Importing ASD-Spectra

Peter Mason, April 2018

Introduction

Malvern Panalytical produces a range of spectrometers that have been popular in a number of application areas since the 1990s. Amongst geologists they are used in various activities from greenfield exploration to ore-grade modelling. They are still known as "ASD" instruments – an acronym for "Analytical Spectral Devices", the company that invented and originally supplied them.

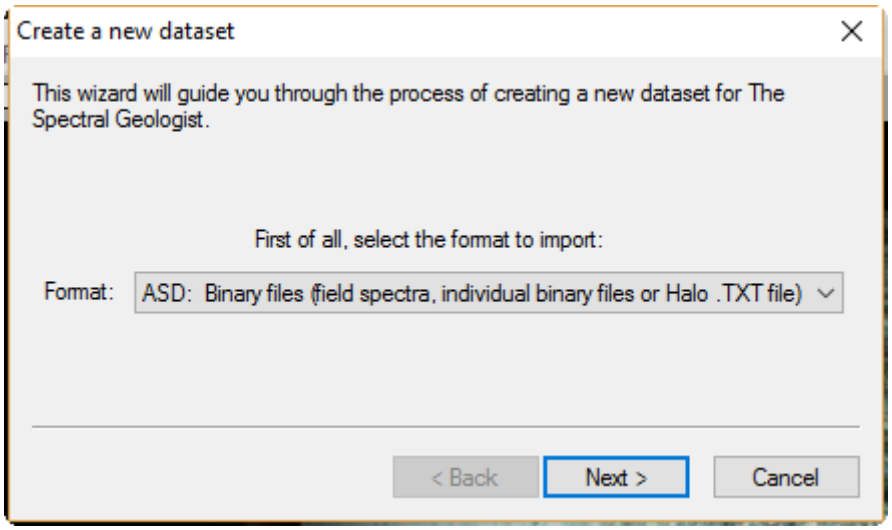
This note describes the options you have when importing spectra from ASD binary files into TSG. Tested instruments are the FieldSpec and TerraSpec range. Other ASD instruments' files haven't been tested in TSG by the author.

Relevant companion notes are "**Importing Photos for Field and Laboratory Datasets**" and "**Dynamic Spectral Imports in TSG**".

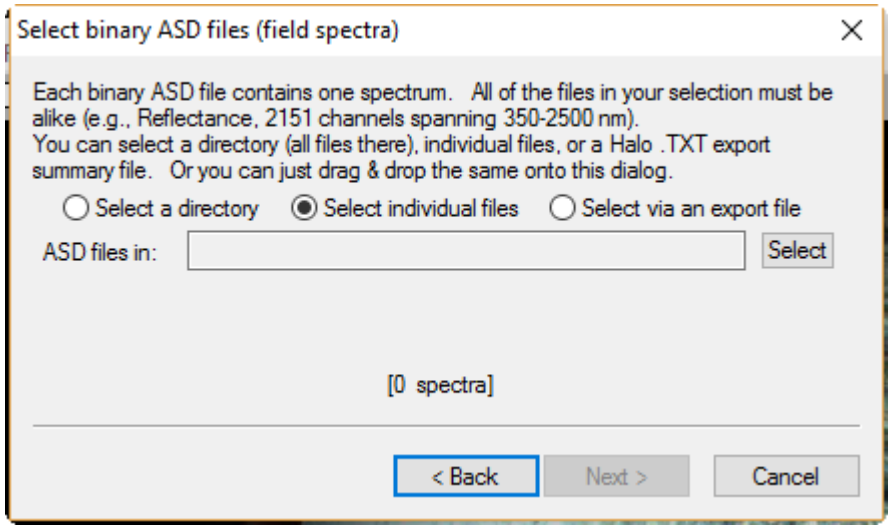
Importing ASD spectra

File selection

- Use TSG's **File -> New** menu or 🗋 toolbar icon to bring up the Import Wizard.
- The wizard's first page is for selecting the file **Format** to import. Select **ASD: Binary files (field spectra, individual binary files or HALO .TXT file)**
- Click **Next**.



The Import wizard will move on to the file-selection / import settings page. (No import settings will be visible yet.)



You have three options here.

1. **Select a directory** is the easiest way to deal with a large number of files. TSG will test each file in the directory (regardless of file extension) and keep the ones that prove to be ASD binary files.
2. **Select individual files** will require that you make the file selection yourself, using <CTRL>click or <SHFT>click pairs in the selection dialog.
3. **Select via an export file** is the way to go if you are working with a FieldSpec HALO and it has given you a .TXT export summary file amongst the binary ASD files.

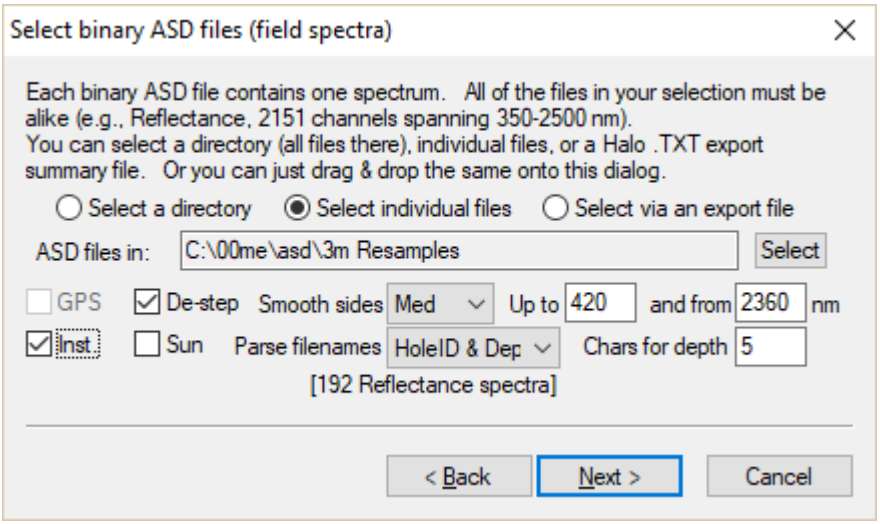
Drag & drop

A shortcut for the above two steps is to drag & drop suitable files or a subdirectory onto the **main TSG window**. For this to work, the binary files' names must have .ASD extensions ***or*** there must be *one* HALO .TXT file.

A lesser shortcut just for the second (file selection) step is to drag & drop files or a directory onto the **file-selection page of the import wizard**. This works like the first shortcut but is more flexible. The binary files' names don't have to have .ASD extensions. TSG will try all given files and keep the ones that are ASD files.

ASD import settings

The various import settings will become visible once you have selected something to import. There is a slight difference here between the ordinary binary-file import and the HALO text-file import. This is what you see for the former; the HALO will be discussed later in this section.



GPS

The **GPS** checkbox will be enabled if TSG found valid GPS info in at least some of the binary files. Turn it on and TSG will import GPS info into TSG scalars **Latitude**, **Longitude** and **Depth (m)** (or **Altitude**). If there is a binary file that does not have valid GPS info then its corresponding scalar values will be NULL.

Note If you have taken JPEG photos to accompany each spectrum then TSG can also extract GPS info from the photos (if your phone / camera put GPS info in them). You can do this in a separate step, after importing spectra. See the companion document "Importing Photos for Field and Laboratory Datasets".

De-step

Inter-detector steps are common, even when the instrument is well calibrated and operated properly. We recommend that you have this correction **on** unless your spectra are from a HALO. It is discussed in more detail later (page 10).

Smoothing

ASD spectra can be noisy on both the short- and long-wavelength sides because the overall instrument response *and* the strength of the illumination are both weaker at the sides. (And compared to a decent spectrometer lamp, sunlight is particularly weak at the long-wavelength side.) So it can be beneficial to do some selective smoothing.
There are three controls for smoothing:

1. A **list** for selecting the smoothing strength (**none**, **low**, **med**, **high**, **xtra**);
2. An "**up to**" field for the last wavelength of the "short" side (smoothing stops here);
3. A "**from**" field for the first wavelength of the "long" side (smoothing starts again here).

Select something other than **none** in the list to enable smoothing. Adjust the **up to** and **from** wavelengths to control how much of the spectrum is smoothed.
Note:

- TSG guesses a default smoothing strength based on the integration time of the first binary file it checks.
- TSG also guesses a default value for **from**. You might want to adjust this. In particular, if sunlight was the illumination source then you might try a (lower than usual) value of 2000 here.
- If you type **–** (just a minus) in either of these fields it means "don't smooth this side".

Inst.

Turn this checkbox on to import two items from each file's ASD header into TSG scalars. The instrument serial number will be imported to the **SerialNum** scalar, and integration count to **IntegCount**.

Sun

Spectra measured with sunlight illumination are very noisy in the 1400 nm region and *impossibly* noisy in the 1900 nm region. (Most sunlight in these regions is absorbed by water vapour in the air.) Some people prefer TSG to wipe out these regions in the spectrum and interpolate over them.
If you turn on the **Sun** checkbox then TSG will check these regions in each spectrum and interpolate over them if they are deemed to be too noisy.

Parse filenames

This list currently has options **None**, **HoleID & Depth**, and **SampleID**. It is for parsing items out of each ASD filename and importing the results into TSG scalars.

HoleID & Depth

This option's for when you use an ASD for manual **core or chip logging** and have taken care to record the hole-name and depth in each filename. TSG will extract these items out of each filename and import them to **HoleID** and **Depth (m)** scalars.
Currently only a straightforward arrangement is supported[1]. Depth follows straight after hole-name and the only control you have is to tell TSG how many characters are for depth. This is done using the **Last chars for depth** field.
e.g., Say one of your filenames is `KLM00200007.asd`. The drill-hole's name is "KLM002" and the depth is 7m. You would specify a value of **5** for "last chars for depth". (The file extension is ignored.)

[1] Additional arrangements may be supported on request. Email peter.mason@csiro.au

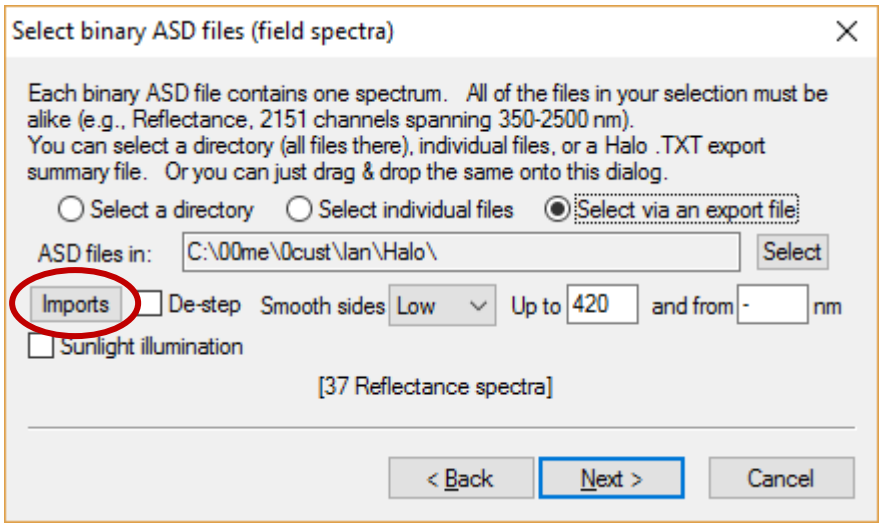
SampleID

This option will search for the last number in each filename and import it to a scalar called **SampleID**

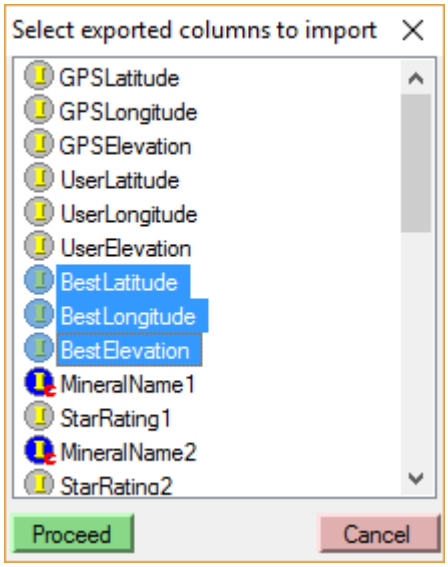
Once you're ready, click **Next** to move on to the next page.

FieldSpec HALO

Like other ASD instruments, the HALO produces one binary ASD file per spectrum and you can import its files as described above. However *it also includes one export summary file in the mix*. This is a text file that has one row per sample. A row includes the path+filename of the sample's binary ASD file, GPS values (where applicable), and the values of analysis scalars (e.g., mineral identification scalars) calculated by the HALO's built-in computer.
You can select the export file instead of selecting binary ASD files. If you do then the TSG import-settings page will look like this:



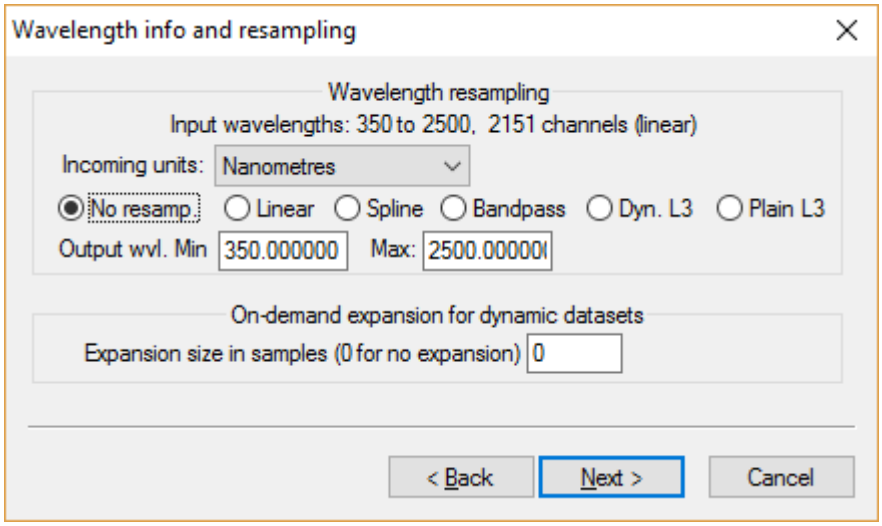
Note there is an **Imports** button where the GPS checkbox used to be. Click this button to get a sub-dialog for selecting the columns to import along with the spectra. It is a multiple-selection dialog – use <CTRL>click or <SHFT>click pairs to select more than one item.
During the import TSG will create a scalar for each column that you select. It checks the contents of each column to decide what sort of TSG scalar to create for the column: numeric (icon) or class (icon).



Aside from scalar imports, the HALO import works like the general ASD import (see above), only the selection of ASD binary files is taken care of by the summary file and de-stepping is not necessary.

Once you're ready, click **Next** to move on to the next page.

Wavelength info and resampling

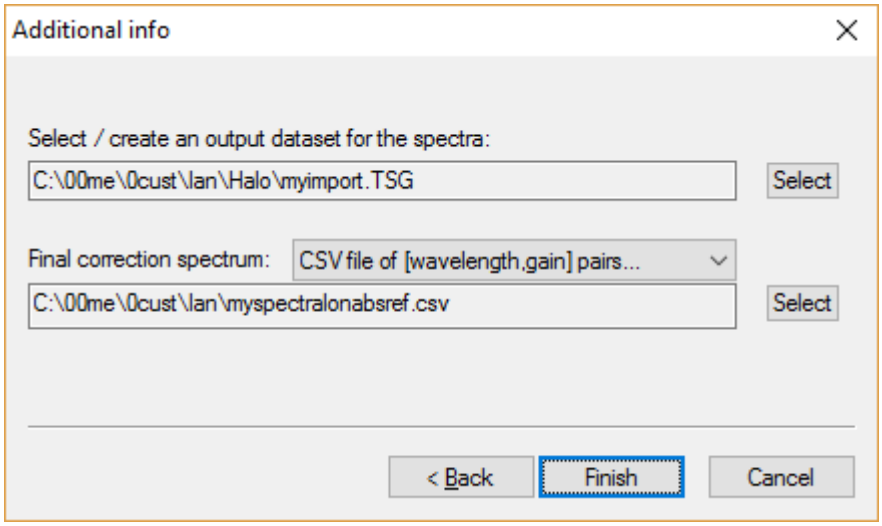


The Input wavelengths label shows the spectral range and number of channels of the incoming spectra. In the graphic above we see the standard spec for a Vis-NIR-SWIR ASD instrument, and can work out that the spectrum is sampled every 1 nm. ((2500-350) / (2151-1) = 1.) All ASD instruments deliver "linear" sampling, which means that the increment from one channel's wavelength to the next is constant.
If you like you can import a subset of the incoming spectral range and / or change the increment to something other than 1 nm (typically something bigger).

- To subset the incoming spectral range, enter a higher value in the **Min** field and / or a lower value in the **Max** field.
- To resample, e.g., to a coarser increment, first select a resampling radio button other than No resamp (e.g., **Linear** or the recommended **Plain L3**.) A third field labelled **Increment** will appear. Type in the increment that you would like.

The Expansion size in samples field is used in connection with dynamic datasets. In short, TSG allows you to add spectra to a dataset at a later time (after doing the first import). If you think that you will be doing this then you can enter a non-zero number here, to leave extra room and speed up the dynamic system when new spectra are added later.
This topic is covered in the companion document "**Dynamic Spectral Imports in TSG**".

Additional info



This is the last page of the import wizard.
TSG requires a filename for the dataset that it will create. (It does not come up with a filename automatically.) Click the top **Select** button to bring up a Windows file-selection dialog, which will let you choose a directory and type in a filename.

The other controls in this page are for selecting a **Final correction spectrum**. Most users will just leave this blank. In the advanced section below (page 9), there is some discussion about using this option to get absolute reflectance. It also has other uses. E.g., If you are measuring samples through the bottom of a glass petri dish and you have the dish's transmission spectrum, calculate the inverse[2] of it and use it here to remove the dish's "colour".

Click **Finish** to start the import. TSG will import the spectra, calculate standard results for them, and finally present you with the open dataset.

[2] 1 / (2*transmission), with the 2* because light is going there & back through the dish.

Advanced topics

ASD binary files

An ASD instrument gives you one binary file per spectrum. The filenames often have an `.ASD` extension but this is not a requirement – there can be any or no file extension. The file format has evolved over the years and TSG supports files from the early 2000s up to the current version (8).

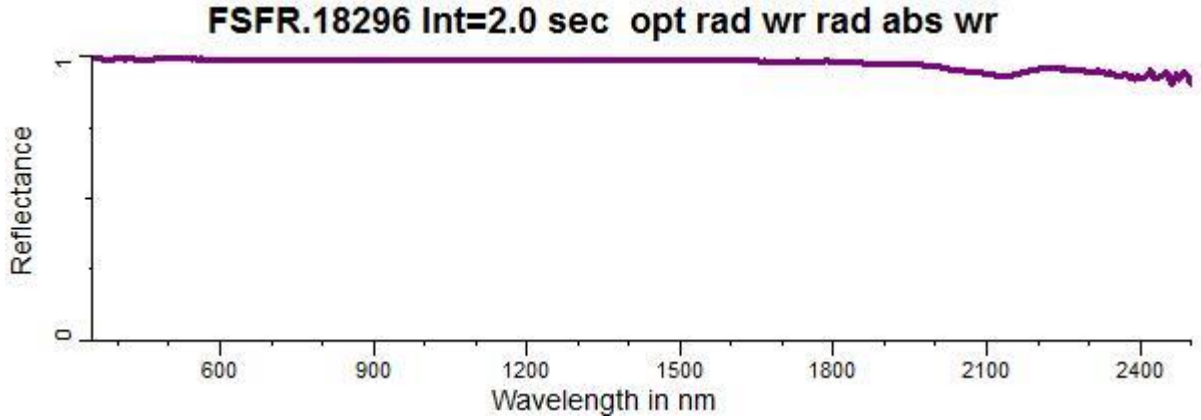
The normal measurement in geological applications is "reflectance" but there are variants. I have seen the following (with approximate[3] sizes for 2151-channel spectra spanning [350, 2500] nm in steps of 1 nm):

Type	Measurement	What's in the file	File size
A	Reflectance	Single-precision reflectance spectrum, sample	9KB
B	Reflectance	Double-precision DN spectrum, sample Double-precision DN spectrum, spectralon	35KB
C	AbsRef	Double-precision DN spectrum, sample Double-precision DN spectrum, spectralon Double-precision AbsRef spectrum, spectralon	52KB
D	Radiance	Double-precision DN spectrum, sample Double-precision AbsRef spectrum, spectralon (lab) Double-precision spectral irradiance, lamp Double-precision DN spectrum, spectralon (lab)	85KB

Relative reflectance ("Reflectance")

Given type A or B, TSG will import relative reflectance. This is reflectance relative to Spectralon.

Spectralon is a very good reflectance standard to use in VNIR-SWIR work. It scatters light quite evenly and has a very bright and almost-flat spectrum over the [350, 2500] nm range. But it is not *perfectly* bright or flat. Spectralon absolute reflectance varies slightly from case to case. Here's a typical example:



This one is about 0.991 (99.1%) at its brightest and decreases with longer wavelengths. It has a characteristic Teflon absorption at around 2136 nm, where it goes down to about 0.931.

[3] Although these are binary files, size may vary due to the possible inclusion of modelling data and (in newer files) an audit log.

In many cases relative reflectance is good enough, especially when working with spectra only measured by one instrument. However for the discerning client[4] it can be a little disappointing. Every spectrum bears the spectral "watermark" of the Spectralon standard that was used. E.g., Sample spectra that ought to be flat around 2136 nm will have a little mound there instead.

Absolute reflectance ("AbsRef")

Given type C, TSG will import absolute reflectance. This is reflectance relative to an ideal (100%, flat) reflectance standard. It is approximated by multiplying (channel by channel) relative reflectance with the Spectralon's absolute reflectance.
If you *have* type-C files then most likely you know what you're doing and are probably getting a little amused at this point. If you have type A or B then TSG may still be able to import AbsRef for you…

D.I.Y. AbsRef

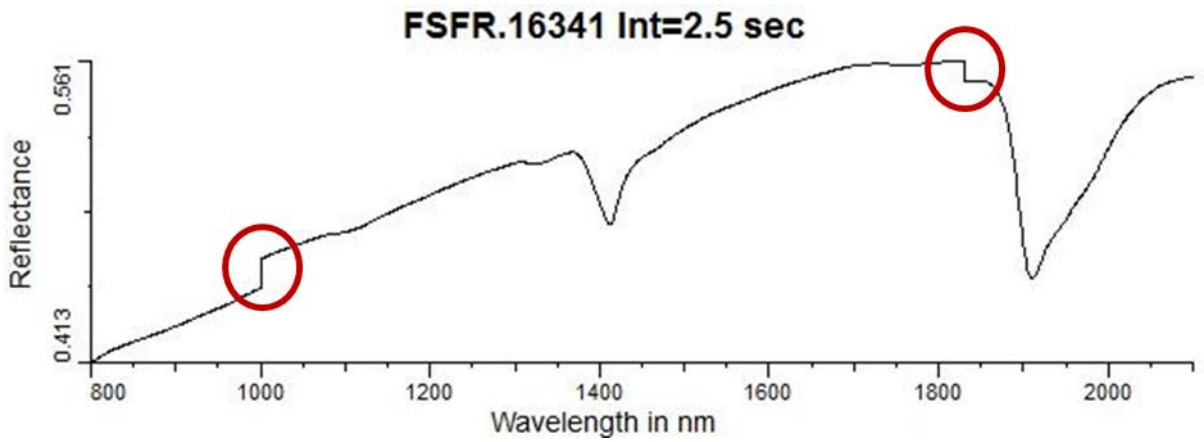
You'll need the absolute reflectance spectrum of your piece of Spectralon. (It should be *your* piece of Spectralon, ideally, not just any piece. Also, *you should consider smoothing the spectrum*. The ones I've seen are quite noisy.) The instrument supplier should be able to provide it to you as it is a reference measurement that should accompany the Spectralon.
TSG wants this spectrum in a CSV (comma-separated values) file with two columns. The first column should be titled `nanometres` and the second `absref`. This spectrum does not have to be sampled like the ASD's but the ASD's spectral range must be covered (normally 350 to 2500 nm).
Once you have this CSV sorted out, you can give it to TSG in the last stage of the Import wizard. (See page 6 above.) TSG will then do the conversion to absolute reflectance during the import.

Radiance

Given type D, TSG will import radiance in units of `w / (m² * sr * nm)`.
Radiance spectra of rocks are dominated by the illumination spectrum (normally sunlight). That isn't everyone's cup of tea, and TSG's reflectance-based unmixing won't make any sense of it at all. Nonetheless radiance can be useful for specific tasks. (e.g., I have heard of it being used for the cal / val work with airborne spectrometers.)
Note that TSG does **not** provide the option to import reflectance from a radiance file. Although there is a "Spectralon DN" spectrum within the file, it is not measured under the same conditions as the "Sample DN" spectrum and may even be a different piece of Spectralon to the one that you use in field work. Therefore it can't be handled like the one within a type-B file. (This Spectralon is measured under special conditions in the lab-based instrument calibration.)

[4] Or generally when working with spectra from various sources, or building a reference library for others to use.

De-stepping



Although we commonly call an ASD instrument "a spectrometer", there are actually *three* spectrometers within a full-spectrum (350 to 2500 nm) instrument. The "splice" points between the spectrometers are commonly at 1000 nm and 1830 nm, and it is common to find steps in reflectance spectra at these points.

These steps *can* be caused by instrument mis-calibration (e.g., stale dark-current correction), but the most common cause is that the detectors each "see" a slightly different patch of surface. This is the case even when a fibre-optic bundle is used in the instrument's fore-optics. Whereas, there normally isn't any *true* correction. Each spectrometer is just telling you what it sees, so to speak. Nonetheless people can't be having with the steps and they must be ironed out.

Turn on TSG's **De-step** checkbox (see page 3) to have the steps corrected. They will be corrected at the splice points recorded for each spectrum[5].

Note I haven't seen steps in HALO specta. I suspect it is due to a combination of specialised fore-optics and on-board step correction. You should not need to use TSG's step correction when importing these spectra.

[5] TSG will guess where the splice points are if given vintage-format binary files that do not contain records of the splice points.