6). We will investigate this further, and possibly allow the user to make small adjustments of α.

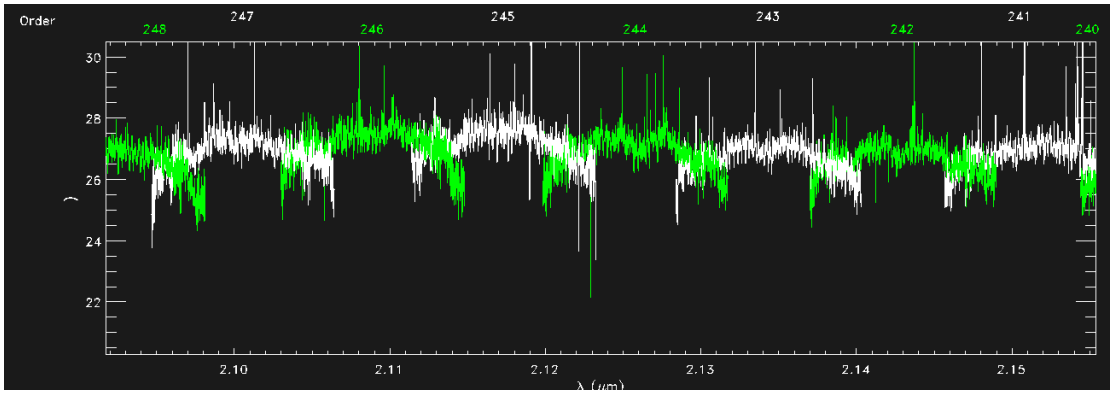


*Figure 12: An observation in the iSHELL H3 mode showing residual order curvature.*

## Order Edges Drop Off

Often, the order edges show a drop. Until we find a solution for this, the user may cut the orders edge at the order merging stage (xmergeorders).

## Wrong Spectral Slope and Large Scale Curvatures

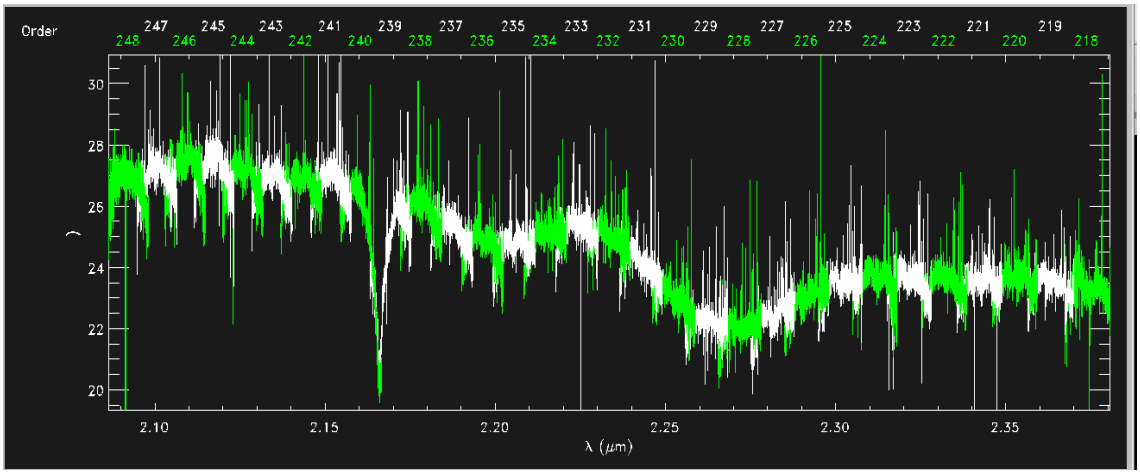


*Figure 13: The broad features at ~2.20 and ~2.27 micron are likely artifacts as a result of features in the flat field. The narrow absorption at ~2.16 micron is real (Br γ).*

We sometimes find broad absorption features in the blaze shape corrected spectra, such as shown in Figure 13. These are likely caused by features in the flat fields used for the blaze shape correction. So far, we have seen them in the iSHELL J1 and K2 modes. We are further investigating the cause and mitigation.

Overall slope differences between the spectra reduced using telluric models and using standard stars are sometimes observed. This may in part be due to the spectral shape of the flat field lamp. We are further investigating the cause and mitigation.

## Narrow Spikes

Occasionally narrow spikes are observed in spectra reduced using model spectra, while they are absent when using standard stars. We suspect this is caused by incorrect non-linearity correction, the effects of which are divided out when using standard stars but not when using models.

## Wavelength Shift Solution Not Robust

We find that when selecting different wavelength regions to determine the wavelength shift (Section 6), different values are found. It works better when narrow regions on single telluric lines are selected. We think that the steep blaze slopes affect the wavelength shift determination and that doing the blaze correction before the shift determination could be a solution. This will need to be implemented.

## Incorrect Header Information

If the FITS header contains wrong header information (e.g., date or slit width), one can override it by replacing the entry ‘header’ with the correct entry in the parameter file teltool_ishell.param. This is very rarely needed, probably only for data obtained during instrument commissioning.

# 9 Future Work

Besides work on the known issues mentioned in section 8, the following non-exhaustive list of improvements are planned for xtellcor_model:

- more accurate and robust matching of molecular columns to the data
- test on 1.50 arcsec wide slit
- integrate into the Spextool for iSHELL distribution
- include more local meteorological data such as PWV columns and pressure
- not all configurations have been tested. Table 1 gives a summary of the status across all iSHELL modes

| ISHELL Mode | Telluric Correction | Blaze Correction |
|---|---|---|
| J0 | Not tested | Not tested |
| J1 | OK | Broad structure across many orders |
| J2 | Needs O2 lines to fit to | Not tested |
| J3 | Needs O2 lines to fit to | Not tested |
| H1 | OK | OK |
| H2 | Not tested | Note tested |
| H3 | OK | Overall slope |
| K1 | Not tested | Not tested |
| K2 | OK | Broad structure across many orders |
| Kgas | Not tested | Not tested |
| K3 | OK | OK |
| L1 | Not tested | Not tested |
| L2 | Not tested | Not tested |
| L3 | Not tested | Not tested |
| Lp1 | OK | OK |
| Lp2 | Not tested | Not tested |
| Lp3 | Not tested | Not tested |
| Lp4 | Not tested | Not tested |
| M1 | O3 residuals | OK |
| M2 | O3 residuals | OK |

*Table 1: Status of Testing Xtellcor_model on iSHELL Modes*

# 10 Change Log

- 12/05/18: updated Beta release (v 0.0.2) on IRTF web page. Includes line profile fitting instead of peak depth fitting and correction of several small bugs.
- 10/18/18: updated Beta release (v 0.0.1) on IRTF web page. Includes items below.
- 10/18/18: output telluric spectrum (.._tellspec.fits) at final step also written in Spextool 5.0.2
- 10/17/18: teltool.pro: take into account gaps in wavelength coverage (such as for iSHELL M-band) when checking if absorption line can be fitted to for column determination
- 10/15/18: Beta release (version 0.0) on IRTF web page

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