

Excel spectroscopic tools to visualize, analyze and manipulate remotely sensed data of planetary bodies.

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1. Introduction

In the context of the future and present missions, tools and techniques are needed to analyze new hyperspectral data of the surfaces of various bodies in the Solar System. Here, we present an interactive Excel tool that provides a quick and easy way to visualize and manipulate laboratory spectroscopic data. The choice of an interactive Microsoft Excel environment was done to make the visualization and use of the manipulated data as simple and fast as possible by a large audience. Our tool works under three different operating systems: Microsoft Windows, MacOSX, and Linux using the opensource project Wine.

2. Overview

Our tool is meant to visualize and analyze the data of an Excel archive. This Excel archive is organized in two sheets. The first sheet contains different columns: *Sample name*, *Reference*, *DOI*, *Spectral range*, *Measured quantity* (e.g., reflectance, absorbance, transmittance, optical constants, etc.), *Lab/instrument*, *Temperature*, *Grain size*, and *Comments*. The second sheet contains the instrumental response of a number of spectrometers organized as follows: instrument names in the first row, and for each instrument two columns: the wavelength set and the spectral resolution (i.e., the full width at half maximum of each spectral channel). In this sheet, one can put additional instrumental responses or update a given instrumental response if necessary.

Each row of the Excel archive represents a chemical compound for which laboratory measurements are available. When multiple temperatures of the measurements of a given sample are also available, a hyperlink under the *Temperature* column directly opens the related ASCII file. This allows a quick view and comparison of the spectra. To this aim, we prepared spectral tools written in Visual Basic for Application (VBA). These tools are easily accessible by right-clicking on specific cells in the Excel spreadsheet, and need no installation of separate add-ons (Figure 1).

The tools are the following:

The *Visualize* tool, which permits the quick-look of the spectral profile as found in the database.

The *Convolve* tool, which convolves the original spectral profile to a specific instrumental function available in a separate sheet of the Excel database.

The *Retrieve_k__Shkuratov_1999* tool, which calculates the absorption coefficient k starting from a reflectance spectrum, and making assumptions about the refractive index n , the porosity, and the grain size of the sample (Shkuratov et al., 1999). Error checks make sure this tool is used only when proper condition apply (for example, if the user attempts to derive k from absorbance, a warning pops up).

All of the three tools allow the user to save the result as a *.txt file or to plot the spectrum and save it as a *.png file.

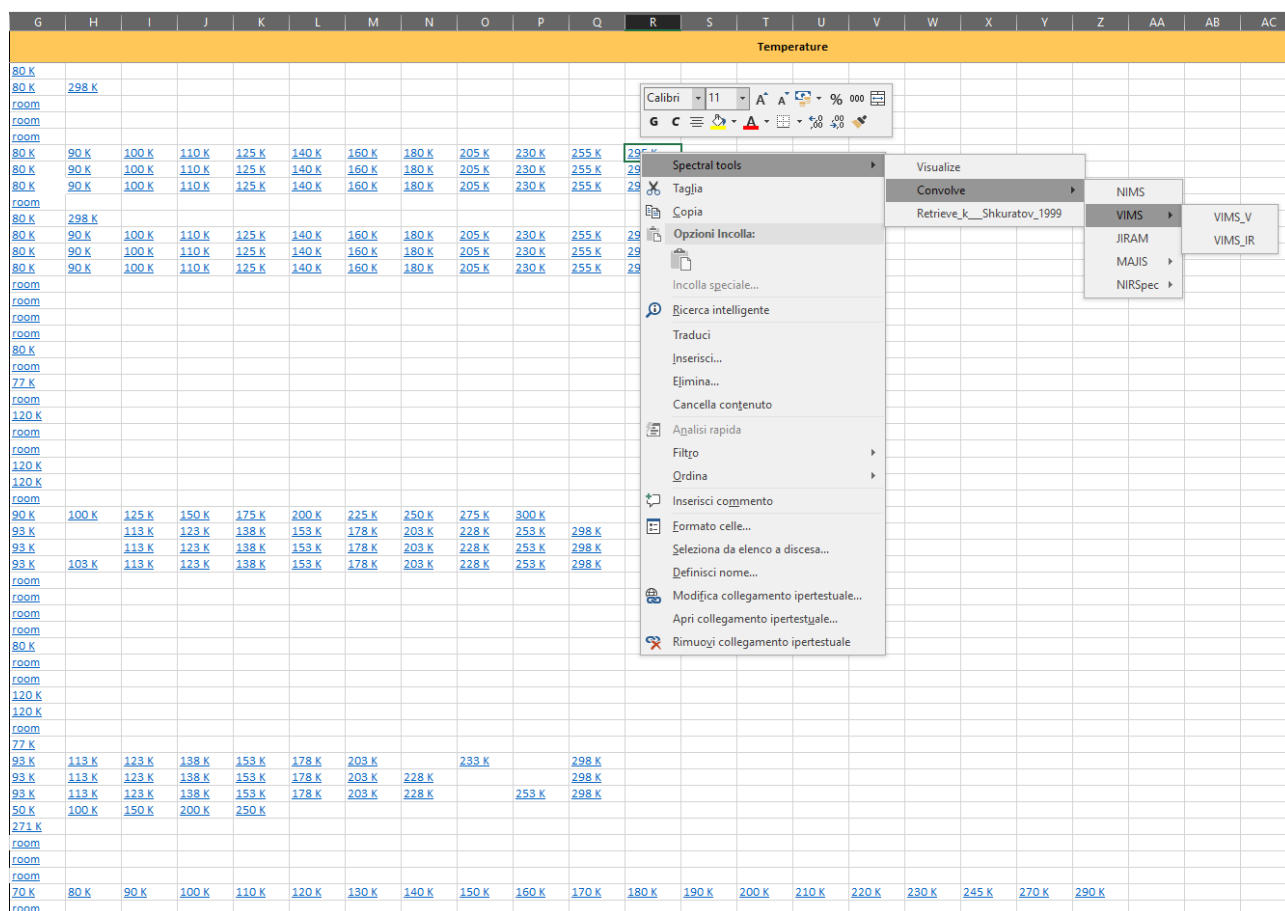


Figure 1. The right click menu Spectral Tools created with VBA Excel.

3. Methods

These tools are Excel macros written in the Visual Basic for Applications (VBA) language. Any user opening this spreadsheet for the first time will need to authorize the use of macros within the Excel environment.

The first tool, *Visualize*, is meant to just display the data as they are in the archive. In this case, the user shall place the mouse on the cell corresponding to a specific chemical compound and temperature value (if multiple temperature values are available). By right-clicking on the cell, a new menu appears among the various existent entries, the Spectral tools menu.

By choosing the Visualize entry (Figure 1), a new Excel Window opens (Figure 2). The new window is the ASCII file visualized in Excel format with the relative plot.

The second tool, *Convolve*, applies a spectral convolution to the laboratory data present in the archive. This is crucial whenever a direct comparison between remotely sensed spectra (e.g., acquired by an imaging spectrometer onboard a spacecraft or by JWST/NIRSpec) and laboratory spectra is needed, or to perform spectral unmixing based on a number of spectral endmembers.

In this tool, the user must first place the mouse on a specific cell representing a given chemical compound and temperature, then choose the Convolve menu by right-clicking the mouse. There the user can choose between several imaging spectrometers

relevant for the exploration of the outer Solar System plus JWST/NIRSpec (Figure 1), and among specific channels (e.g., VIS or IR) if the instrument has more than one.

After the desired option is selected, the program performs a convolution of the laboratory spectrum to the wavelength set and spectral resolution of the instrument (as found in the second sheet of the main Excel archive). Once the convolution is completed, the result is displayed in a new window. Figure 3 shows an example of what can be obtained.

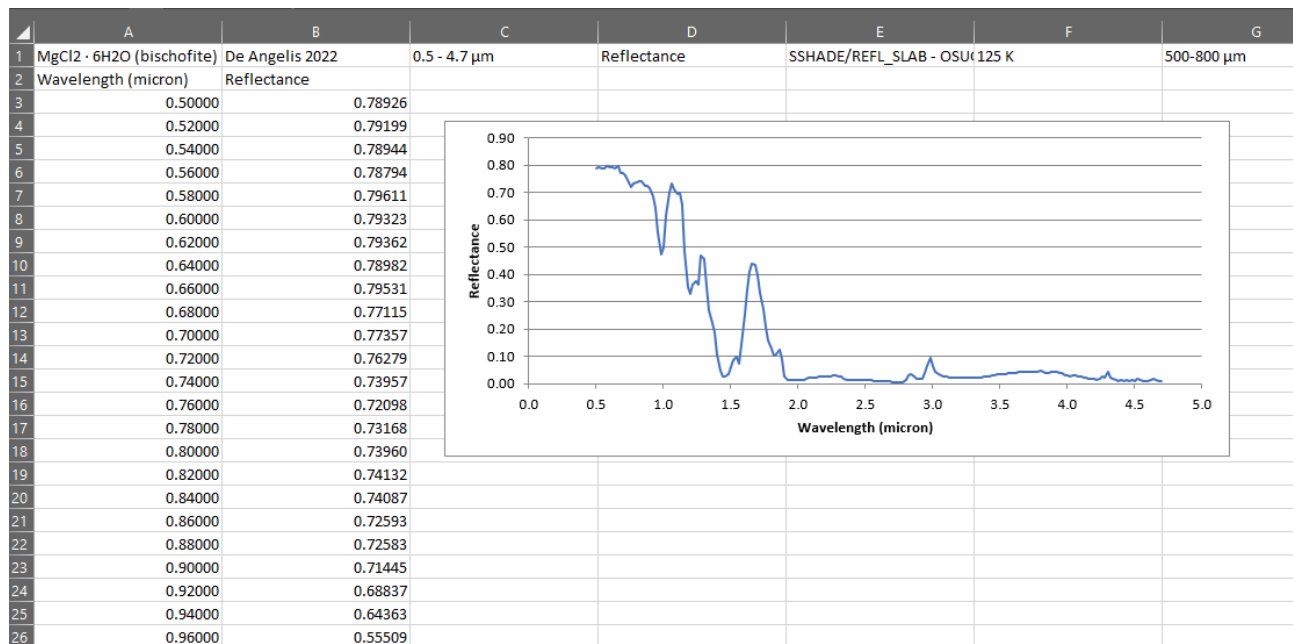


Figure 2. An example of the Visualize output.

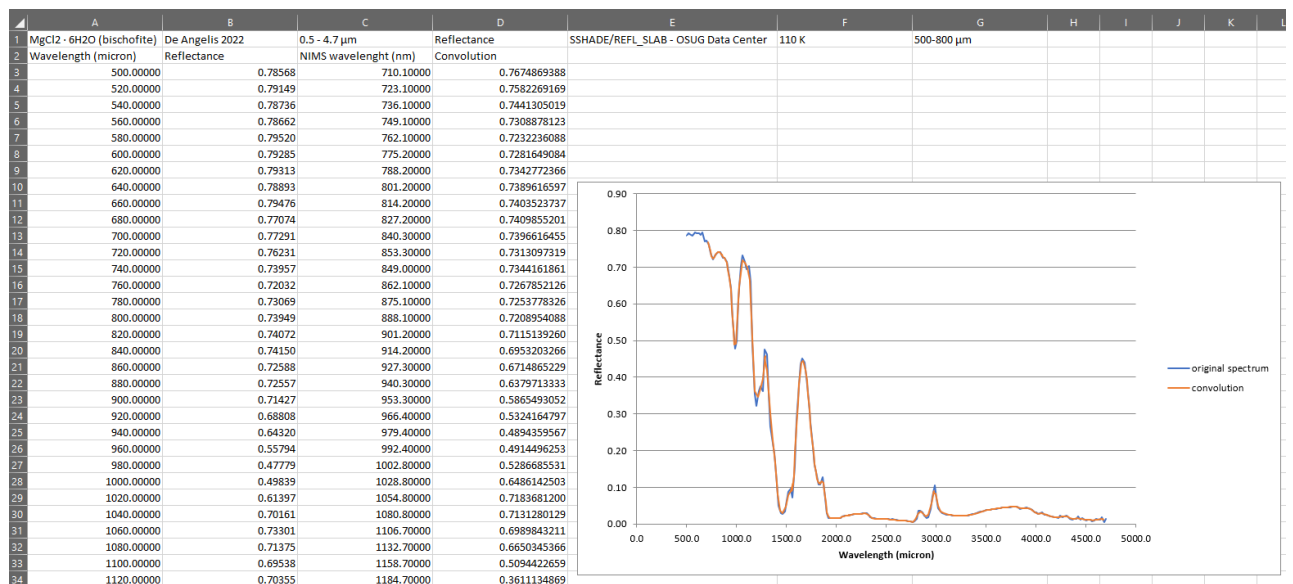


Figure 3. An example of the Convolve output.

The third and last tool derives the absorption coefficient k of a chemical compound with the semi-empirical approach of Shkuratov et al. (1999), starting from the knowledge of the reflectance spectrum and making assumptions on the refractive index n , the porosity, and the grain size of the sample.

In this case, the user must choose the *Retrieve_k___Shkuratov_1999* option in the right-click menu. This will open an interactive Excel window (Figure 4). There, the user can specify the grain size (in microns), the porosity, and the scalar value of the refractive index (assumed to be constant throughout the spectral range) following the red arrow, and then pressing the button “Calculate k ” on the right.

	A	B	C	D	E	F	G	H
1	INSERT INPUT VALUES FOR THE ALGORITHM:							
2								
3		Grain Size (micron)	Porosity (between 0 and 1)	Real refractive index (scalar quantity)				Calculate k
4								
5	Values -->							
6								
7								
8				OR go back to the main Excel catalogue and select the cell corresponding to the desired n profile (column G). Then push THIS button.				
9								
10								
11								
12								
13				OR select an external n file				
14								
15								
16								
17								
18								

Figure 4. This new calculation sheet opens after clicking *Retrieve_k___Shkuratov_1999*.

Two other buttons offer an alternative to using a scalar value for the refractive index n . The first button allows the user to choose a refractive index file available in the archive, while the second button opens and reads an external n ASCII file (provided that it has the same formatting used for all the ASCII files in our archive). In the first case, the user must go back to the main Excel catalogue and place the mouse on the cell corresponding to the desired n profile (column G). Then the user must switch to the interactive windows and push the button named: “OR go back to the main Excel catalogue and select the cell corresponding to the desired n profile (column G)”. In the second case, a “Open Folder and Select File” window pops up, allowing the user to choose an external ASCII file.

In both cases, the selected refractive index spectrum is first interpolated to the same wavelength set of the laboratory data, then the absorption coefficient k is derived using the refractive index spectrum instead of a scalar value of n in the Shkuratov approach. In all cases, the k value is tabulated next to the n column (Figure 5). In the second sheet (Figure 6), a dialog box will appear saying: “ k retrieval is completed. Do you want to calculate k again with other parameters? If you choose no and you want to calculate k later, cancel the n and k column in the first sheet and insert new parameters in this second sheet.”

	A	B	C	D	E	F	G	H	I	J	K
1	CaCO3 (calcium carbonate)	ReLab Database	0.3 - 2.8 μm	Reflectance	Brown Un room	0 - 45 μm	sample path name: SF-BFJ-002/C1SF02				
2	Wavelength(micron)	Reflectance	n	k							
3	0.3	0.82956	1.72139032	1.2097476E-06							
4	0.305	0.81655	1.718164862	1.4496101E-06							
5	0.31	0.825	1.715338939	1.3298333E-06							
6	0.315	0.82604	1.712513017	1.3359526E-06							
7	0.32	0.82441	1.709687094	1.3877324E-06							
8	0.325	0.82907	1.707202061	1.3303548E-06							
9	0.33	0.82988	1.704963879	1.3385956E-06							

Figure 5. An example of the *Retrieve_k*___Shkuratov_1999 output in the first sheet.

After having obtained the absorption coefficient k , new buttons will appear, which will allow the user to convolve the spectral profile of k with some specific instrumental profiles among those available (imaging spectrometers and JWST/NIRSpec), without the need to save an ASCII file and put it in the database.

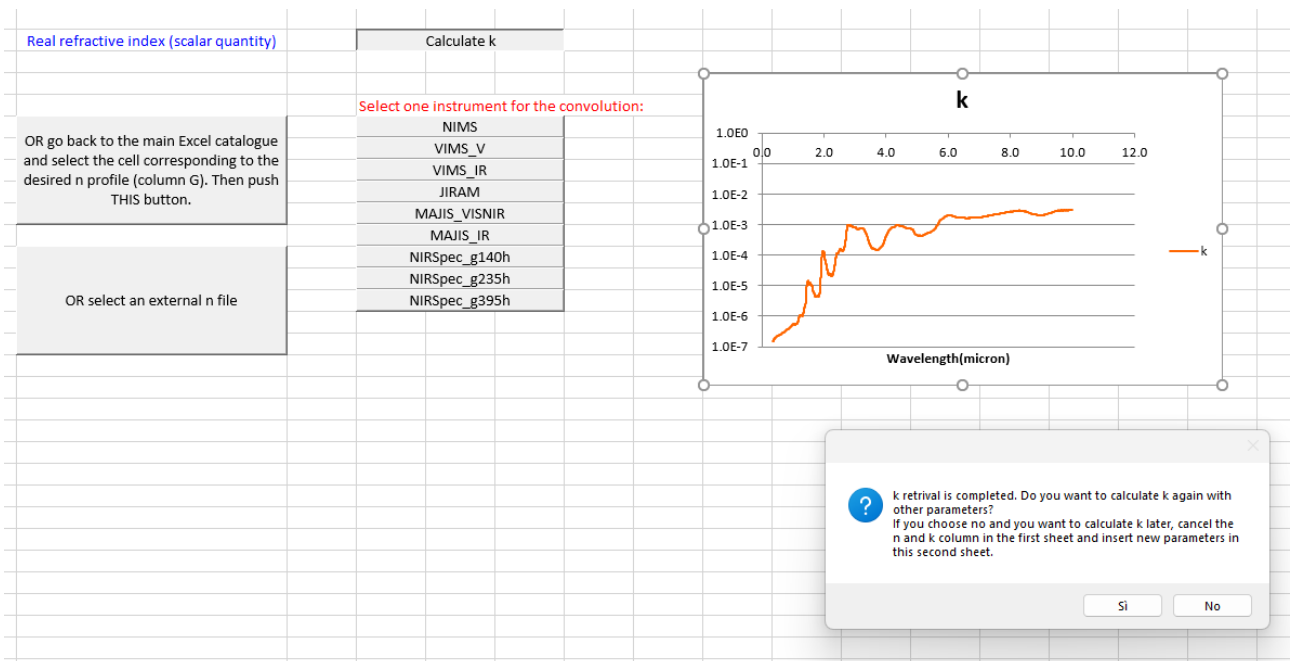


Figure 6. An example of the *Retrieve_k*___Shkuratov_1999 output, second sheet.

At the end of these computations, that is after Visualize, Convolve and Retrieve, a new menu appears in the right-click menu on the output sheet: "Save calculation" (Figure 7). It gives the user the possibility to save the data as an ASCII file or as a plot in the *.png file format. When the user selects an option, a folder window opens, allowing one to save the file in the desired local directory.

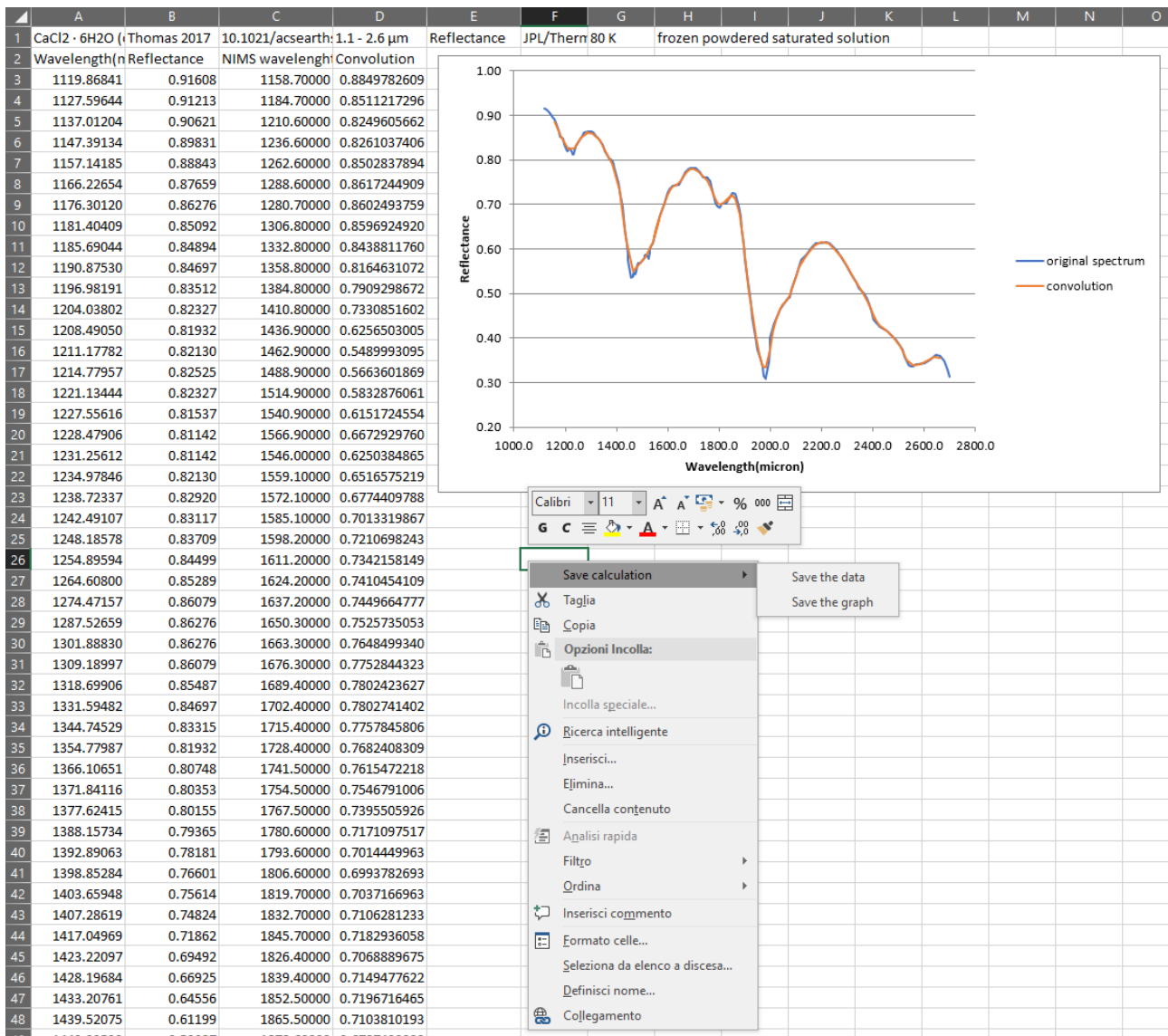


Figure 7. Once the computation is done, the save options appear in the menu in the new Excel file.

4. Installation

To use this Excel archive there is no need to install separate add-ons. The package is self-consistent and provided in the form of an Excel sheet with macros. It includes examples in the first and second Excel sheets on how to set up the data.

The tools are ready to be distributed and they are available sending an email to alessandra.cofano@inaf.it. When used for publications, it is kindly requested to cite its DOI.

5. Conclusions

These spectroscopic tools in Excel provide a quick and easy way to manipulate data. To validate the outputs, the results from the convolution tool were compared with a convolution tool existing in the Harris ENVI software, while the derivation of k using

the Skhuratov approach was double-checked with other studies such as Roush et al. (2007).

6. References

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