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AVASOFT 8

SOFTWARE

Operation and Installation Manual

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AvaSoft

Version 8.12

User's Manual

November 2020

Table of Contents

1 AvaSoft Installation

Before you connect the AvaSpec spectrometer to the USB port of your computer, you need to install the AvaSoft software first.

AvaSoft version 8 is a 32-bit application that can be installed on the following operating systems:

- 32-bit Windows Windows 7/Windows 8/Windows 10
- 64-bit Windows Windows 7/Windows 8/Windows 10

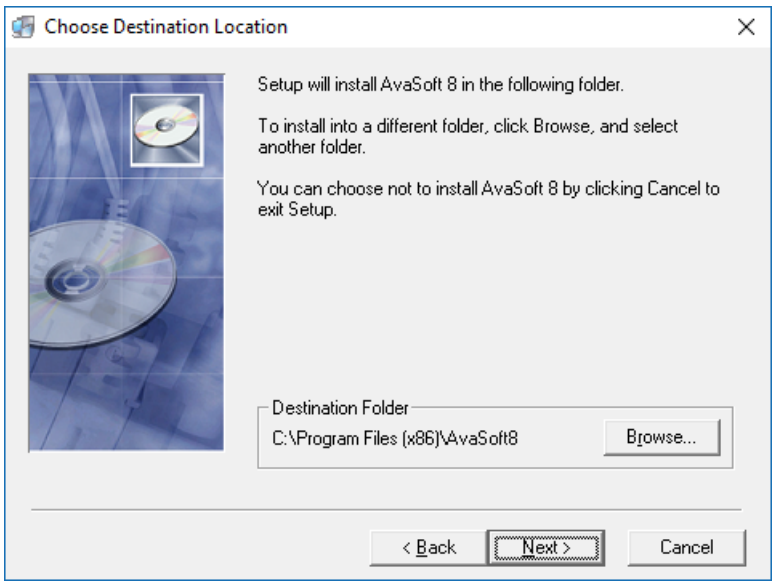
1.1 Installation Program

To install your AvaSpec spectrometer please go to *www.avantes.com/gettingstarted*
Here you can find all the information you need. For installing the AvaSoft software click on the software icon or go to *https://www.avantes.com/support/software*

Please note that you need to register and login to install the software

AvaSoft 8 can be installed for any of the AvaSpec-USB2, AvaSpec-Mini and AvaSpec-EVO spectrometers.

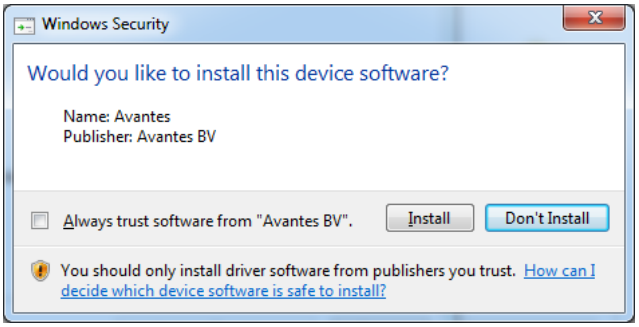
Installation Dialogs
The setup program will check the system configuration of the computer. If no problems are detected, the first dialog is the “Welcome” dialog with some general information. In the next dialog, the destination directory for the AvaSoft software can be changed. The default destination directory is C:\Program Files (x86)\AvaSoft8. If you want to install the software to a different directory, click the Browse button, select a new directory and click OK. If the specified directory does not exist, it will be created.



After this, the “Start Installation” dialog is shown. After clicking the “Next” button, the installation program starts installing files.

During the installation, the install program will check if the WinUSB driver has been installed on the PC. In some earlier AvaSoft versions (and only on 32bit versions of Windows), an Avantes kernel USB driver was installed for AS5216 spectrometers.

The install program will launch the Device Driver Installation Wizard to install the WinUSB driver. The driver package has been signed by Avantes. If asked by your operating system, please select the ‘Install’ button to install the WinUSB driver.



The last dialog in the Device Driver Installation Wizard displays whether the WinUSB driver has been installed correctly. If you experience problems here, please refer to Appendix A, which describes some special cases.

After all files have been installed, the “Installation Complete” dialog shows up. Click Finish.

Connecting the hardware
Connect the USB connector to a USB port on your computer with the supplied USB cable. Windows will install the driver silently, in general without displaying any dialogs.

1.2 Launching the Software

AvaSoft can be started from the Windows Start Menu. Under ‘Start’, ‘All Programs’, a group “AVANTES Software” has been added, which has an entry for the AvaSoft 8 program and an entry for the AvaSoft 8 helpfile.

There will also be an AvaSoft 8 icon on the desktop that you can click.

After starting the AvaSoft 8 software, a welcome window will be displayed that will show the spectrometers that are connected.

The AvaSoft 8 windows will be displayed next. Refer to section 4 for a description of the different windows. A “Quick Start” can be found in section 2 if you want to start measuring immediately. Depending on the AvaSoft version (Basic or Full) and the extra add-on modules that were ordered for your spectrometer, more applications are available in AvaSoft 8, which are described in sections 4.6 to 4.11.

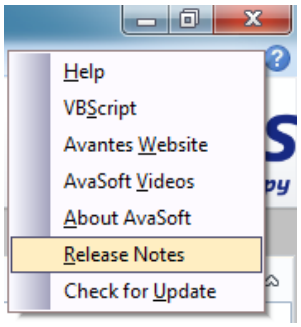
2 Quick Start: Measuring and Saving a Spectrum

1. After starting AvaSoft, the Start button in the upper left corner of the screen needs to be clicked to start measuring. The F2 function key may be used as well to start (or stop) a measurement.
2. Connect a fiber or probe to the light source and to the spectrometer input port(s) and set up the experiment for taking a reference spectrum.
3. Optimal smoothing is preset and stored on board in the EEPROM.
4. Now turn on the light source. Usually some sort of spectrum may be seen on the screen, but it is possible that too much or too little light reaches the spectrometer at the present data collection settings. Too much light means that, over a certain wavelength range, the signal is saturated shown as a straight line at the maximum counts and the appearance of the label "saturated" in the spectrometer window of the channel. This can usually be solved by a shorter integration time. The integration time can be changed in the spectrometer window (by pressing the cogwheel icon, by directly changing the ms value, or by pressing the Auto-configure Integration time button. Try to adjust the integration time, such that the maximum count over the wavelength range is around 90% of the full ADC scale (59000 counts for a 16bit ADC). When at minimum integration time the signal is still too high, an attenuator, a neutral density filter or fibers with a smaller diameter may be used. When not enough light reaches the spectrometer, likewise a longer integration time should be entered.
5. When a good spectrum is displayed, turn off the light source.
6. Now save the Dark data. This can be done by clicking the dark bulb icon in the spectrometer window, or the one on the left top of the screen with the mouse. Always use Save Dark after the integration time has been changed.
7. Turn on the light source again. Save the present spectrum as a reference by clicking the bright bulb icon (next to the dark one). Always use Save Reference after the integration time has been changed. Now the measure mode can be changed to e.g. Absorbance (A button) or Transmittance (T button). To have a better look at the amplitude versus wavelength, the Assign Cursor button can be clicked in the Tools menu. A vertical line is then displayed in the graph. If the mouse cursor is placed nearby this line, the shape of the mouse cursor changes from an arrow to a 'splitter' shape. If this shape is displayed, the left mouse button can be used to drag (keep left mouse button down) the line with the mouse towards a new position. Moving this line shows the corresponding values of wavelength and amplitude in the status line of the screen. By clicking the stop button (or the F2 key), the data acquisition is stopped and the last acquired spectrum is shown in static mode. The data acquisition can be started again by clicking the same button, which now displays 'Start', or the F2 key.
8. To save the spectrum (in the mode chosen before), choose 'File'-'Save' from the menu.
9. To improve the Signal/Noise ratio, a number of spectra may be averaged. To do this, the value in the spectrometer window (below the integration time) can be increased. The new value will take effect when you press the 'Set' button.

3 Differences from Earlier Versions of AvaSoft

AvaSoft8 represents a major change when comparing it to earlier versions of AvaSoft; AvaSoft7. The software was completely rewritten and made much more modular, resulting in better stability and maintainability, essential for a program of this complexity.

- The look and feel of the software was modernized, using Office like ribbons and buttons.
- You can open new windows at will and view them either docked or as separate windows. This means you can now use bigger or multiple screens much more effectively.
- The limit of 8 spectrometers was removed.
- The limit of 8 time series was removed.
- Separation of measurement screens and spectrometer setup screens.
- You can now open more windows for the same channel, viewing multiple measurement modes at the same time.
- The number of files saved is substantially lowered. Multiple channels can be saved in a single file and StoreToRam/3D sessions are saved in a single file.
- Better management of experiments and of the data file directories on your PC.
- Several measurement modes were added, such as a separate Scope minus Dark mode, separate Reflectance and Transmittance modes and separate Absolute and Relative Irradiance modes.
- A logarithmic scale was added.
- A visible color spectrum scale was added.



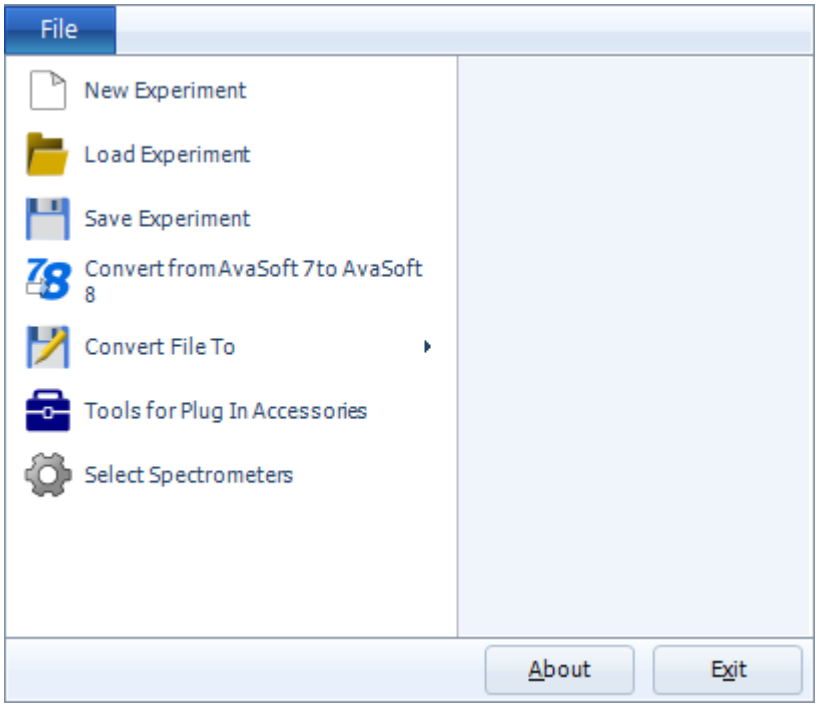
The release notes for AvaSoft8 versions can be found by clicking the ‘question mark’ button in the upper right corner, followed by selecting the Release Notes menu option.

4 The AvaSoft Windows

AvaSoft 8 has a multiple document interface structure. The main program consists of the top ribbon, the left side Experiment window and the left side Spectrometer windows.

The largest part of the screen consists of the client windows, a variable number of which can be opened by the user. With these client windows, the different applications are opened. Some of these applications are always present, like the Spectrum, Spectrum3D and TimeSeries applications. Others, like the Chemometry, Color, or Irradiance applications, are installed later, as a plug-in application. The client windows can be undocked from the main window and positioned on other parts of the screen, even outside of the main window.

4.1 Main window

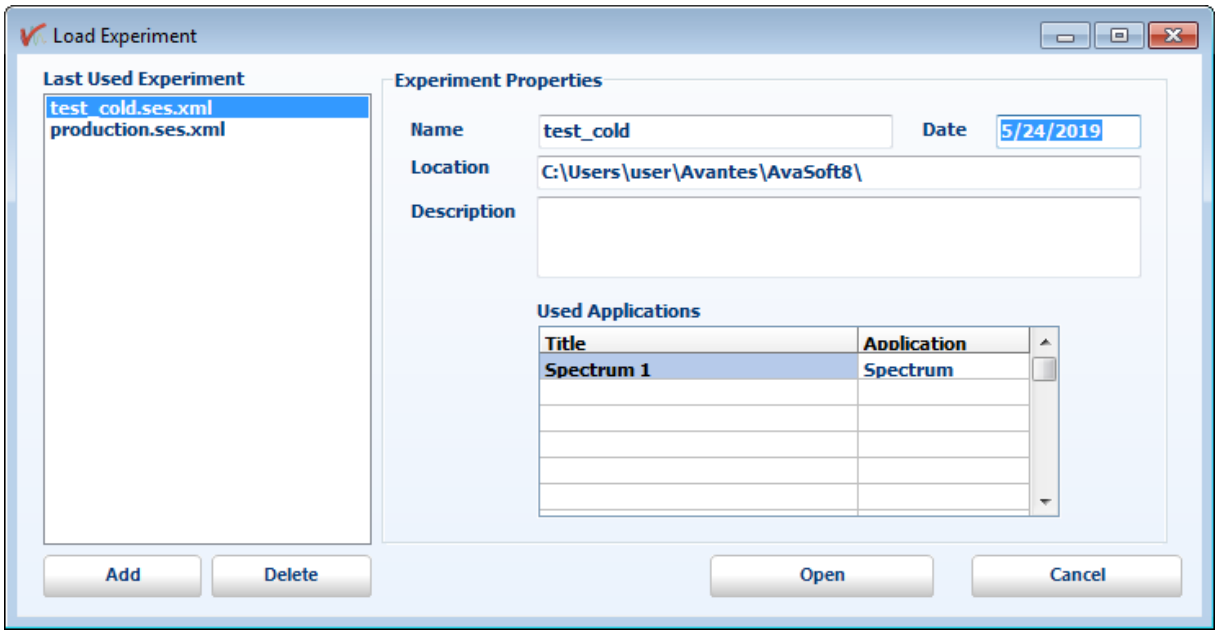


4.1.1 'File' tab, 'New Experiment' Menu Option

Allows you to start a new experiment.

4.1.2 'File' tab, 'Load Experiment' Menu Option

Loads the setup data for a session.

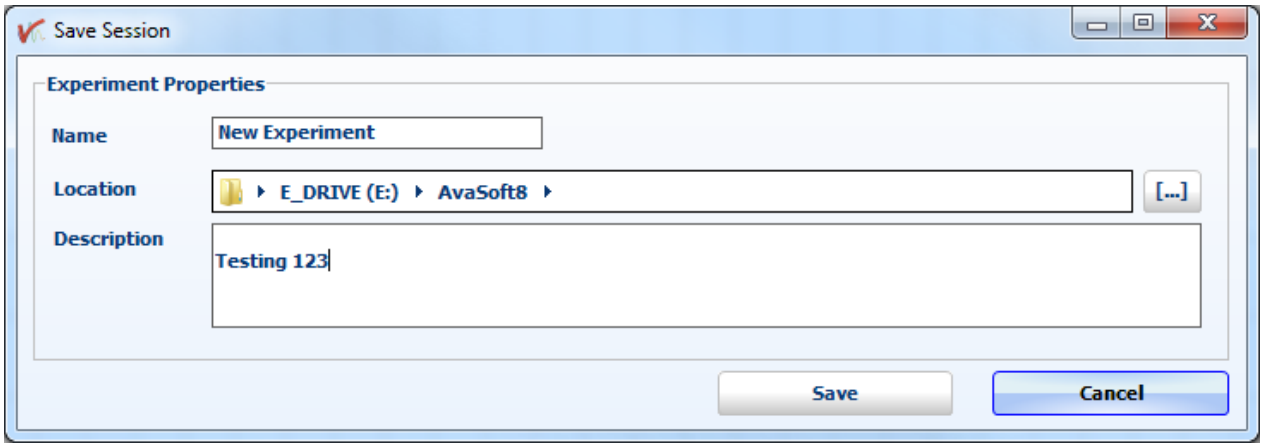


Doubleclick on the session you want to open, or select the session you want and click the 'Open' button.

You can add (an)other session file(s) to the list by clicking the 'Add Experiment' button and selecting the corresponding file(s) on disk.
Clicking the "Delete" button will remove the session from the list and will raise a question if the experiment file itself should be removed too.

4.1.3 'File' tab, 'Save Experiment' Menu Option

Saves the setup data for the current session.



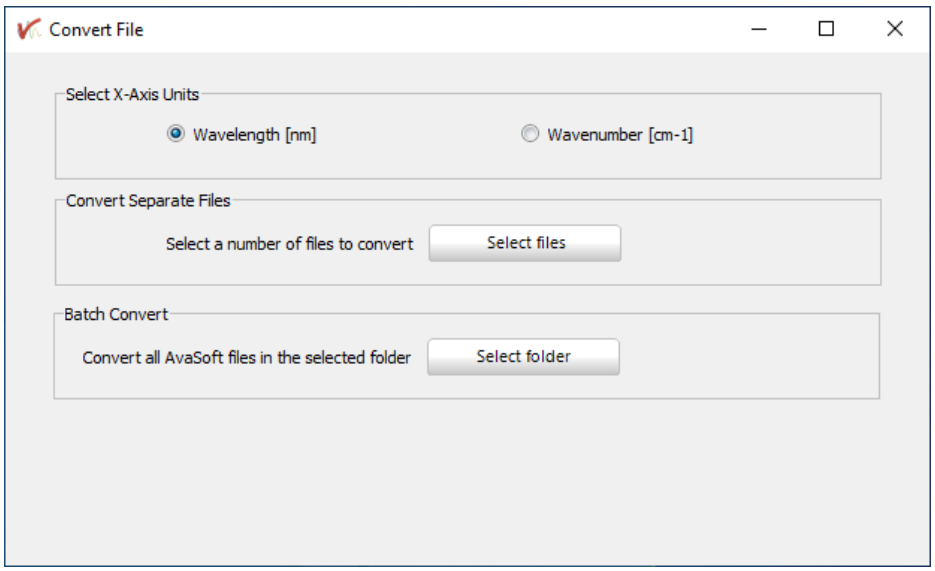
The current experiment setup will be saved to disk. Enter a session name, the directory on disk where the file will be saved and a description. Next press the 'Save' button.

4.1.4 'File' tab, 'Convert from AvaSoft 7 to AvaSoft 8' Menu Option

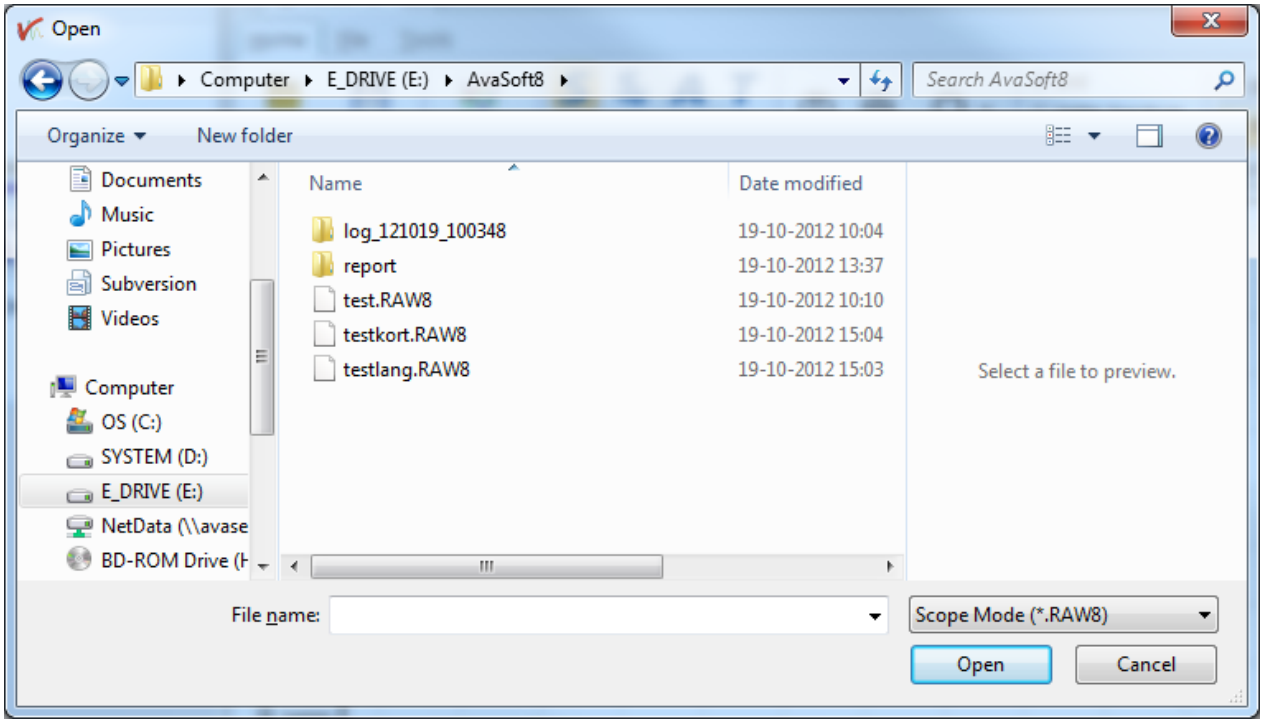
This selection starts a batch converter for AvaSoft 7 files. Note that you can also open AvaSoft 7 files in the Spectrum application, described in section 4.4.

4.1.5 'File' tab, 'Convert File To ASCII/Excel/JCAMP/GRAMS' Menu Option

This option allows you to convert files that were saved earlier to different formats. If you select 'To ASCII', you can first select the x-axis units, and whether you want to convert separately selected files, or all files in a selected subdirectory.



Next, a window shows all files in the current measure mode. In the example below, the measure mode is 'Scope Mode', so the extension of the earlier saved spectra is *.RAW8.



To select graphic files that were saved in another measure mode, e.g. absorbance, click  behind the Mode display, and pick the desired measure mode.

To select graphic files from another folder or drive, click  behind the current folder name. Selecting multiple filenames can be realized by using the CTRL or SHIFT key in combination with the mouse. If the CTRL key is pressed, all the files that are clicked by the mouse will be selected for conversion. If the SHIFT key is pressed, all the files in between two clicked files will be selected for conversion. Select the name of the file(s) to be converted to ASCII and click the Open button. To leave this dialog without converting files, click the Cancel button.

Extensions of binary files:

- RAW8 Scope Mode
- RWD8 Scope Corrected for Dark Mode
- ABS8 Absorbance Mode
- TRM8 Transmittance Mode
- RFL8 Reflectance Mode
- IRR8 Absolute Irradiance Mode
- RIR8 Relative Irradiance Mode
- RMN8 Raman Scope Mode
- RMD8 Raman Scope Corrected for Dark Mode

Two or more channels in a merge group can be stored in file with an extension that adds an ‘x’ character. For example the extension RAW8x is used for a merge group in scope mode. Please note that only the separate spectra are stored in this file, and not a merged spectrum. A continuous merged spectrum can afterwards be obtained from a RAW8x file, and saved e.g. in ASCII format.
All converted text files start with a header with information for the graphic file that has been converted. The header shows:

- the comment line
- the integration time
- the number of scans that has been averaged
- the number of pixels used for smoothing
- the serial number of the spectrometer that was used to save the data

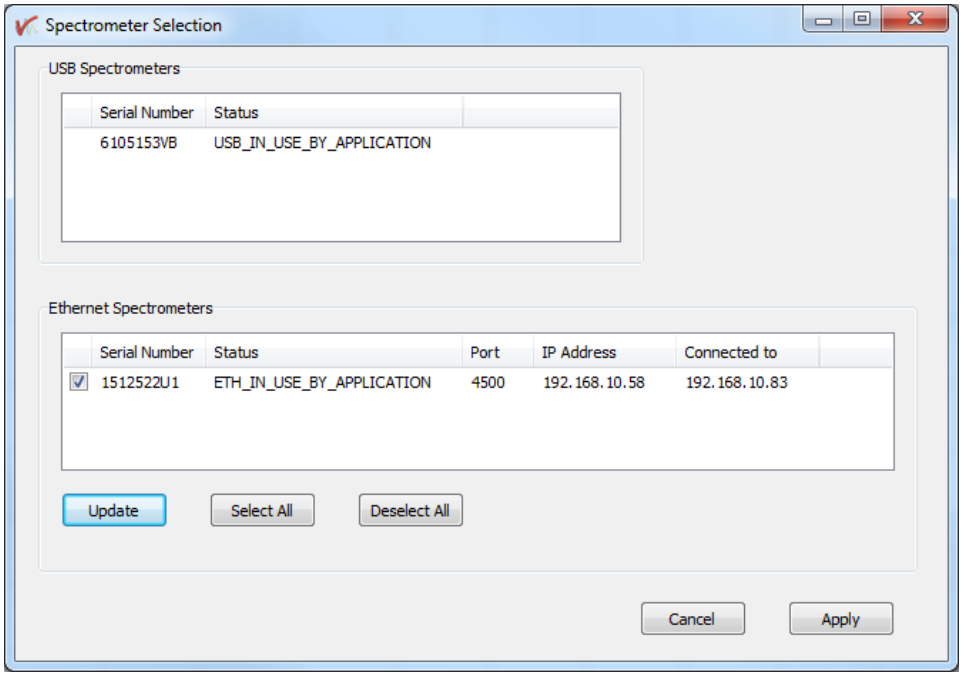
The data in a converted scope mode file is given in four columns. The first column gives the wavelength in nanometers, the second one the scope data, the third the dark data and the fourth the reference data.
The data in the converted files for all other modes is presented in five columns. The fifth column gives the calculated value that the mode offers.

4.1.6 ‘File’ tab, ‘Tools for Plug In accessories’ Menu Option

This selection allows you to install available plug-in options to the program.

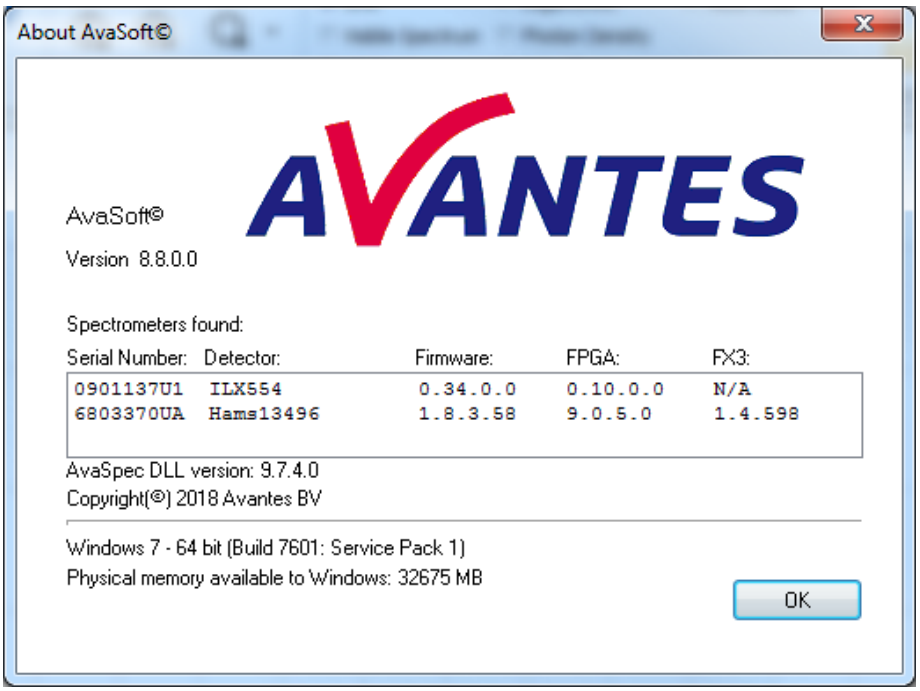
4.1.7 ‘File’ tab, ‘Select Spectrometers’ Menu Option

This selection opens a form that lets you select Ethernet spectrometers. The top box lists all spectrometers connected by USB. The bottom box will list all spectrometers connected by Ethernet, after pressing the ‘Update’ button. Depending on your network, you might need to press ‘Update’ several times. The check box in front of each Ethernet spectrometer controls whether the spectrometer will be opened in AvaSoft. You can check each checkbox individually, or use the ‘Select All’ and ‘Deselect All’ buttons to select or deselect all available spectrometers at once. The ‘Apply’ button will save your settings, the ‘Cancel’ button lets you leave without changes. See also section 4.1.15.5 about including spectrometers with Ethernet communication in AvaSoft and Appendix C for general background information about Ethernet communication.



4.1.8 'File' tab, 'About' Button

This brings up the About Box which shows some information about the AvaSoft version that is being used, the serial numbers of the spectrometers that are connected, detector types, firmware and FPGA versions, the AvaSpec DLL version, the Windows version of the computer and the available memory.



4.1.9 'File' tab, 'Exit' Button

Closes AvaSoft

4.1.10 'Home' ribbon tab, 'Start/Stop' Button

The Start/Stop button can be used to display data real-time or to take a snapshot. It applies to all spectrometers that are connected. As an alternative, the F2 function key can be used as well.

Pull down menu:
- Single measurement
- Continuous
- Store to Ram
- L.I.B.S.
- Autosave Spectra Enabled

In **'Single' mode**, a single measurement is made on all spectrometers.
In **'Continuous' mode**, a series of measurements is performed. A new measurement is started automatically after the previous one is finished. This is repeated until the 'Stop' button is pushed.
In **'StoreToRam' mode**, a fixed number of measurements is made, without the overhead of the communication interface. The number to StoreToRam scans can be set in the spectrometer settings. The scans are stored in the internal memory of the AvaSpec, and the results are only sent to the computer after the last measurement has been made.

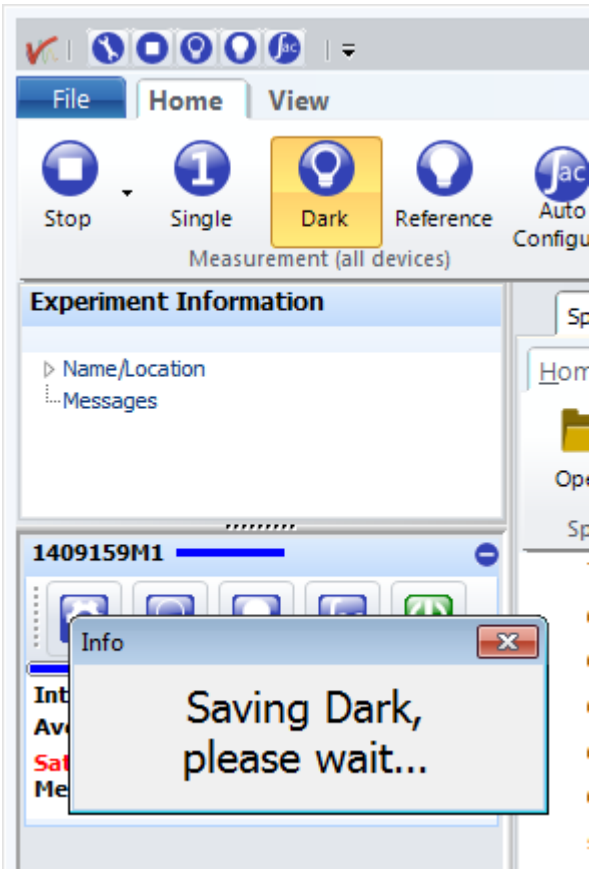
'L.I.B.S.' mode is a special mode of the program that has to be enabled in the 'Options' first.
'Autosave Spectra Enabled' is used when logging all scans to disk. In 'Options', 'Save Spectra Periodically', you must select the number of scans and optional time delays. You can also select here whether you want the scans to be saved as separate files, or as a single StoreToRam format file.

4.1.11 'Home' ribbon tab, 'Single' Button

This is equivalent to the 'Single' measurement option of the Start/Stop button.

4.1.12 'Home' ribbon tab, 'Dark' Button

This will save the dark data for all spectrometers. The color of the corresponding Save Dark icons in the spectrometer windows will change to green when ready.
A message box will indicate saving the dark data is in progress:

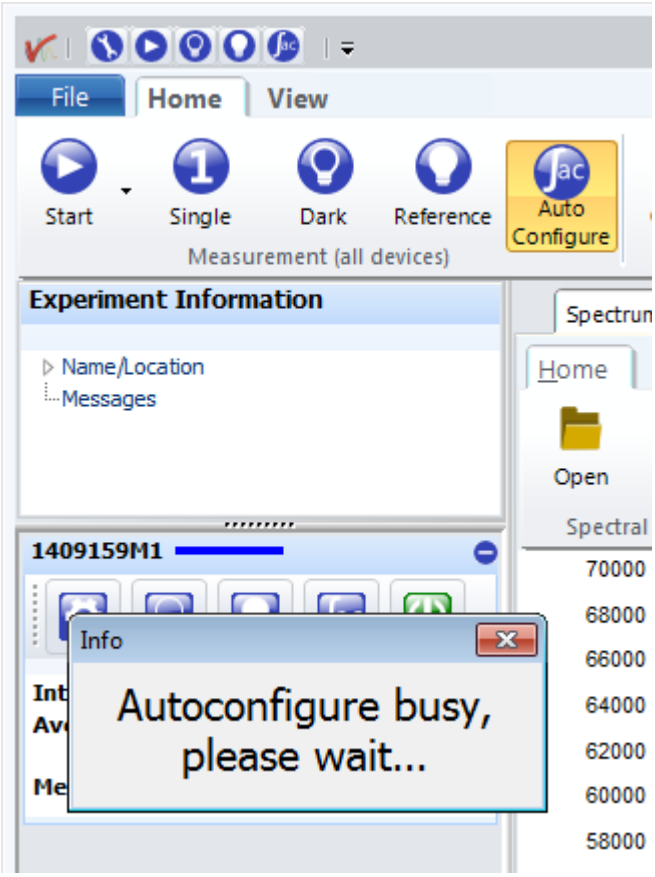


4.1.13 'Home' ribbon tab, 'Reference' Button

This will save the reference data for all spectrometers. The color of the corresponding Save Reference icons in the spectrometer windows will change to green.

4.1.14 'Home' ribbon tab, 'Auto Configure' Button

This will Auto Configure the integration time for all spectrometers. Depending on the maximum counts in the last scan, the integration time will be increased/decreased automatically until a scope signal of about 90% of the full scale is measured. The number of averages is set to a target cycle time of 500 ms, with a minimum value of 2 and a maximum value of 100 averages. You can edit the target cycle time in the AutoConfigure Options.
A message box will be shown when the Auto Configure is in progress:



4.1.15 'Home' ribbon tab, 'Options' Button

4.1.15.1 Save Options

- Auto Increment Filename:
  Here you can set the way the filename is patterned when using filenames that are auto incremented when you save multiple scans. You can base the name on your experiment, on the name of the window (plugin caption), or you can define it yourself. It is also possible to add a date stamp or a time stamp to the name.
- Suppress Save Comments Dialog:
  You can select this option to prevent having to enter a comment for every saved scan, when you want to save many files.
- Suppress ASCII Header:
  You can select this header when you want to save readings without header, e.g. when you want to import them into another application.

The wavelength values of the detectors supported by AvaSoft are not evenly spaced (or equidistant). For highest accuracy, our output files reflect this, and this behavior is fully supported by the respective SPC and DX output file standards,
Some third party programs, however, cannot handle non-evenly spaced wavelength values. You may need to use the following options with these programs:

- Save to ASCII in Equidistant Format:
  Normally, the readings are saved per pixel. The pixel array is not perfectly linear in wavelength, however. In case your application needs perfectly spaced wavelengths, you can select this option, and the readings will be interpolated. You can enter start and stop wavelengths, and wavelength increments.
- Save to JCAMP-DX in Equidistant Format:
  JCAMP-DX can be used with equidistant x values or with non-equidistant x values. With equidistant x values, the readings will be interpolated. AvaSoft 7 did not offer this choice, it would always output equidistant JCAMP files.
- Save to GRAMS-SPC in Equidistant Format:
  GRAMS-SPC can also be used with equidistant x values or with non-equidistant x values. With equidistant x values, the readings will be interpolated. AvaSoft 7 did not offer this choice, it would always output equidistant GRAMS-SPC files.
- Save log information
  When this option is enabled, two log files will be created: avaspec.dll.log (in the users root folder) and AvaSoft8.log (in the user\Avantes\AvaSoft8 folder). These log files may be useful when Avantes Support is looking into a reported problem.
  NOTE: enabling this option will slow down AvaSoft8.

4.1.15.2 Export Options

This option allows you to change the number of decimals that is used in exported spectra. You can set both the number of decimals of wavelength values and of measurement values.

4.1.15.3 Look and Feel

The on screen spectral line width in AvaSoft can be changed here. Only after restarting AvaSoft the new line width will be shown. Recommended value is 1 or 2, a value of 0 means no change will be made.

4.1.15.4 Windows Options

We have seen some problems with PC's relating to power management.
On some PCs, measurement stops as soon as the screen saver kicks in. In this option screen, you can disable the screen saver during measurement.
Some PCs try to conserve battery capacity by cutting the power to the USB ports, and fail to notice ongoing measurements. In this screen, you can also disable power saving.

4.1.15.5 USB vs Ethernet

This option allows you to use AvaSpec devices with the AS7010 board when connected through their Ethernet interface. If you want to connect your spectrometer through the Ethernet interface, select the bottom radio button 'Ethernet/USB', press 'OK' and restart AvaSoft. This selection will not affect spectrometers without an Ethernet port.
See also section 4.1.7 about selecting the Ethernet spectrometers

4.1.15.6 Save Spectra Periodically

When saving multiple scans, you select the number to scan here, and also the time delay before the start of the saving, and the time delay between consecutive savings. Only raw files are stored here. If you have selected merging in the Merge Channel Settings, the scans will be saved as raw8/raw8x files, with all channels combined in a single file per scan. If merging is off, the scans will be saved as raw8 files, one file per spectrometer and per scan.

You can also select to save data as a single StoreToRam file here. You can load and view this file in a 3D spectrum window, where you may also save the data into separate files. Another way to save spectra periodically is available in live mode see 'Save Live Output Periodically' Button.

4.1.15.7 Correct for Drift Channel

Introduction

When measuring the reflectance of a white reference tile or the transmittance of a reference solution against time, the output should theoretically remain 100% +/- noise. In practice the output value will not remain exactly fluctuating round 100%, but the signal can slowly drift away. The cause for this drift in the measurement system can be a change in temperature in the optical bench which causes micro bending of the components that focus the light at the detector, but also a drift in the light source that is used to illuminate the reference sample.
To correct for the drift in the system, it needs to be measured first. If a 2-or multiple-channel spectrometer is available, the measured deviation from 100% at a reference channel can be used to compensate the measured data at the sample channel. The sample and reference data can be measured simultaneously and the measured data at the reference sample can be used directly to correct the sample data. Disadvantage of the "correct for drift by spectrometer channel" is that the data for reference and sample are measured by using two optical benches which may react differently to temperature changes. If the drift is mainly caused by the light source (such as a difference in flash intensity of the AvaLight-XE), this method of correction is recommended.
A disadvantage of this method is that it will not correct for drift caused by temperature changes of the optical bench.

Correct for Drift by Spectrometer Channel

This option is only available if the spectrometer system has one or more slave channels. One spectrometer channel will be used as a reference channel, which will continuously measure the reference spectrum (e.g. the white tile in reflectance measurements or the cuvette holding the reference solution in transmittance measurements). Changes in this reference signal, e.g. because of drift in the light source, will be used to correct the data of the other (selected) spectrometer channels. The wavelength range over which the data can be corrected will be the overlapping wavelength range between reference spectrometer channel and the spectrometer channel to be corrected.
The option screen will be shown in which the reference channel and one or more (depending on the number of spectrometer channels that are available) channels to be corrected can be selected. After selecting the right setup, click the OK button
To disable the correct for drift option, the menu option must be set to off again.

4.1.15.8 External Trigger Settings

If the external trigger setting is enabled the spectrometer will wait until a TTL signal at pin 6[1] of the DB26 connector gets high and will then start the integration time. The delay between the rising edge of the TTL pulse and the start of the integration time cycle depends on the spectrometer type.

The table shows for each detector the fastest response to an external trigger pulse. Note that the start of the integration time can be delayed further by setting the integration delay parameter. The integration delay parameter can be set under L.I.B.S Mode – Measurement Settings.

[1] Please note that pin numbers are valid for DB26 connectors on -USB2 and –EVO spectrometers

Spectrometer Type	Minimum Delay [µs]	Maximum Delay [µs]
AvaSpec-128-USB2	9	60
AvaSpec-256-USB2	0.80	0.84
AvaSpec-1024-USB2	0.80	0.84
AvaSpec-2048-USB2	1.28	1.30
AvaSpec-2048L-USB2	3.28	3.30
AvaSpec-3648-USB2 (clearbuffer mode)	0.28	0.30
AvaSpec-NIR256-1.7, AvaSpec-NIR256-1.7-EVO AvaSpec-NIR256-2.5-HSC	536.48	536.73
AvaSpec-NIR512-2.5-HSC	531.74	533.93
AvaSpec-NIR512-1.7-EVO AvaSpec-NIR512-2.5-HSC-EVO	527.64	529.83
AvaSpec-NIR256-1.7TEC, AvaSpec-NIR256-2.2TEC	4.92*	5.75*
AvaSpec-NIR512-1.7TEC, AvaSpec-NIR512-2.2TEC	4.92**	5.75**
AvaSpec-2048x14-USB2	-2170	0
AvaSpec-2048x16-USB2	-1820	0
AvaSpec-2048x64-USB2	-2400	0
AvaSpec-2048x64TEC-USB2	-9700	0
AvaSpec-HS1024x58-USB2	-5220	0
AvaSpec-HS1024x122-USB2	-6240	0
AvaSpec-2048XL-USB2	0.37	0.39
AvaSpec-2048CL-EVO	0.90	0.92
AvaSpec-4096CL-EVO	0.90	0.92

* = 4.92 – 5.75 µs with FPGA version 6.4 and later, 137.5 – 138.3 µs with FPGA version 6.3
** = 4.92 – 5.75 µs with FPGA version 6.4 and later, 251.1 – 252.8 µs with FPGA version 6.3

Single Scan Trigger
If you use external triggering in Store to Ram mode, all measurements will be taken after the first trigger is received. When using an EVO series spectrometer, you can select whether you want to take all scans after the first trigger (uncheck the checkbox), or whether you want to take a single scan after each trigger (check the checkbox).
The single scan triggering selection does not work on AS5216 spectrometers. It is, however, possible to install a custom firmware version that will implement the single scan triggering feature.

Trigger Type Edge
When this mode is selected one or multiple scans will be started at the rising edge of a TTL pulse at pin 6[2] of the DB26 connector. The delay between the rising edge and the actual start of the integration time can be found in the table above.

Trigger Type Level
When this mode is selected the spectrometer will start to accumulate data (take scans at the selected integration time) at the rising edge of the TTL pulse and will continue to do so as long as the TTL signal remains high. When the signal becomes low, the average of the accumulated data (except for the last scan) will be displayed or saved. This mode is especially useful for conveying belt applications, when a product needs to be scanned, independent of the transport speed.

[2] Please note that pin numbers are valid for DB26 connectors on -USB2 and –EVO spectrometers

Scans per trigger
If a number of scans is set to a value higher than 1, the spectrometer will accumulate multiple scans on every rising edge of the external TTL trigger. This setting is overruled when level triggered is enabled.

4.1.15.9 Use Non-linearity Correction

If you have ordered a non-linearity-correction calibration with your spectrometer, you can enable or disable the feature here.

4.1.15.10 Laser Induced Breakdown Spectroscopy

Enable L.I.B.S.:
You must check this box to enable L.I.B.S. The other options choices will now be shown.

L.I.B.S. Mode:
Depending on your detector, you can select one of 3 modes here.
Spectrometer Triggers Laser. This option is only enabled with the AvaSpec-2048-USB2 and the AvaSpec-2048XL-USB spectrometers
Laser Triggers Spectrometer. This option can be selected with all spectrometers.
Laser Triggers PreScan Spectrometer. This option is only available with the AvaSpec-3648-USB2 spectrometer.

Measurement Settings:
You can set the number of measurements here, including the number of averages per scan.
If you check the Autosave Measurements box, the spectra will be saved after each measurement and can be displayed afterwards like any other saved measurement.
The integration delay can be set either fixed or variable. If the 'Variable' checkbox is left unchecked, the required fixed integration time delay can be entered. If the 'Variable' checkbox is checked, you can enter the first and the final integration time delay. The integration time delay for all measurements in between will be linearly interpolated.

Spectrometer Triggers Laser:
The LIBS settings in the lower box of the window are only relevant in the first mode, where the TTL-Out is used to trigger the laser.
Interval between scans:
This setting determines the frequency at which the laser is fired.
The Pulse Width parameter is the width for the laser pulse in microseconds during which the TTL-Out is set.
External Trigger options can be set to:

- Off, meaning the measurement sequence is software controlled. The frequency of the TTL-Out is determined by the "Interval between scans [ms]" parameter.
- First, meaning the first scan is controlled by an external hardware trigger. Then every next scan in the measurement sequence is started by the software, using the "Interval between scans [ms]" parameter to determine the frequency of the TTL-Out.
- All, meaning every scan is started on hardware trigger, optionally using the Laser Delay parameter.

The spectrometer will be setup in external trigger mode and requires one external trigger input for each scan (totaling Number of measurements * Averages trigger signals) to complete the sequence. The "Time Between scans [ms]" parameter becomes irrelevant when using this setting, because the frequency will be determined by the frequency of the trigger pulses received.

The Laser Delay parameter is the time in microseconds between receiving the external trigger and sending out the Laser pulse to fire the laser.

To check the exact pin numbers of the TTL-Out and external trigger I/O signals for your spectrometer, please have a look at the AvaSpec Operating Manual.

4.1.15.11 Merge Channel Settings

You can merge overlapping multiple channels into a merge group. The Merge Channel Settings screen lets you select which channels will be combined in merge groups. See Appendix D for more information.

4.1.15.12 Electronic Optical accessories

This selection will let you use devices like the Fiber Optic Multiplexer, the Fiber Optic Switch, the AvaAbsorb, the Beam Combiner or the Beam Splitter with AvaSoft 8. Please refer to the manuals that accompany these options.

4.1.15.13 AutoConfigure Options

When you connect multiple spectrometers that use integration times that differ substantially, it is advisable to use the available time for the ones with smaller integration times productively by increasing the number of averages. You will then have less noise, and it will not impact the total cycle time of your measurement. The AutoConfigure option will change the number of averages to make use of available time. The default cycle time used in the calculation of the number of averages is 500 ms. You can edit this number here, to fine tune the behavior of this calculation.

4.1.16 'Home' ribbon tab, 'Sync' Button

Pull down menu:

- No Hardware Synchronization
- Master: spectrometer ID

Synchronization will let you start multiple spectrometers at the exact same time, with either software or hardware triggering.
If you just connect many spectrometers (especially over USB), and start measuring, you will find that Windows will favor some of them, while others might not be handled at all. Synchronization will be necessary in this case.
For synchronization of scans a master spectrometer needs to be assigned. In rack-mounted setups, usually the leftmost spectrometer (as seen from the front) is assigned to be the dedicated master by Avantes. The other spectrometers are then dedicated slave spectrometers. Please note that separate spectrometers need to be connected with synchronization cables for this option to work, otherwise only the master spectrometer will scan just once, and the program will start to wait for data that will not arrive. You can switch off the synchronization by selecting the top option again (No Hardware Synchronization). Avantes rack-mounts are already fitted with these cables.
An alternative to synchronization is to use parallel external hardware triggering. As of late 2020, Avantes has started to wire all rack-mounted setups both with synchronization cables and parallel hardware triggering cables. In these setups, AvaSoft will copy the External Trigger Settings for the master to all dedicated slave spectrometers as well. Hardware triggering of the master will then trigger all of the slave spectrometers as well.

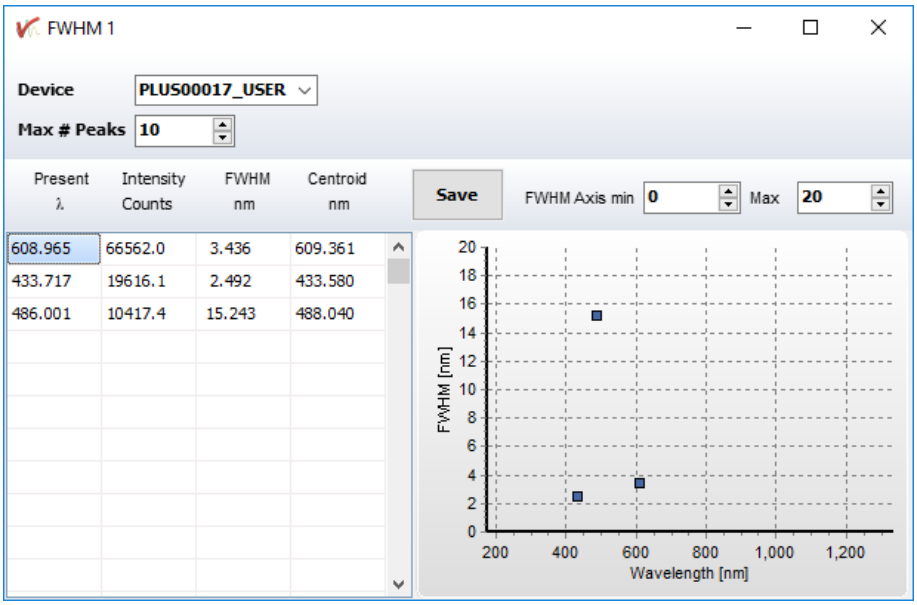
4.1.17 'Home' ribbon tab, 'Tools' Button

A pull down menu is shown with two choices:

4.1.17.1 Full Width Half Max (FWHM)

The Full Width Half Maximum of a peak is the bandwidth (in nanometers) for which the intensity is higher than half of the maximum intensity of that peak. This utility is used mostly measuring the output of laser diodes. For correct FWHM calculations, the intensity needs to be corrected for the dark data. Therefore it is recommended to enable the 'Dynamic Dark' option or measure in Scope minus Dark mode.

The FWHM is displayed in a table and in a graph.



On the left side of the window is the table. Every row of the table contains the Wavelength, Intensity, FWHM and the Centroid Wavelength of a Peak. These values are displayed and updated after each scan.

On the right side of the window is the graph. Every Peak (a table row) is represented by a dot. The minimum and maximum value of the vertical axis of the graph can be changed.

The channel selector at the top of the FWHM dialog can be useful if there are multiple spectrometers connected, and you want to switch between channels.

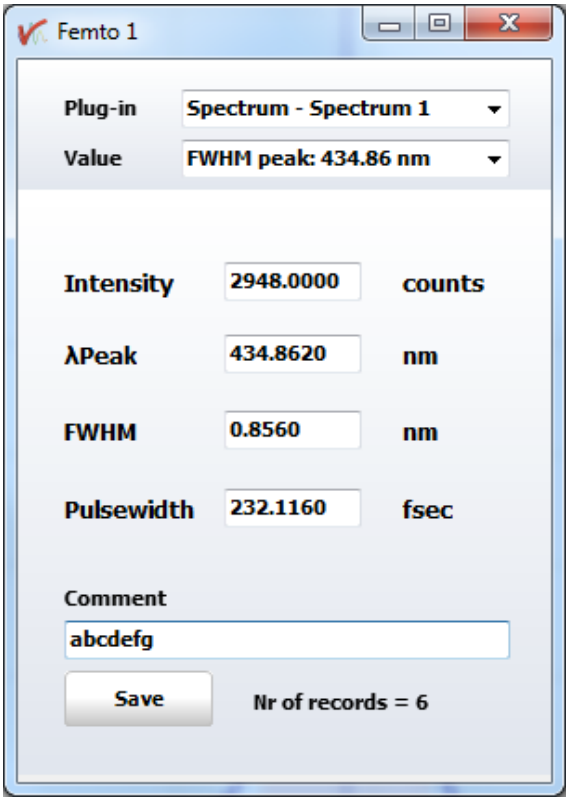
The results can be saved any time by clicking the Save button. The file is a text file with the file extension .fwm. It can be opened with any text editor, e.g. notepad.

Centroid Wavelength: The total wavelength intensity left and right from the centroid wavelength (integral) is the same.

4.1.17.2 Peak Tracing (pulsewidth fsec)

This application will let you calculate a laser pulsewidth from the wavelength and FWHM of a peak. First zoom in on peak of interest and use right mouse button to determine peak and

FWHM, next select Peak Tracing via ‘Tools’ button. In Femto window (see figure below) peak wavelength can be entered so that it can be monitored.



When Save button is pressed results are written to a text file named Femto Peak Tracing.lad

4.1.18 ‘Home’ ribbon tab, Application Buttons

4.1.18.1 ‘Spectrum’ Button

This button will open a new spectrum application window. The spectrum application is described in section 4.4.

4.1.18.2 ‘Spectrum3D’ Button

This button will open a new 3D spectrum application window. The spectrum3D application is described in section 4.5.

4.1.18.3 ‘TimeSeries’ Button

This button will open a new Timeseries application window. This application is described in section 4.6. If there are more applications enabled for your spectrometer, you can open new application windows with extra buttons to the right of the ‘TimeSeries’ button.

4.1.19 'View' ribbon tab, 'Dock All' Button

This button will redock all undocked windows.

4.1.20 'View' ribbon tab, 'Tile in Grid' Button

This button will arrange all windows in a grid, each window will be undocked.

4.1.21 'View' ribbon tab, 'Tile Vertically' Button

This button will arrange all windows side by side, each window will be undocked.

4.1.22 'View' ribbon tab, 'Tile Horizontally' Button

This button will arrange all windows from top to bottom. Each window will be undocked.

4.1.23 'View' ribbon tab, 'Set Panel Indicators' Button

Pull down menu:

- Progress Bar
- Scan Counter
- Detector Temp and Setpoint

The spectrometer windows display a number of parameters that change with each scan. In this menu, you can choose which ones to show. The detector temperature and setpoint will only be shown in the spectrometer window if your spectrometer is TE cooled.

4.1.24 'Help' menu

4.1.24.1 'Help'

This menu entry will open the AvaSoft 8 Manual.

4.1.24.2 'VBScript'

This menu entry will open the Visual Basic Script Language Reference. You can use VBScript in a specific type of Time Series.

4.1.24.3 'Avantes Website'

This menu entry will open the Avantes website in your default web browser.

4.1.24.4 'AvaSoft Videos'

This menu entry will open the YouTube website containing Avantes videos in your default web browser, allowing you to view these videos.

4.1.24.5 'About AvaSoft'

This menu entry will show the AvaSoft About box, which shows extensive version information, like the AvaSoft version being used, the AvaSpec DLL version being used and some information on the connected spectrometers, including their firmware versions.

4.1.24.6 'Release Notes'

This menu entry shows release notes for each AvaSoft 8 version.

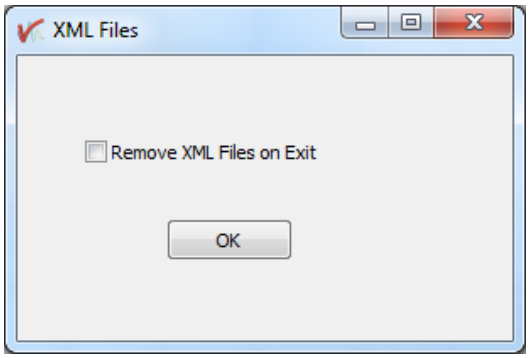
4.1.24.7 'Check for Update'

This menu entry checks your AvaSoft 8 version against the version that is currently available on the Avantes website, and will prompt you to download a newer version, once available. Please note that you will need to register on the Avantes website before you can download the latest version of AvaSoft.

4.1.24.8 'Remove XML Files'

This menu entry allows you to remove the XML settings files from your home directory, allowing you to start AvaSoft in a clean, defined state. Please note that the files are not actually deleted, but moved to a new subdirectory called e.g. 'oldxmlfiles_190301130709', the name containing a date/time stamp. You can always retrieve your old settings files from this backup directory.

Selecting the menu entry will show the following form:



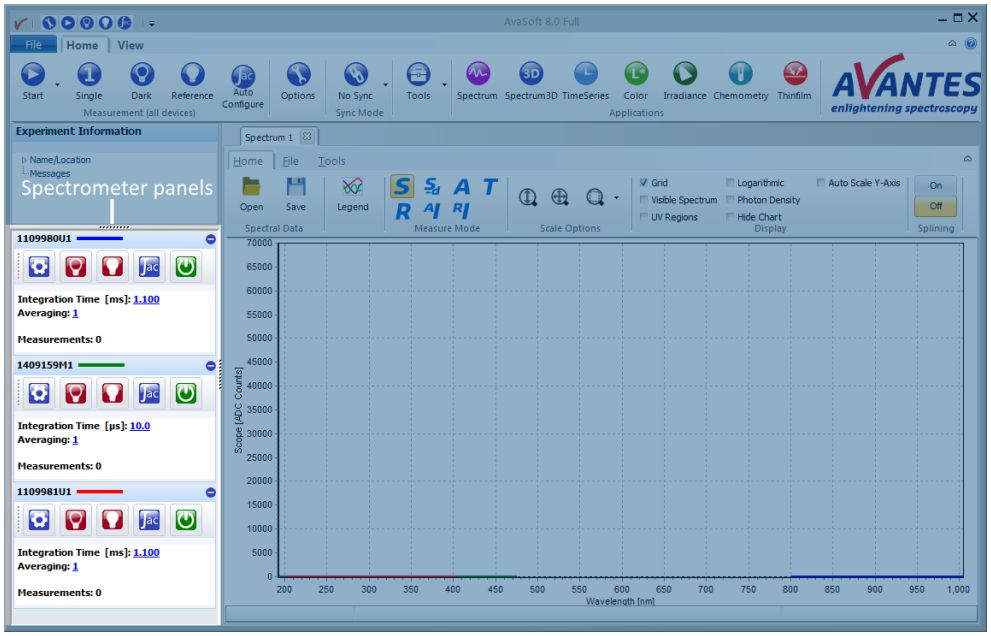
To remove the XML settings files, please check the box in the form and press the 'OK' button. Next close AvaSoft and restart it. On startup, you will see the 'Register AvaSoft 8' form, that shows you have now started with clean, defined settings.

4.2 Experiment Window

Allows you to set the name and folder location of your experiment, which allows you to control where data files are saved.
The setup data for the experiments can be saved to and reloaded from disk, which allows you to continue experiments where you left off, without reentering all of the setup data.
You can load and save the setup data from the main window, under the 'File' tab, with the 'Load Experiment' and 'Save Experiment' buttons.

4.3 Spectrometer Window

The spectrometer window holds the panels for all spectrometers:



You can drag & drop these panels to change the order of the spectrometers shown in this window, see paragraph 4.3.1.

4.3.1 Sorting the spectrometer panels

By simply dragging and dropping a spectrometer panel, you can change the order of the spectrometers as they are shown in the spectrometer window. Dragging and dropping is done by “grabbing” the panel on the title bar and moving it to the position you want it to be.

The order is automatically saved, so when you start AvaSoft again, the same order will be used. When saving your session to an experiment file, the spectrometer order is saved as well.

4.3.2 Friendly name ‘Spectrometer Settings’ dialog

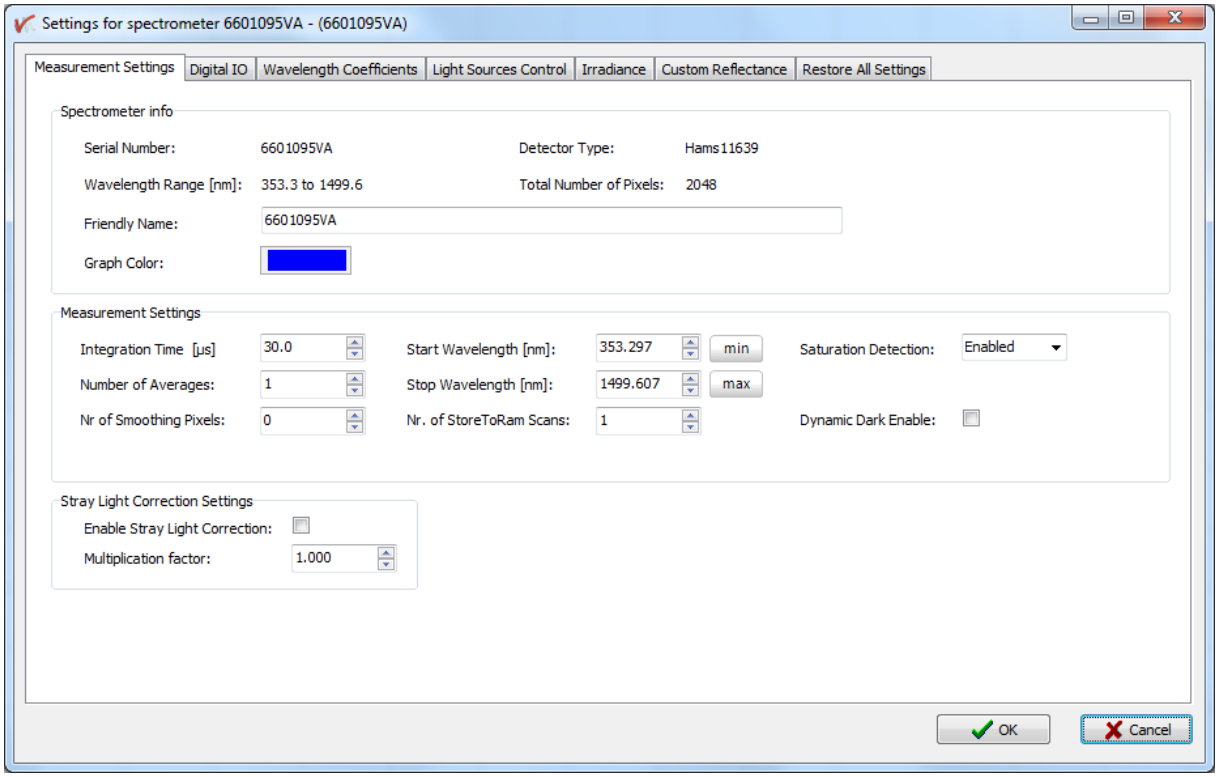
You can change the color of the line in the ‘Graph Parameters’ dialog, after pressing the ‘Legend’ button, described in the ‘Spectrum’ application, see section 4.3.4.1

4.3.3 Collapse / Expand button

Use the buttons to free up screen space, and to show the spectrometer window again, when necessary.

4.3.4 ‘Spectrometer Settings’ Button

4.3.4.1 Measurements Settings



This screen allows you to set the **Friendly Name** of the spectrometer, which will be shown in most screens of the program. You can also set **Integration Time**, **Number of Averages** and smoothing number, **Start** and **Stop Wavelength** (you can reduce the number of pixels the spectrometer uses here, which may significantly speed up processing and reduce the size of data files).

The next option you can set is **Saturation Detection.** The 16-bit A/D converter in the AvaSpec results in raw Scope pixel values between 0 and 65535 counts. If the value of 65535 counts is measured at one or more pixels, then these pixels are called to be saturated or overexposed. Since saturated pixels can disturb the measurement results, a lot of attention has been given in AvaSoft to detect saturation and to notify the user if a measurement contains saturated pixels. This notification is done in such a way that the user can always decide to ignore the saturation, for example if the saturation happens at pixels that are not in the wavelength range the user is interested in. Saturation can usually be solved by selecting a shorter integration time. When at minimum integration the signal is still too high, an attenuator, a neutral density filter or fibers with a smaller diameter may be used.
In AvaSoft, the default setting for Saturation Detection is 'Enabled'. It can also to set to 'Disabled'. Saturation is indicated in the Spectrometer Window that contains a 'Saturated' Panel Indicator. In case of saturation, the label 'saturated' will become visible here.

This is useful for measurements in transmittance, absorbance and irradiance mode, because in these modes saturation cannot be observed by looking at the number of counts, like in scope mode. But even in scope mode, a spectrum can contain saturated pixels also when this is not directly obvious from the graph. Examples are:

- Smoothing. The maximum pixel value of a peak can be saturated, but is averaged with neighbor pixels which may not be saturated.
- The correct for dynamic dark algorithm subtracts the dark values that are measured at the optical black pixels from the spectral data. Therefore, the saturation level of 65535 counts will never be reached with correct for dynamic dark ON. The saturation detection in AvaSoft is done before the data is corrected for dynamic dark, so it will also detect saturation with dynamic dark ON.
- Monitor resolution. Most of the time, the detector will contain more pixels than the monitor pixels in the graph. Since not each detector pixel can be drawn at the monitor, a sharp peak at one detector pixel can be saturated although this is not visible at the monitor. Use the zoom function if you want to verify if this is the cause of saturation.
- Zoomed in. Saturation can also happen at a wavelength range that is not visible because the graph is not at full scale.

Under all these circumstances, the “saturation” label will be shown in the spectrometer window of the channel for which one or more pixels are saturated.

To get a smoother spectrum without losing information it is important to set the right **Smoothing** parameter in the software. The optimal smoothing parameter depends on the distance between the pixels at the detector array and the light beam that enters the spectrometer. For the AvaSpec-2048, the distance between the pixels on the CCD-array is 14 micron.

With a 200 micron fiber (no slit installed) connected, the optical pixel resolution is about 14.3 CCD-pixels. With a smoothing parameter set to 7, each pixel will be averaged with 7 left and 7 right neighbor pixels. Averaging over 15 pixels with a pitch distance between the CCD pixels of 14 micron will cover 15*14 = 210 micron at the CCD array. Using a fiber diameter of 200 micron means that we will lose resolution when setting the smoothing parameter to 7. Theoretically the optimal smoothing parameter is therefore 6. The formula is `((slit size/pixel size) – 1)/2`.

In the table below, the recommended smoothing values for the AvaSpec spectrometer are listed as a function of the light beam that enters the spectrometer. This light beam is the fiber core diameter, or if a smaller slit has been installed in the spectrometer, the slit width. Note that this table shows the optimal smoothing without losing resolution. If resolution is not an important issue, a higher smoothing parameter can be set to decrease noise against the price of less resolution.

Slit or Fiber	**AvaSpec-128** **Pixel 63.5 µm**	**AvaSpec-256 1024** **Pixel 25 µm**	**AvaSpec-HS 1024x58 1024x122** **Pixel 24 µm**	**AvaSpec-2048, 2048L, 2048x14, 2048x16, 2048x64, 2048XL 2048CL** **Pixel 14 µm**	**AvaSpec-4096CL 3648** **Pixel 7-8 µm**	**AvaSpec-NIR256** **Pixel 50 µm**	**AvaSpec-NIR512** **Pixel 25 µm**
10µm	n.a.	n.a.	0	0	0	n.a.	n.a.
25µm	n.a.	0	0	0-1	1	n.a.	0
50µm	0	0-1	0-1	1-2	2-3	0	0-1

100µm	0-1	1-2	1-2	3	5-6	0-1	1-2
200µm	1	3-4	3-4	6-7	12	1-2	3-4
400µm	2-3	7-8	7-8	13-14	24-25	3-4	7-8
500µm	3-4	9-10	9-10	17	31	4-5	9-10
600µm	4	11-12	11-12	21	37	5-6	11-12

You can set the number of scans for **StoreToRam** mode.

This mode allows you to measure a fixed amount of scans as fast as possible, without the overhead of USB communications. The scans are stored in the internal memory of the AvaSpec, and the results are only sent to the computer after the last measurement has been made.

You can, for example, store as much as 1013 full pixel scans with the AvaSpec-2048-USB2, which has 2048 pixels and a fastest integration cycle of 1.05 msec. By limiting the wavelength range in the measurement ('Setup', 'Wavelength Calibration Coefficients', change the 'Start at' and 'Stop at' fields) you can extend the number of scans.

When you use a spectrometer with more pixels, the number of full pixel scans is proportionally less. The AvaSpec-2048Mini and the AvaSpec-2048L-EVO have much more memory, theoretically allowing for 7783 and 16383 scans of 2048 pixels respectively. All spectrometers allow you to extend the amount of Store To Ram scans by limiting the wavelength range. Memory use and the 3D chart in AvaSoft 8 will, however, be a limiting factor in the use of very high numbers of scans.

Note that the time needed to transport the data to the computer (after the measurement has been made), can be as long as 50 seconds, if you select a very large number of scans.

Only for AvaSpec NIR spectrometers an extra option **Sensitivity Mode** exists below the Saturation Detection option. This mode can be set to Low Noise or High Sensitivity.
The Toshiba detector, TCD1304 (3648 pixels), can be used in 2 different control modes:

1. The Prescan mode (default mode with option "Prescan enabled" set to on).
   In this mode the Toshiba detector will generate automatically an additional prescan for every request from the PC, the first scan contains non-linear data and will be rejected, the 2nd scan contains linear data and will be showed on the screen and/or saved. This prescan mode is default and should be used in most applications, like with averaging (only one prescan is generated for a nr of averages), with the use of an AvaLight-XE (one or more flashes per scan) and with multichannel spectrometers. The advantage of this mode is a very stable and linear spectrum. The disadvantage of this mode is that a minor (<5%) image of the previous scan (ghost spectrum) is included in the signal.
   This mode cannot be used for fast external trigger and accurate timing, since the start of the scan is always delayed with the integration time (min. 3.7 ms).

2. The Clear-Buffer mode (option "Prescan enabled" set to off)
   In this mode the Toshiba detector buffer will be cleared, before a scan is taken. This clear-buffer mode should be used when timing is important, like with fast external triggering. The advantage of this mode is that a scan will start at the time of an external trigger, the disadvantage of this mode is that after clearing the buffer, the detector will have a minor

threshold, in which small signals (<2000 counts) will not appear and with different integration times the detector is not linear.

Another option you can select in the ‘Measurement Settings’ is **Dynamic Dark** mode.

The pixels of the CCD detector are thermally sensitive, which causes a small dark current, even without exposure to light. To get an approximation of this dark current, the signal of some optical black pixels of the detector can be taken and subtracted from the raw scope data. This will happen if the correct for dynamic dark option is enabled. As these optical black pixels have the same thermal behaviour as the active pixels, the correction is dynamic.
Some detector types (AvaSpec-2048/2048L/3648) include dedicated optical black pixels. At these optical black pixels, the intensity and thermal behaviour is the same as the active data pixels, if no light falls on the detector. Enabling dynamic dark correction will therefore result in a baseline fluctuating round zero, and measurement data will be less sensitive for temperature changes than with dynamic dark correction off.

Some NIR detector types (NIR256-2.0TEC, NIR256-2.5TEC) and the AvaSpec-2048CL also support dynamic dark, because a few datapixels are blackened during fabrication of the optical bench. These blackened pixels can then be used for dynamic dark correction.

For spectrometers with dedicated optical black or blackened pixels, the correct for dynamic dark option can be switched on or off by clicking this menu option. The option is on if the menu option is preceded by a checkmark which is the default state. If the connected spectrometers don’t have optical black or blackened pixels, the correct for dynamic dark menu option will not be available. This is also the case for the back illuminated detectors in the AvaSpec-2048x14, 2048x16 and 2048x64, 1024x58, 1024x122, 2048XL. These detectors don’t include optical black pixels, but a few elements in the shift register are used for correcting the raw data.

Note that this option is different from the dark current that needs to be saved before any transmittance or absorbance measurements can be taken (Save Dark Spectrum button). If the correct for dynamic dark option has been changed, it will be necessary to save a new dark and reference spectrum because the raw data has been changed.

Stray Light Correction Settings

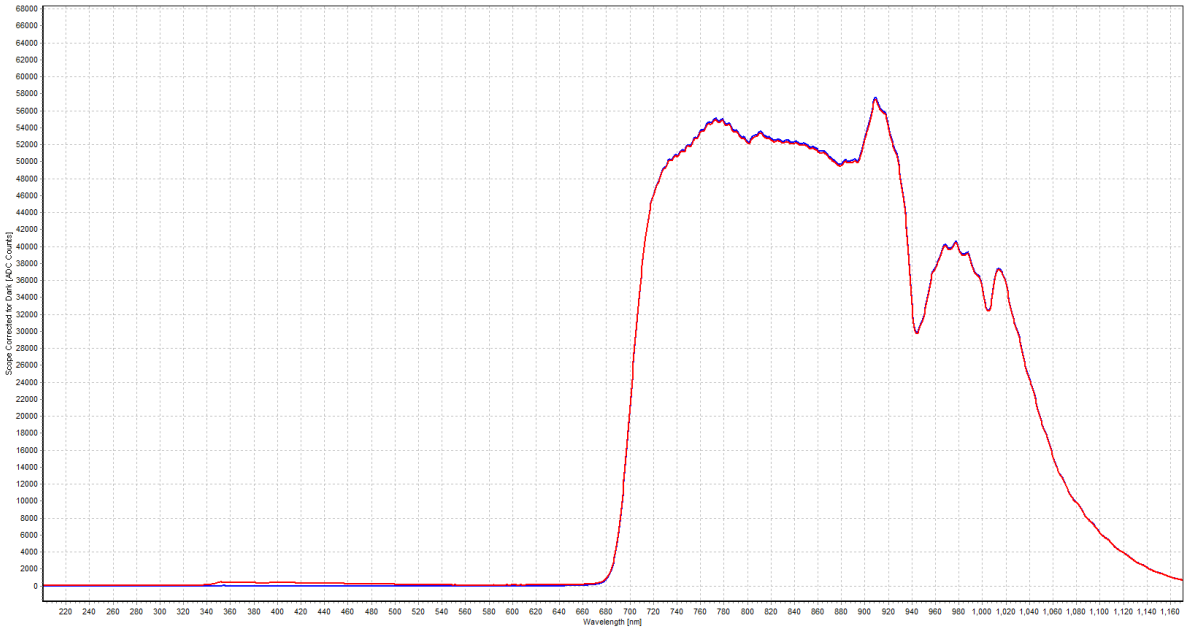
If your spectrometer has been calibrated for Stray Light Correction, an additional box will appear in this screen. It allows you to enable or disable the Stray Light Correction by checking or clearing the appropriate checkbox.

You will e.g. need to disable the Stray Light Correction when using an irradiance calibration that has been recorded without Stray Light Correction.

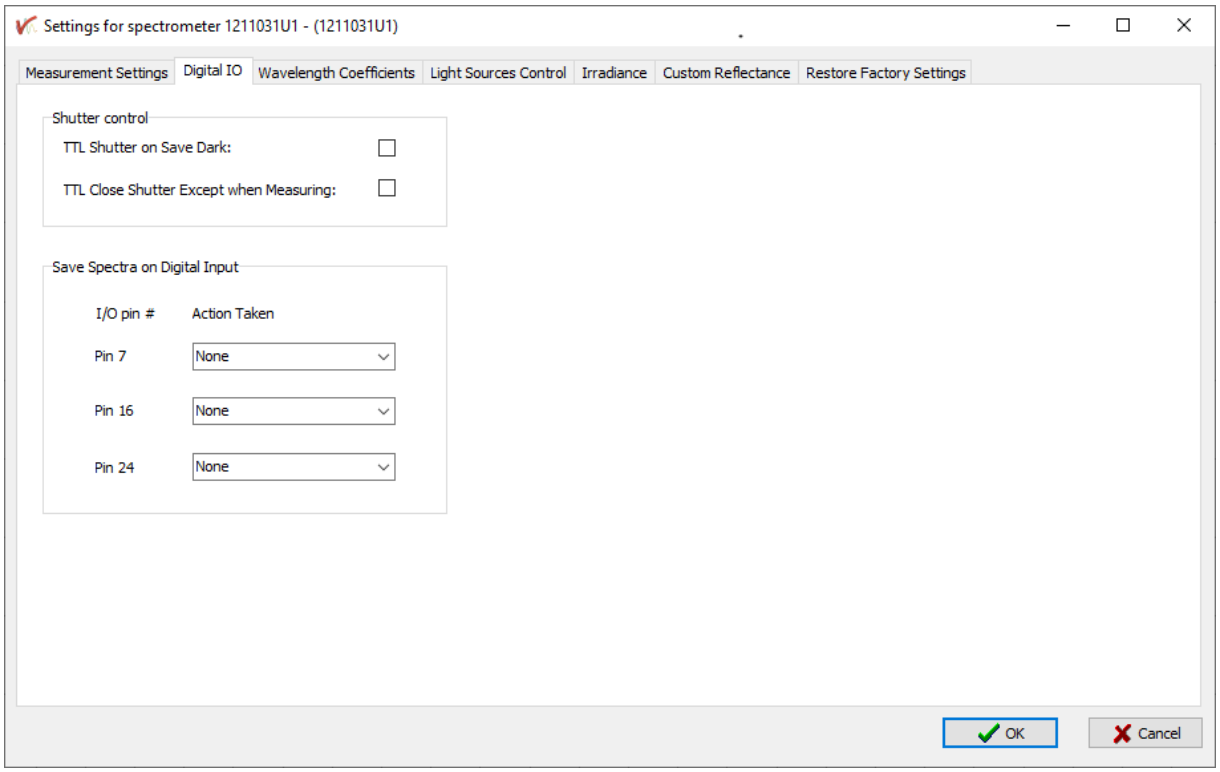
If Stray Light Correction is enabled, you must also enable Dynamic Dark if it is available, as the calibration will also have been done with Dynamic Dark enabled, if it is available.

You can also change the Multiplication factor that will be used in the correction algorithm. It has a range of 0.0 – 4.0, where 0.0 means no correction and 4.0 means maximum correction. The default value is 1.0. The spectrometer was calibrated for Stray Light Correction with a 200 micron fiber. For some configurations, you could use the multiplication factor e.g. to compensate for using a fiber of a different size.

The effect of the Stray Light Correction is shown in the figure below. The spectrum of a halogen light source using a 695 nm long pass filter is shown, with and without the Stray Light Correction. Note that the corrected blue line shows considerably less counts in the are below 695 nm.



4.3.4.2 Digital IO



TTL Shutter on Save Dark
To use the automatic TTL Shutter on Save Dark option, an interface cable needs to be connected from the spectrometer to the light source with shutter (AvaLight-HAL-S, AvaLight-DHc, AvaLight-D(H)-S-(DUV)). The interface cable between TTL-shutter and spectrometer is a 26 pin to 15 pin cable (IC-DB26-2).

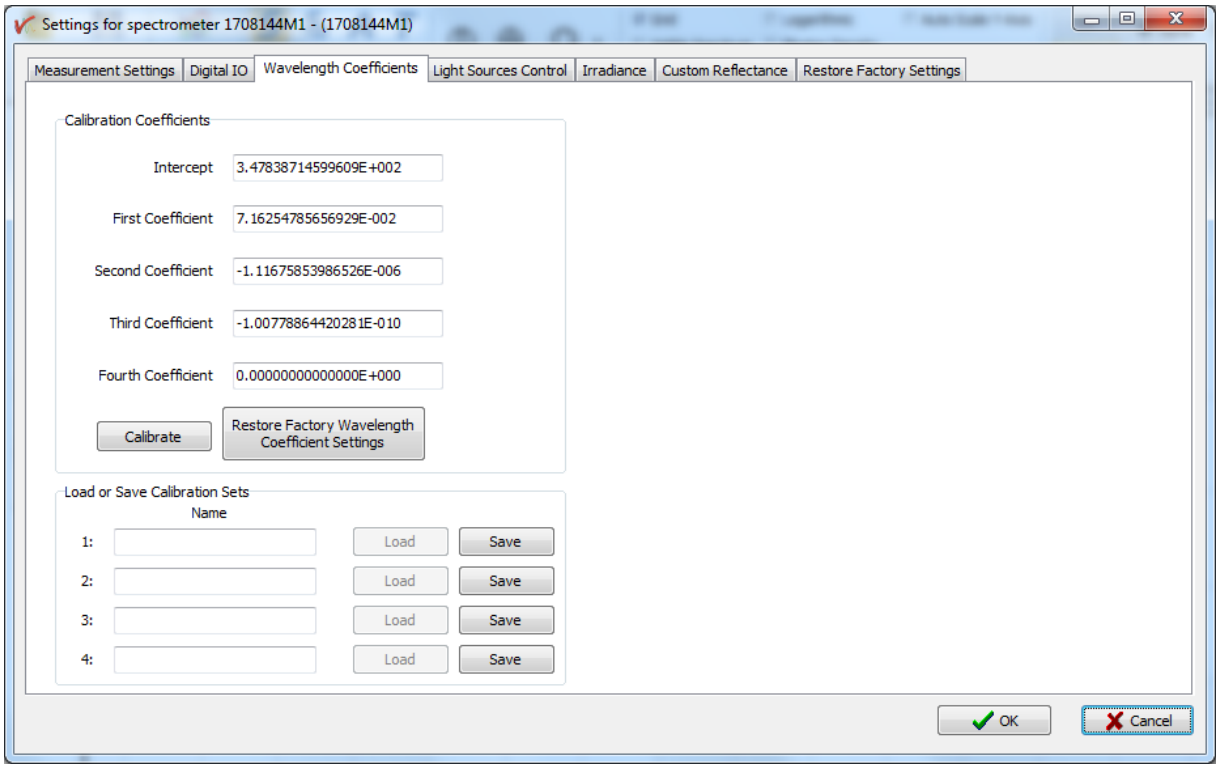
The TTL switch at the light source needs to be in TTL-position. In AvaSoft, the menu option 'Activate TTL Shutter on Save Dark' needs to be enabled in the Digital IO screen. If this option is enabled, the TTL will close the shutter of the light source at the moment the dark data is saved. After the dark has been saved, the shutter will be opened automatically.

TTL Close Shutter Except when Measuring
When this setting is enabled, the TTL Shutter will be closed when no measurement is active.
This option can be used when the sample being measured is degrading when exposed to the (for example UV) lightsource.

Save Spectra on Digital Input
The DB26 connector pins 7, 16 and 24[3] may be used to connect external switches, such as photo switches, to save a spectrum, reference or dark. This is especially useful for automated sampling in a process control environment with periodical updates of dark and reference signals. It is recommended to enable the Activate TTL shutter on Save Dark in combination with the Save dark on Digital Input setting. You can select the action taken on each pin in the Digital IO form.

[3] Please note that pin numbers are valid for DB26 connectors on -USB2 and –EVO spectrometers

4.3.4.3 Wavelength Coefficients



In this dialog, you can manually change the wavelength calibration coefficients, you can perform a new wavelength calibration and you can restore the original factory calibration which is stored in EEPROM.

The wavelength λ that corresponds to a pixel number (pixnr) in the detector in the spectrometer can be calculated by the following equation:

$$\lambda = Intercept + X1*pixnr + X2*pixnr^2 + X3*pixnr^3 + X4*pixnr^4$$

in which Intercept and X1 to X4 correspond to Intercept and First to Fourth Coefficient in the screen above. For example, if we want to calculate the wavelength at pixel number 1000, using the numbers in the screen above, the wavelength becomes:

```
λ =    409,672 +
       0,28770*1000 +
       -9.54557E-6*1000*1000 +
       -1,40802E-9*1000*1000*1000
  =    686,418 nm.
```

In the ‘Load or Save Calibration Sets’ panel, you can enter a file name and save the current set of calibration coefficients to disk. You can also load a previously saved calibration set from disk. A maximum of 4 calibration sets can be stored with each spectrometer.

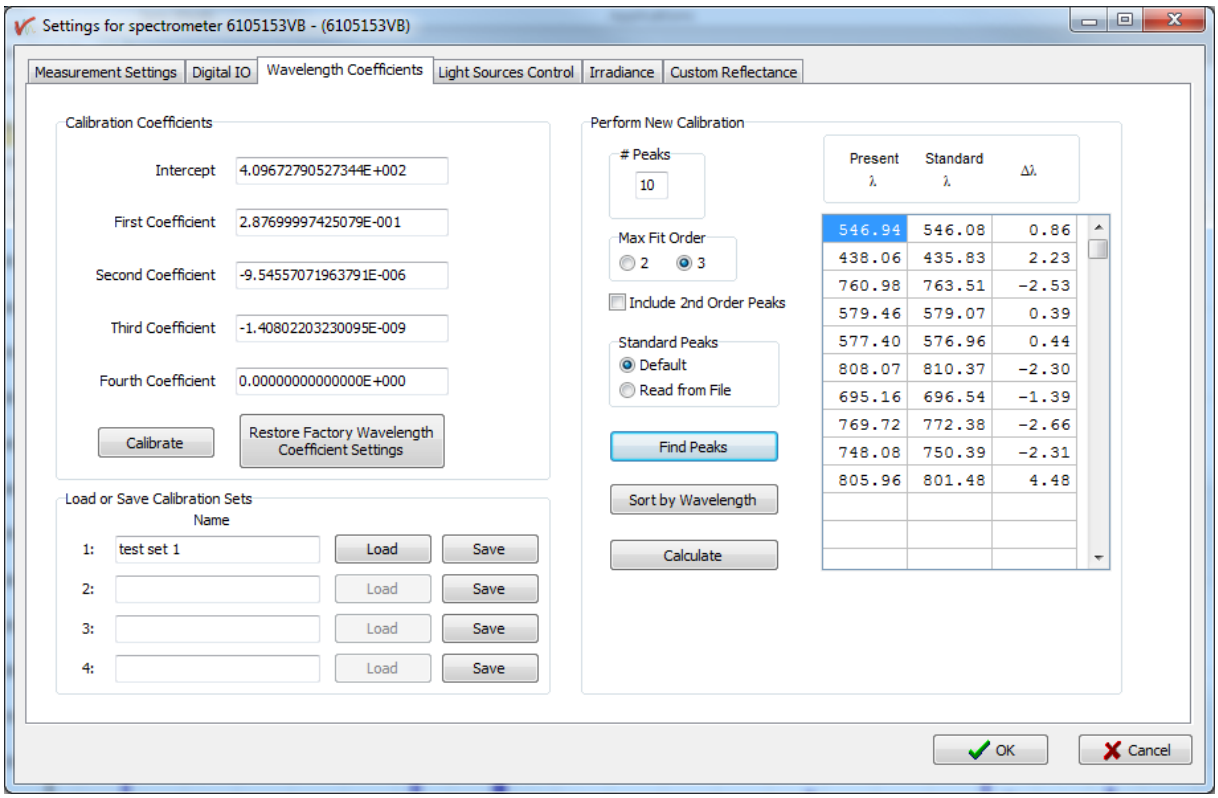
If a Wavelength Calibration light source is available, together with suitable optical fibers, an automatic wavelength calibration can be performed. Press the ‘Calibrate’ button to show the right part of the form. The peaks for the Mercury-Argon calibration source (AvaLight-CAL) are loaded by default. It is also possible to import the peaks that will be used in the calibration from a file by selecting the “Read from File” radio button above the “Find Peaks” button. This option allows you to import peaks for

different calibration sources such as the AvaLight-CAL-NEON or AvaLight-CAL-AR. The files that can be imported are in ASCII format and can be edited with any text editor, e.g. Notepad.

The extension for these files is ".lit" and the data is presented in three columns:

<wavelength in nm> <intensity in arbitrary units> <peak order>

An important precondition for a successful auto calibration is the absence of saturation. The easiest way to assure this is to select the 'Saturation Detection' option in measurement settings (see section 4.3.4.1). If the spectrometer is saturated at minimum integration time, a fiber with smaller core diameter (e.g. FC-IR008-2) needs to be used. As an alternative, the incoming light can be attenuated e.g. by using an attenuator (FOA-Inline) or neutral density filter.

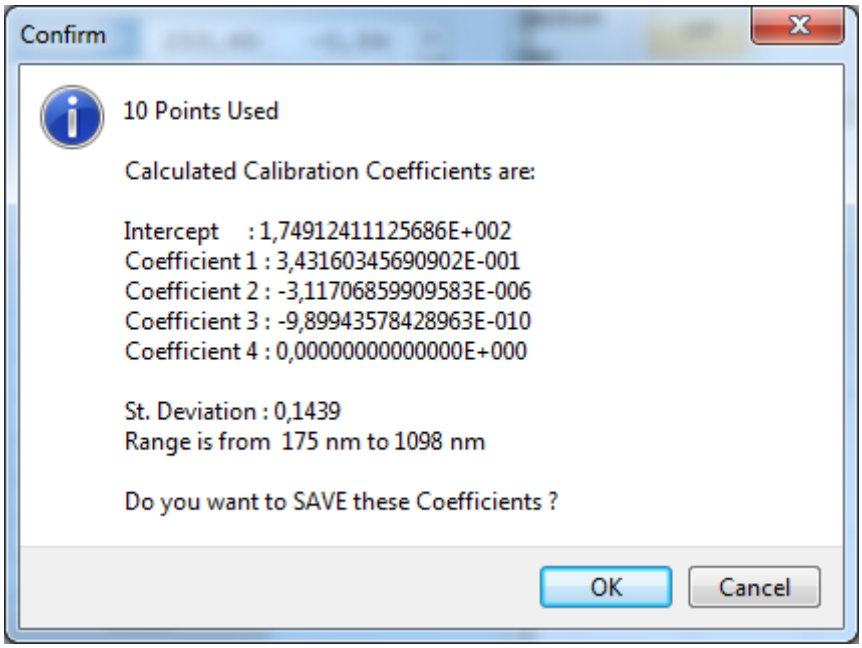


Perform New Calibration
The procedure to perform an auto calibration is as follows:

- Connect the fiber to the AvaLight-CAL light source and to the spectrometer channel to be calibrated.
- Choose a suitable integration time so as not to saturate the detector. The peaks can be seen in scope mode.
- Show the 'Calibrate' panel on the right side of the form by pressing the 'Calibrate' button.
- Pressing the 'Find Peaks' button will make the program look for a number of peaks; initially it will look for 5 peaks.
- The number of peaks to look for can be altered. A new search can be performed by pressing the 'Find Peaks' button again. The peaks are shown in 3 columns. The first column shows the position of the peaks found. The second column shows the position of a suggested standard peak, if available. The last column lists the difference between the first two columns. You can edit the values of the second column by selecting them with the mouse.
- Select the polynomial order. In most cases a third order polynomial will show an excellent fit (see figure above)

- The “include 2nd order peaks” option can be enabled if second or third order peaks should be added to the list of available literature peaks (e.g. 507.30 nm as second order peak for 253.65). In most spectrometers, the second order effects are eliminated by filters or coatings, but if these options have not been added to the spectrometer, and second order peaks are available, then these can be included in the calibration. The central column cells will be marked green if a second order peak is found and yellow if a third order peak is found.
- Press the ‘Calculate’ button. If your calibration is successful, you will be asked to confirm new coefficients.

Select ‘OK’ and the new calibration will be applied immediately.

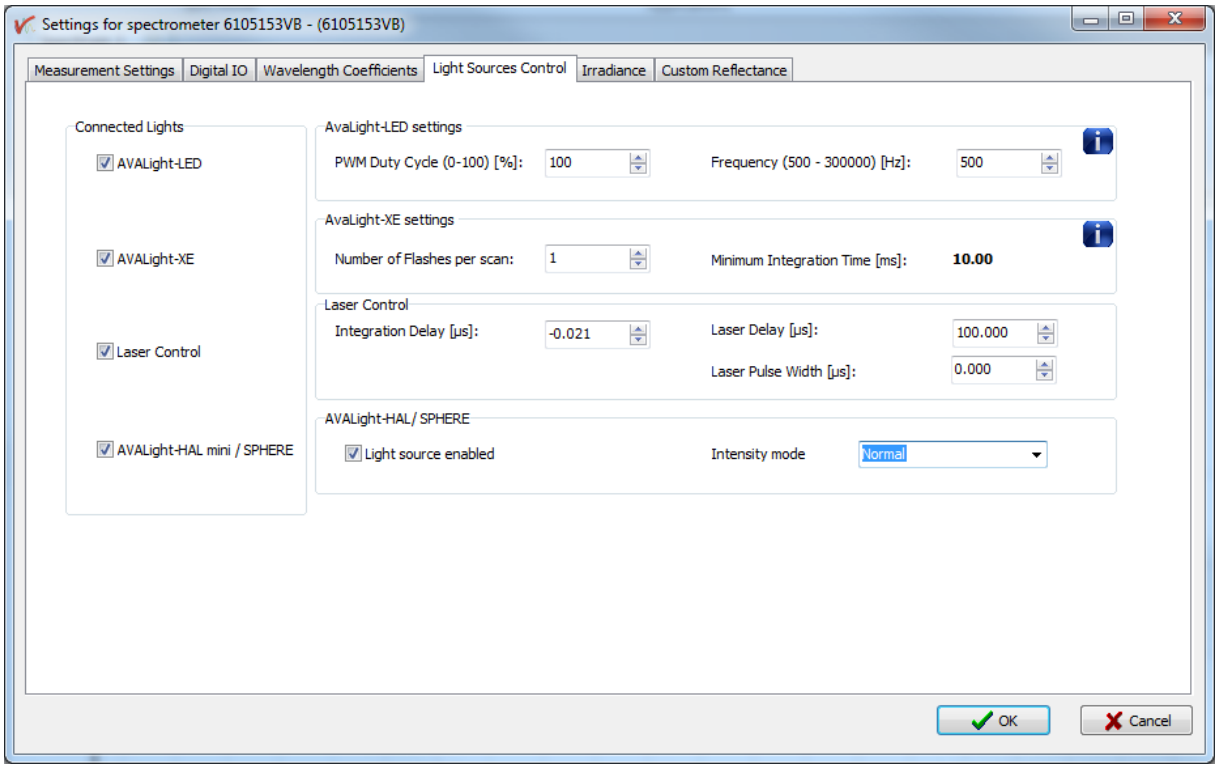


At least 3 peaks are needed to successfully complete a new calibration. Try to calibrate with more peaks. Selecting too many peaks can however lead to peaks that cannot be matched with standard wavelengths.

Restoring the Original Calibration
It is possible to restore the calibration coefficients to their original values, i.e. the values that AvaSoft was shipped with. If a new calibration was performed with a limited number of peaks, or over a limited wavelength range, the results could be less favorable. You can undo unwanted changes to the calibration by clicking the ‘Restore Factory Settings’ button.

The ‘Restore Factory Settings’ button restores the original wavelength calibration coefficients that were saved to the EEPROM during factory calibration.

4.3.4.4 Light Sources Control



The AvaLight-LED needs to be attached to a AvaSpec-USB2 by connecting an IC-DB26-2 interface cable between the high density 26 pole Sub-D connectors at the AvaSpec-USB2 and the 15-pole DB connector of the AvaLight –LED (DO1 – pin11[4]).

The frequency can be set between 500 Hz and 300 kHz, the duty cycle between 0 and 100%.
If used with a multichannel system, all channels can have their own independent PWM setting for both frequency and duty cycle. To disable the PWM output, simply enter 0 under the Duty Cycle.

This AvaLight-XE option can be used to enable or disable an external strobe (an AvaLight-XE or AvaLight-XE-HP) attached to an AvaSpec spectrometer. The measured light intensity of the AvaLight-XE is independent of the integration time in AvaSoft. To increase light intensity, the number of pulses per integration interval should be increased. The maximum frequency at which the AvaLight-XE operates is 100 Hz. This means that the minimum integration time for 1 pulse per scan is 10 ms. When setting the number of pulses e.g. to 3, the minimum integration time becomes 30 ms. It is recommended to keep the integration time as low as possible to avoid unnecessary increase of noise.

The AvaLight-XE needs to be attached to an AvaSpec-USB2 or AvaSpec-EVO by connecting an IC-DB26-2 interface cable between the high density 26 pole Sub-D connectors at the AvaSpec-USB2 and the 15-pole DB connector of the AvaLight -XE. If used with a multichannel system, make sure that the AvaLight-XE is connected to the master sync spectrometer, only the number of flashes per scan set for the master sync spectrometer will determine flash rate. To disable the strobe, simply enter 0 under the Number of Flashes per scan.

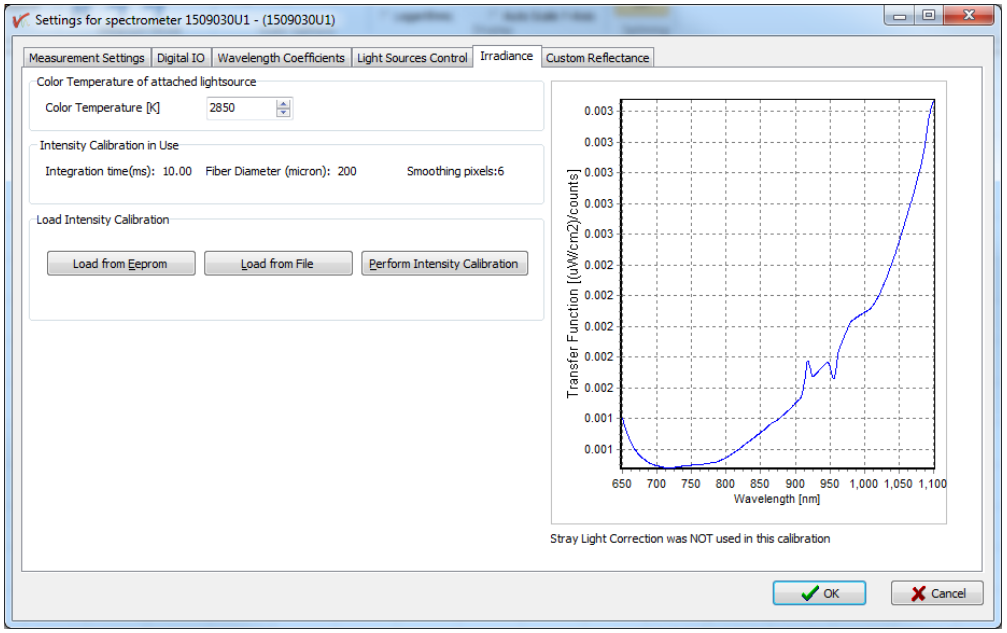
The Laser Control option lets you select Integration Delay, Laser Delay and Laser Pulse Width.
The Laser Pulse Width is the time in microseconds that the TTL signal is set.

[4] Please note that pin numbers are valid for DB26 connectors on -USB2 and –EVO spectrometers

The Laser Delay parameter is the time in microseconds between receiving the external trigger and sending out the Laser pulse to fire the laser.
The Integration Delay is the time delay in microseconds between the laser output pulse and the start of the integration time cycle.

The AvaLight-HAL mini/SPHERE option lets you operate this light source by software. When you check the 'light source enabled' checkbox, the lamp is switched on (pin 2[5] on the HD26 is asserted) The drop down box on the right lets you select between Normal mode, Long Life mode and High Intensity mode. Asserting pin 21[6] on the HD26 selects Long Life mode and asserting pin 22[7] on the HD26 selects High Power mode.

4.3.4.5 Irradiance



The Color Temperature value of your light source is used in the calculation of relative irradiance. A standard value for the Color Temperature is 2850 °K, you can use this value e.g. for the Avalight-Hal light source with default jumper setting.

Before you can measure absolute irradiance data, you must load an intensity calibration. An intensity calibration file contains the data which is necessary to convert the Scope data to Irradiance data. If the spectrometer system has multiple channels, it is important to know that the calibration data for each spectrometer channel are saved in a separate file. To measure irradiance data at more spectrometer channels simultaneously, the calibration file for each spectrometer channel needs to be loaded first. After loading an intensity calibration file, a graph is displayed which shows the data transfer function for the loaded channel. The irradiance spectrum is calculated by multiplying the measured scope data (from which a saved dark spectrum is subtracted) with this data transfer function.

The intensity calibration is loaded from EEPROM by default. However, if multiple calibrations are available for a spectrometer, the EEPROM calibration can be overruled by loading a calibration from

[5] Please note that pin numbers are valid for DB26 connectors on -USB2 and –EVO spectrometers
[6] (idem)
[7] (idem)

file. The filename that holds the intensity calibration needs to include the serial number of the spectrometer channel.

Please note that you must match the setting of the Stray Light Correction of your irradiance measurements with that of the irradiance calibration. Do not use a calibration that was recorded with Stray Light Correction, when this feature has been turned off, or vice versa. A mismatch will result in a warning when loading the calibration. After loading an intensity calibration from file or EEPROM, a line will be displayed under the data transfer function, indicating if the intensity calibration has been performed with or without straylight correction.

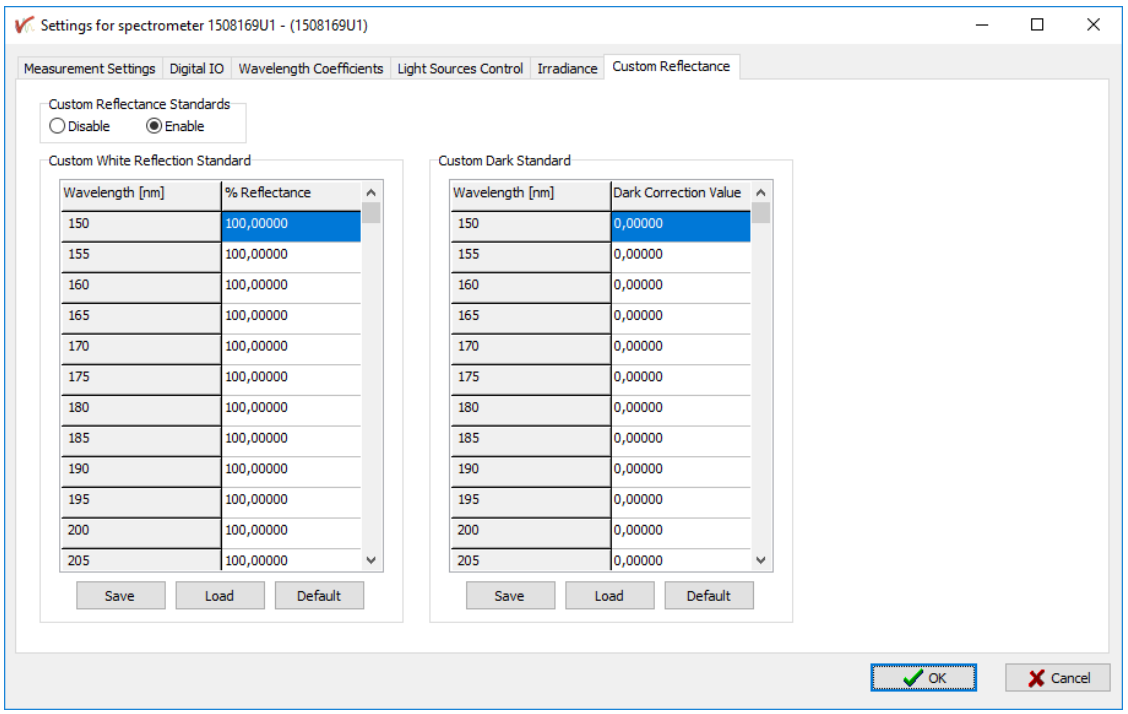
If a calibrated light source such as the AvaLight-HAL-CAL or AvaLight-DH-CAL is available, an intensity calibration can be performed.

The following settings need to be entered before starting the intensity calibration:

- Calibration Lampfile
- CC-UV/VIS, Fiber or AvaSphere sample port diameter

For a detailed description of an irradiance calibration, please refer to section 4.1.10 ('Home' ribbon tab, 'Start/Stop' Button).

4.3.4.6 Custom Reflectance



In Transmittance/Reflectance Mode, the transmittance/reflectance at pixel n is calculated using the current sample, reference and dark data sets in the following equations:

$$T_n = CW_n * \left(\frac{sample_n - dark'_n}{ref_n - dark'_n} \right)$$

where

$$dark'_n = dark_n - CD_n * ref_n / 100$$

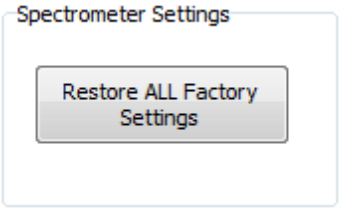
CW_n is the Custom White Reflectance Reference factor at pixel n. In earlier versions of AvaSoft, this factor was set to 100 for each pixel and could not be modified. In AvaSoft version 6 and later, the custom reflectance reference factor is set to 100 by default, but can be set to different values if needed. If the reflectance spectrum of a “white” calibration tile is known, the data can be read from a file, or entered in a table in AvaSoft. The resulting custom reference data can be saved and loaded under a user defined filename. The values can be reset to the default 100% (for white) and 0% (for dark).

CD_n is the Custom Dark factor. In earlier versions of AvaSoft 8.6.3, the Custom Dark factor was set to 0 for each pixel, and could not be modified. In AvaSoft 8.6.3 and later, the Custom Dark factor is set to 0 by default, but can be set to different values if needed. The factor can be set in the table and saved or loaded under a user defined filename.

Click the “Enable” radio button in the “Custom Reflectance Standard” box, and then OK in the Settings dialog to use the customized reference data in AvaSoft.

4.3.4.7 Restore Factory Settings

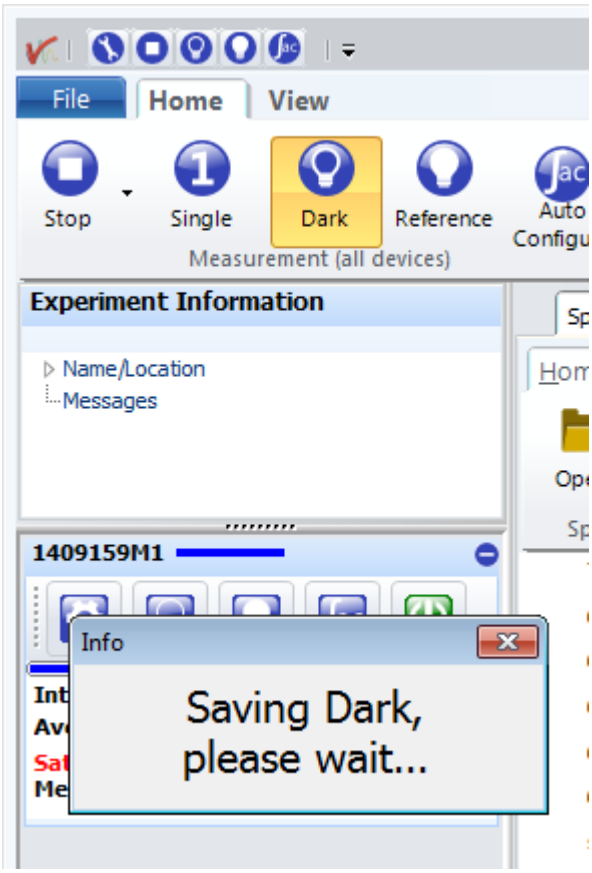
Click the ‘Restore ALL Factory Settings’ button in this screen if you want to restore the original settings that were saved to Eeprom in the factory. Please note that this function is only implemented for the Mini and EVO spectrometers.



This will restore ALL settings of the spectrometer, not just the wavelength calibration coefficients, which can be restored from the Wavelength Coefficients screen.
Please note that AvaSoft buffers these settings in an XML file on disk. You also have to restart AvaSoft here to start with fresh XML files that reflect the original factory settings.

4.3.5 ‘Save Dark Spectrum’ Button

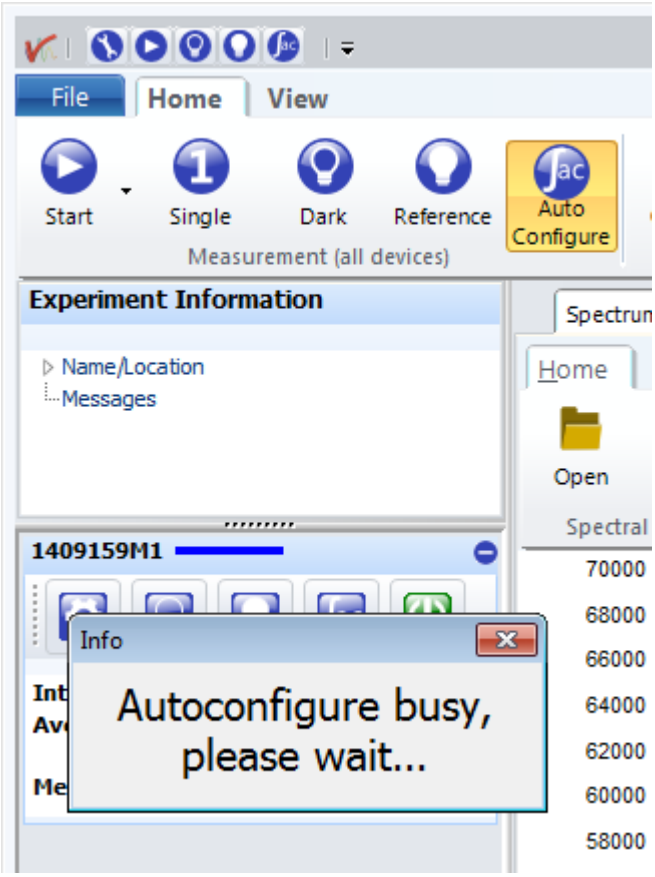
This will save the dark data. The color of the button will change to green when ready.
A message box will indicate saving the dark data is in progress:



4.3.6 'Save Reference Spectrum' Button

4.3.7 'Autoconfigure' Button

After this button is clicked, AvaSoft starts searching for an optimal integration time. Depending on the maximum counts in the last scan, the integration time will be increased/decreased automatically until a scope signal of about 90% of the full scale is measured.
A message box will be shown when the Auto Configure is in progress:



4.3.8 'Activate / Deactivate' Button

This allows you to disable output for this spectrometer, e.g. when you do not want to use a channel in a multi-channel system. The color of the button will then change to red and the other buttons will be grayed and inactivated.

4.3.9 'Progress Bar' Panel Indicator

If using long integration times or a high number of averages, it can take a few or more seconds before a new scan is received by the application. To get an indication about how much time it will take until the next scan arrives, a progress bar can be displayed. After enabling the progress bar by clicking the menu option, it will be displayed after the next scan has arrived. The progress bar will be shown only if the time between scans is more than one second. The time between scans is roughly the integration time, multiplied with the number of averages. However, if the number of averages is high, the time between scans can get longer because of the overhead time that is spent on transmitting the high number of average spectra to the PC.

4.3.10 'Integration Time [ms]' Panel Indicator

If you click the number, an edit box will appear, allowing you to change the value.

This option changes the CCD readout frequency and therefore the exposure- or integration time of the CCD detector. The longer the integration time, the more light is exposed to the detector during a single scan, so the higher the signal. If the integration time is set too long, too much light reaches the detector. The result is that, over some wavelength range, the signal extends the maximum counts (65535 for the 16bit ADC) or in extreme case shows as a straight line at any arbitrary height, even near zero. Entering a shorter integration time can usually solve this. Try to adjust the integration time, such that the maximum count over the wavelength range is around 90% of the full ADC scale (59000 counts for the 16bit ADC). When at minimum integration the signal is still too high, an attenuator, a neutral density filter or fibers with a smaller diameter may be used. When not enough light reaches the spectrometer, likewise a longer integration time should be entered. It's also possible to let AvaSoft search for a good integration time by clicking the Autoconfigure button. If measurements are done in a mode in which reference and dark data are required (all modes except the Scope modes), then new reference and dark spectra need to be saved after the integration time has been changed.

4.3.11 'Averaging' Panel Indicator

If you click the number, an edit box will appear, allowing you to change the value.
With this option, the number of scans to average can be set. A spectrum will be displayed every time this number of scans has been made. This spectrum is the average of the number of scans set here.

4.3.12 'Saturated' Panel Indicator

This field is used to indicate that the spectrometer is receiving too much light at a certain wavelength range (These ADC counts are evaluated before correcting for dynamic dark, smoothing or averaging), in which case the label 'saturated' will become visible.

4.3.13 'Stray Light Correction messages' Panel Indicator

This field is used to indicate possible error or warning messages that are issued when using the Stray Light Correction feature. An extended explanation will be shown as a popup label, when you move the mouse cursor over the error or warning message.
Possible messages are:

- DARK_OK in green: 'No Errors'
- ERROR_1 in red: 'Dark is not up to date'. Dark must be up to date for the Stray Light Correction algorithm to give correct results.
- ERROR_2 in red: 'Dynamic Dark is switched off'. You must enable Dynamic Dark if it is available, as this setting was also used in the calibration of the Stray Light Correction.
- SAVE_DARK! in blue: 'Dark may not be up to date, e.g. Integration Time has changed'. Warning issued when the status of the dark spectrum has changed, e.g. after changing the Integration Time.
- WARNING_4 in blue: 'Reference may not be up to date'. Issued when the reference spectrum was recorded without Stray Light Correction.

4.3.14 'Custom Reflectance' Panel Indicator

This field is used to indicate that the Custom Reflectance setting is active, in which case the label "CR" will become visible.

4.3.15 'Measurements' Panel Indicator

The number of scans taken since the start button was clicked.

4.3.16 'Detector Temp and Setpoint' Panel Indicator

Shows the present detector temperature and the setpoint value for the NIR2.2/2.5 and the TE Cooled USB2 spectrometers.

4.4 Spectrum Application Window

This offers a traditional 2D display of signal versus wavelength. You can load earlier measurements from disk, or show live measurements from attached spectrometers. In Store To Ram mode, only the last measurement of a series is shown.

4.4.1 'Home' Ribbon Tab, 'Open' Button

Loads spectral data in AvaSoft 8 binary format.

4.4.2 'Home' Ribbon Tab, 'Save' Button

Saves spectral data in AvaSoft 8 binary format.

4.4.3 'Home' Ribbon Tab, 'Legend' Button

Shows information about the series present in the chart. You can edit visibility of the series, splining of the line, color of the line and width of the line. The default line width value of 2 can be changed with persistence via Option menu item Look and feel. Allowed width range is 1 to 10. If the series was loaded from disk, you can remove it here by pressing the 'Remove' button. You can also add an integral calculation to each of the series. The start and stop wavelength of the integral calculation can be set, as well as a factor that is applied. Integrals can also be removed in this screen.

4.4.4 'Home' Ribbon Tab, 'Scope Mode' Button

This mode will show a real time raw data signal, with on the Y-axis the read out of the AD-converter and on the X-axis the calculated wavelength.

4.4.5 'Home' Ribbon Tab, 'Scope minus Dark Mode' Button

This mode will also show a real time raw data signal, but corrected for the dark signal that is set.

4.4.6 'Home' Ribbon Tab, 'Absorbance Mode' Button

In Absorbance Mode, the absorbance at pixel n is calculated using the current sample, reference and dark data sets in the following equation:

$$A_n = -\log\left(\frac{sample_n - dark_n}{ref_n - dark_n}\right)$$

4.4.7 'Home' Ribbon Tab, 'Transmittance Mode' Button

In Transmittance Mode, the transmittance at pixel n is calculated using the current sample, reference and dark data sets in the following equation:

$$T_n = 100 * \left(\frac{sample_n - dark_n}{ref_n - dark_n} \right)$$

4.4.8 'Home' Ribbon Tab, 'Reflectance Mode' Button

In Reflectance Mode, the reflectance at pixel n is calculated using the current sample, reference and dark data sets in the following equation:

$$R_n = 100 * \left(\frac{sample_n - dark_n}{ref_n - dark_n} \right)$$

As described in the spectrometer settings section, both the reference (white) percentage of 100 and the dark value can be customized.

4.4.9 'Home' Ribbon Tab, 'Absolute Irradiance Mode' Button

If the Absolute Irradiance Measurements Module has been ordered with AvaSoft, this option will show the absolute energy output in µWatt/cm^2/nm. An elaborate description about the experimental setup in case of absolute irradiance can be found in the section describing the irradiance application.

4.4.10 'Home' Ribbon Tab, 'Relative Irradiance Mode' Button

If the absolute irradiance application is not available, a light source of known color temperature is needed as a reference, for example the AvaLight-HAL with color temperatures of 2850K at default jumper setting. The **relative** radiance energy at wavelength λ is then calculated using the current sample, the reference and the dark data sets:

$$S_\lambda = B_\lambda * (sample_\lambda - dark_\lambda)$$

Where B_λ is the computed component of the spectral distribution of the blackbody radiant emittance (at user selected temperature in degrees Kelvin), divided by the current reference data at wavelength λ

4.4.11 'Home' Ribbon Tab, 'Auto Scale Y-axis' Button

By using this option, the graph will be rescaled on-line. A maximum signal will be shown at about 75% of the vertical scale.

4.4.12 'Home' Ribbon Tab, 'Graphic Reset' Button

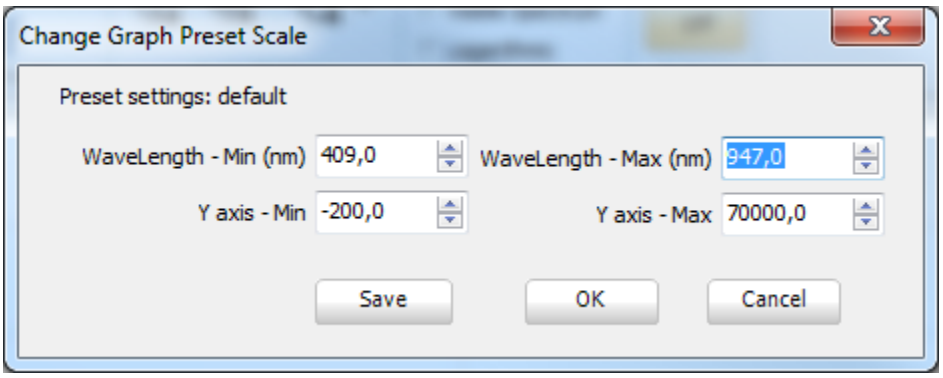
When selecting this option, the graph will be reset to the default X- and Y-axes.

4.4.13 'Home' Ribbon Tab, 'Preset Scale' Button

Pull down menu:

- Edit
- Save Current Scale

Pressing this button will set a preset scale. To preset a scale, you can save the current scale as preset scale by selecting the bottom option from the pull down menu.
You can also edit the scale first, with the following form that will appear after selecting 'Edit' from the pull down menu.



4.4.14 'Home' Ribbon Tab, 'Grid' Checkbox

With the Grid Enable option activated, a grid will be displayed in the graph.

4.4.15 'Home' Ribbon Tab, 'Visible Spectrum' Checkbox

If you select this option, a background will appear that shows the colors of the visible spectrum at the corresponding wavelengths from 380 to 780 nm.

4.4.16 'Home' Ribbon Tab, 'UV Regions' Checkbox

If you select this option, a background will appear that highlights the UV regions at the corresponding wavelengths from 100 to 400 nm.

4.4.17 'Home' Ribbon Tab, 'Logarithmic' Checkbox

If you select this option, the Y axis will be displayed with a logarithmic scale, rather than a linear one.

4.4.18 'Home' Ribbon Tab, 'Photon Density' Checkbox

This option will change the Y axis to Photon Counts [uMol/s/m2/nm]. It only applies in Absolute Irradiance mode.

4.4.19 'Home' Ribbon Tab, 'Hide Chart' Checkbox

Use this option to completely hide the Chart from the screen.

4.4.20 'Home' Ribbon Tab, 'Auto Scale Y-Axis' Checkbox

If you select this option, the graph will be automatically rescaled after each measurement. A maximum signal will be shown at about 75% of the vertical scale.

4.4.21 'Home' Ribbon Tab, 'Wave Numbers' Checkbox

This option allows you to change the unit on the X-Axis from Wavelength [nm] to Wavenumber [cm-1]. Please note that this is only implemented in the Spectrum application. The main screen, the spectrometer settings, all other applications only support display of wavelengths. The only other location wavenumbers are implemented is the file conversion in the main window.

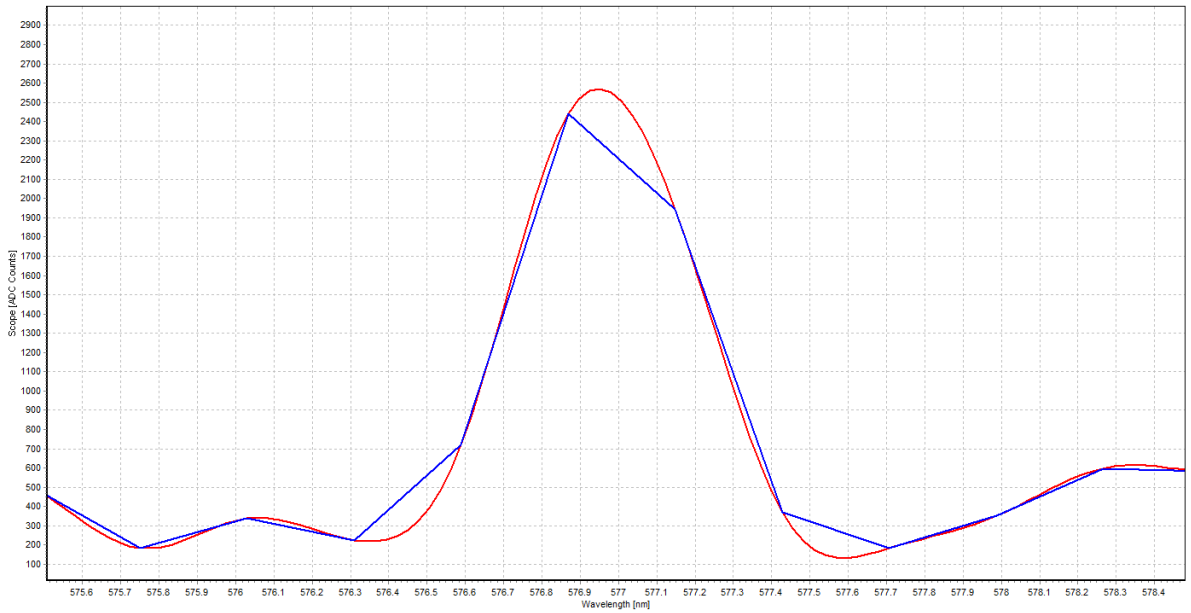
4.4.22 'Home' Ribbon Tab, 'Invert X-Axis' Checkbox

This changes the order of the x-axis from ascending to descending. Note that this option does not change the order of the data in exported files.

4.4.23 'Home' Ribbon Tab, 'Splining' Radio button

This will switch on a cubic spline interpolation of the spectrum.
The spline interpolation can be useful for applications in which the output of line sources (like laser diodes) is displayed, or for other applications which require a high resolution. Note that for the AvaSpec-2048 with 2048 pixels, the effect of spline interpolation is not visible if the data is shown at full scale. The monitor resolution will probably be less than 2048 pixels. The effect of spline interpolation can only be visualized if the number of detector pixels that are displayed is smaller than the number of monitor pixels at the x-axis.

In the figure below, the effect of spline interpolation is illustrated. The blue line shows the AD counts for about 10 pixels, connected by a straight line (linear interpolation). The data for the red line is exactly the same, but this time the cubic spline interpolation algorithm has been applied, resulting in data which is smooth in the first derivative and continuous in the second derivative.



4.4.24 'Home' Ribbon Tab, 'First Derivative' Radio button

This will show a first derivative of the spectral data, calculated as a (delta y / delta x) value for each pixel.

4.4.25 'Home' Ribbon Tab, 'Second Derivative' Radio button

This will show a second derivative of the spectral data, calculated as a (delta(delta y) / delta x) value for each pixel.

4.4.26 'File' Ribbon Tab, 'Open Spectral Data' Button

Loads spectral data in AvaSoft 8 binary format. This option is repeated from the 'Home' menu.

4.4.27 'File' Ribbon Tab, 'Import V7 Spectral Data' Button

Loads spectral data in AvaSoft 7 binary format.

4.4.28 'File' Ribbon Tab, 'Save Spectral Data' Button

Saves spectral data in AvaSoft 8 binary format. This option is repeated from the 'Home' menu.

4.4.29 'File' Ribbon Tab, 'Export Spectral Data' Button

Pull down menu:

- ASCII
- Excel (New File)
- Excel (Existing File)
- JCAMP
- GRAMS
- Active FWHM (ASCII)

Saves spectral data in one of several popular formats. Note that this only exports the LIVE data. To convert existing files, please use the 'Convert File To' option in the main window.

You can export to Excel either to a new file, or to an existing Excel file. In the latter case, you will get a dialog to choose the existing excel file. The data will be added in a column to the right of the existing data in a separate tab sheet per spectrometer used.
Please note that Excel must be installed to use this feature. Some versions of Excel (notably the 2010 'Starter' version) do not support the OLE Automation that is used here.

Note that ASCII, JCAMP and GRAMS can be optionally saved in equidistant format (meaning the points are evenly spaced on the x axis). You will have to select this in the 'Save Options' menu, which you can access by clicking the 'Options' button in the main form.

The last option lets you export a table of all selected FWHM values in the window to ASCII.

4.4.30 'File' Ribbon Tab, 'Copy Graph' Button

This will store the graph on the clipboard, allowing you to paste it into other applications.

4.4.31 'File' Ribbon Tab, 'Save Graph As' Button

Pull down menu:

- Rich Text Format (*.rtf)
- Windows Bitmap (*.bmp)
- Compressed bitmap (*.jpg)
- Portable Network Graphics (*.png)
- Acrobat Reader (*.pdf)

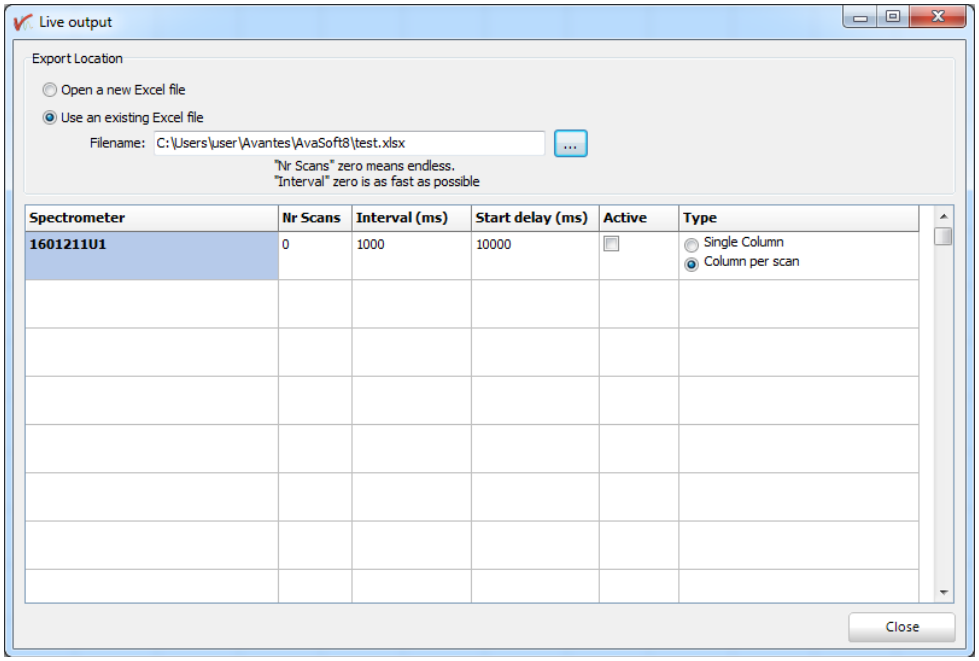
Saves the graph in one of several popular formats. Note that the .rtf format is a Microsoft format that will open in MS Word. The saved file holds a .png graph that you can extract from it if necessary.
The .pdf format that we export does not support transparency. If your graph has transparent parts (e.g. when if contains an integral), please select a different format.

4.4.32 'File' Ribbon Tab, 'Print Graph' Button

Will open a standard Windows Print dialog.

4.4.33 'File' Ribbon Tab, 'Live Excel Output' Button

Will save live spectral data to Excel, either to a single column, where new data overwrites the old, or to a new column per scan. You can export to Excel either to a new file, or to an existing Excel file.



You can set the number of scans, the scan interval and the start delay (the delay before the first scan is saved) in the appropriate columns. You can set endless saving by selecting 0 scans. Check the 'Active' box to enable the export. Select the type of scanning in the rightmost column. 'Single Column' will overwrite the scan data each time into the same column, 'Column per scan' will extend the spreadsheet with each new scan.

4.4.34 'File' Ribbon Tab, 'Save Live Output Periodically' Button

Saves complete live spectral data periodically, in AvaSoft 8 format. Remember to first set this option when spectrometer is not started before being able to save later in 'Live' output mode. On the bottom of the AvaSoft screen a message will appear with text "Live Output Enabled" Also live merged spectral data can be stored in scope mode to disk automatically after selection of a merge group channel. Filenames can be configured to include a time stamp and/or date stamp. The output can be either in binary or ASCII format. When the output is in ASCII, the number of wavelength and measurement decimals can be defined in the export options  , which is part of the global options.

4.4.35 'Tools' Ribbon Tab, 'New Integral' Button

You can also add an integral calculation to each of the series. The start and stop wavelength of the integral calculation can be set, as well as a factor that is applied. Integrals can be removed in the screen that is shown after pressing Legend button.

4.4.36 'Tools' Ribbon Tab, 'Magnify Tool On' Button

Switches on the Magnify tool. You can select the magnification in the pull down menu.

4.4.37 'Tools' Ribbon Tab, 'Magnify Tool Off' Button

Switches off the Magnify tool.

4.4.38 'Tools' Ribbon Tab, 'Assign Cursor' Button

Pull down menu:
- 'None'
- Spectrometer ID

You can assign a cursor to a Chart series here. The cursor consists of a vertical and a horizontal line. If you hover over a line, the mouse cursor will change into a 'splitter' shape, if you then press the left mouse button, you can drag the line to another position. The vertical line will snap to the next pixel position.

The status line will display the cursor position with a value for the wavelength and the amplitude. You can remove the cursor by selecting 'None' in the pull down menu.

4.4.39 'Tools' Ribbon Tab, Cursor Wavelength Edit Box

You can place the vertical cursor line on a specific wavelength by entering the value in the edit box and pressing the 'OK' button.

4.4.40 'Tools' Ribbon Tab, 'Spectrum Chart Name' Button

This option allows you to change the name of the application window.

4.4.41 'Tools' Ribbon Tab, 'Base Line On' Button

This will show a horizontal line on the screen, with a value on the left side of the screen. You can move the line up and down by moving the mouse over it until the cursor changes into a 'splitter' shape. Next press down the left mouse button and drag the line up or down.

4.4.42 'Tools' Ribbon Tab, 'Base Line Off' Button

This will hide the horizontal line.

4.4.43 'Tools' Ribbon Tab, 'Show Legend' Checkbox

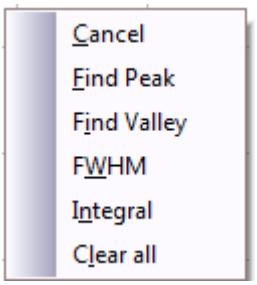
If you check this box, a legend will be shown to the right of the chart. Note that this take up a lot of screen space, as it shows the Friendly name, which can be up to 64 characters.

4.4.44 Status Bar

The status bar at the bottom of the spectrum application window is used to display wavelength and intensity data for the cursor

4.4.45 Peak Submenu

When you click the right button of your mouse in the graphical region, a pop up menu will be shown.



Click ‘Cancel’ to go back.
Click ‘Find Peak’ to position a cursor line on the peak nearest to the mouse position. The following procedure is used:

- The wavelength is determined from the position the mouse click occurred.
- The data from closest pixel is retrieved
- The direction to search for the peak is determined from the neighbor pixels. If both neighbor pixels have a lower value at the Y-axis than the current pixel, the current pixel is already a peak. If only one of the neighbor pixel values is higher than the current pixel value, the peak will be searched in the direction of this higher pixel. If both neighbor pixels have a higher value at the Y-axis than the current pixel, the current pixel is in a valley. The peak will in this case be searched in the direction of this neighbor pixel with the highest value.
- The cursor starts moving in the direction, as determined under 3), until it reaches a pixel of which the value is not higher than the last one evaluated. At this pixel the cursor stops.

Click ‘Find Valley’ to position a cursor line on the valley nearest to the mouse position. This uses the same procure.
Click ‘FWHM’ to calculate an FWHM value of the peak the mouse is over. An area of the chart will be marked in a transparent color with the FWHM width. The FWHM value will be printed to the top right of this area.
Click ‘Integral’ to add an integral value.
Click ‘Clear All’ to clear all Peak, Valley and FWHM markings.

If more than one spectrum is being displayed, a dialog will popup that lets you select which spectrum will be used by the peak finder or the FWHM calculator.

4.4.46 Find Peaks or Valleys by CTRL or SHIFT + Right Mouse Button Click

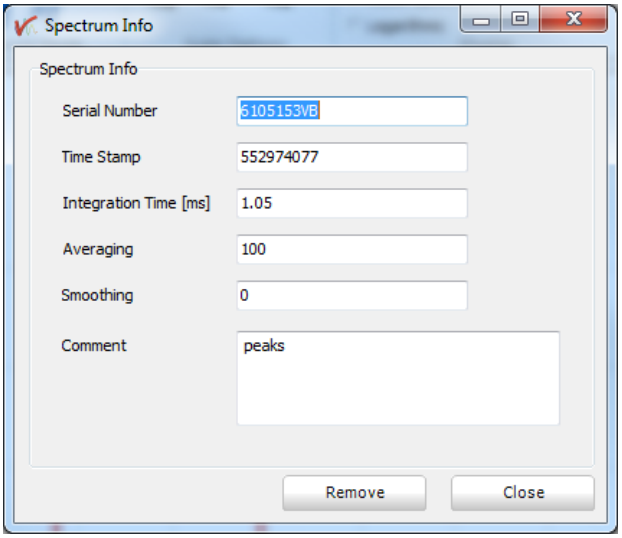
If the cursor is visible, you can use it to find the value of valleys or peaks.
When the right mouse button is clicked in the graphical region, while the CTRL key is down, AvaSoft will follow the procedure described above to run the cursor to the closest peak:

By holding down the SHIFT key instead of the CTRL key, the same procedure will be used to move to the closest valley.

To mark a peak for which the FWHM values need to be calculated, press the ALT key, and click with the right mouse button on this peak.

If more than one spectrum is being displayed, a dialog will popup that lets you select which spectrum will be used by the peak finder or the FWHM calculator.

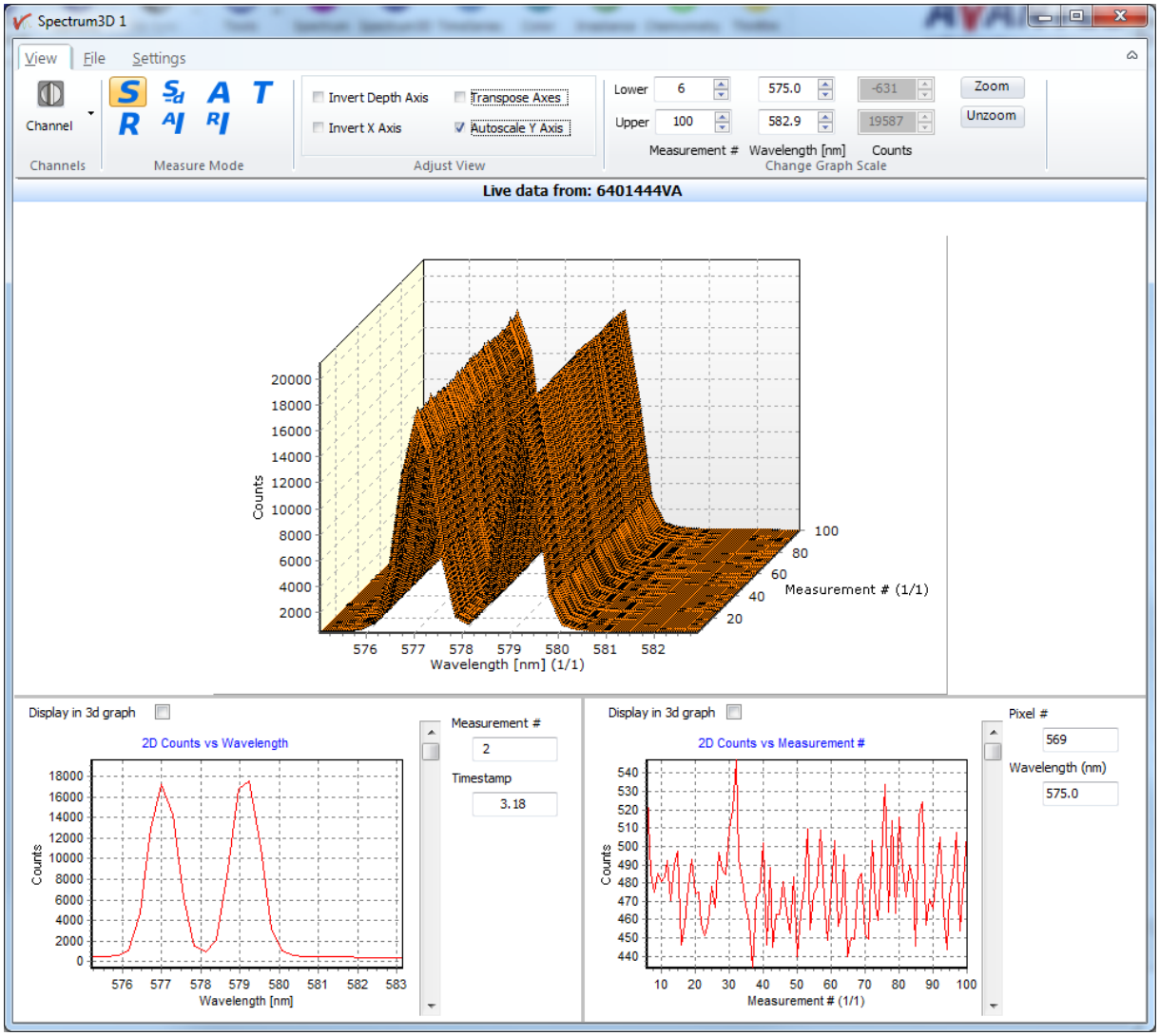
4.4.47 Spectrum Info Window



If you left click on a graph series in the graphical region, a window will appear with some info about the spectrum that is shown in the graph. You can also remove the series by pressing the ‘Remove’ button.

4.5 Spectrum3D Window

This shows a 3D display of your data against both wavelength and measurement number. You can load and display earlier date from disk, or you can display live date from attached spectrometers in Store To Ram mode. The window includes two charts in 2D, which show data against wavelength and data against measurement number.



The view of the 3D graph can be adjusted by inverting the Depth axis and the X axis. These axes can also be transposed, which enables a side view of the graph.
The Y axis is auto scaled by default, this can be undone by unchecking the option in the ‘Adjust View’ box.

The 2D graphs both have a scrollbar, which allows you to change the third dimension. It is also possible to display the position of each 2D graph in the 3D graph by displaying a separate highlighted line that sections the 3D graph. This feature is turned on and off with the ‘Display in 3D Graph’ checkbox at the top-right position of each 2D graph.

The amount of data in the 3D graph and the second 2D graph (Counts vs. Time) has been limited to prevent computer overload. If more data is present, only one out a calculated number of scans or pixels is shown. Zooming the graphs will reveal more detail. The fraction of the data that is shown is indicated in the title of the relevant axis.

E.g. ‘Measurement # (1/10)’ means that only one out of every 10 scans is shown.

Note that the first 2D graph (Counts vs. Wavelength) always shows all of the data present. It is therefore possible to show this graph as a highlighted line in the 3D graph that shows more detail than the 3D graph itself shows. Zooming in will show more detail in the 3D graph, which will eventually correct the discrepancy.

You can zoom both 2D graphs and the 3D graph will zoom to the selected range after double clicking the 2D graph. The selected range will then also be shown in the manual selection boxes described below.

Unzooming the 2D graphs will also unzoom the 3D graph. Note that zooming and unzooming the 2D graphs is performed the same way as in the main screen of AvaSoft:

You zoom the graph by clicking the top-left corner of your area to select, hold down the left mouse button, then draw a rectangle and release the mouse button at the lower-right corner of the area to select.

You unzoom the graph by clicking anywhere on the graph, hold down the left mouse button, then drag a rectangle towards the top and left and release the mouse button at any position.
You can pan the 2D graphs by holding down the middle mouse button.

It is also possible to manually select the ranges by entering values in the ‘Measurement #’, ‘Wavelength [nm]’ and ‘Counts’ boxes, and pressing the ‘Zoom’ button. Note that changing the ‘Counts’ will only have an effect if the ‘Autoscale Y-axis’ option is unchecked. The ‘Unzoom’ button will undo all your changes.

After your selection is made, you can save the scans to disk by pressing the ‘Save Separate Files’ button. Each scan will result in a file written to disk, a .raw8 file in scope mode.
If you save the .raw8 files to Excel, using AvaSoft ‘File’-‘Convert File To’-‘Excel’ in the main screen, the timestamp values from the scans will be written into Excel in row 6 of each data column, allowing you to use these timestamp values in calculations.

The files are numbered consecutively, a five digit number is affixed to the filename you enter in the dialog. The starting number of the sequence is the lower limit of the range of selected scans. Only the presence of a previous version of this file will trigger an overwrite warning in the dialog. All consecutive scans will silently overwrite previous versions with the same filename.

Note that the scans that are saved are all full scans, only the values entered in ‘Measurement #’ boxes have an effect here. If you want to limit the wavelength range in the files, you will have to do this in the spectrometer settings screen, as described above.

Although it is possible to use the Spectrum3D application to measure huge amounts of scans with a limited wavelength range, we strongly advise you to save only a limited amount of scans.
If you select 50000 scans to save, the huge number of small files to save will bring your computer to a near standstill.
For this reason, a warning has been built in when you want to save more than 2500 scans.

You can save the graphs to disk by pressing the ‘Save (rtf) Graph’ button. You can first enter a comment line, which will be included on the page. Next, you can enter the filename that will be used to save the graphs. The three graphs will be saved in PNG format, embedded in a single, one page .RTF file. You can open this file with Microsoft Word, edit it, extract the graphs, change the size of the graphs, etc.
You can also export the 3D graph to a number of formats by selecting a format from the ‘Export Graph’ button. You can select between .bmp, .jpg, .png and .pdf formats.

4.5.1 'View' Ribbon Tab, 'Channel' Button

You can select the channel here, in case you have multiple spectrometers attached.

4.5.2 'View' Ribbon Tab, Measure Mode Selection

Please refer to sections 4.4.4 to 4.4.10 for an explanation of the measure modes.

4.5.3 'View' Ribbon Tab, Adjust View Selection

Allows predefined changes in the display of the 3D graph.

Invert Depth Axis:	This changes the order of the depth axis from ascending to descending.
Invert X Axis:	This changes the order of the x axis from ascending to descending.
Transpose Axes:	Swaps the wavelength and measurement # axes.
Autoscale Y Axis:	Uncheck this if you want to manually change the scale of the y axis.

4.5.4 'View' Ribbon Tab, Change Graph Scale

You can manually set the axis scales of the 3D graph here. Press the 'Zoom' button after changing the values. Press 'Unzoom' to return to the full scale. Note that changing the values for 'Counts' will only work if the 'Autoscale Y-axis' option is unchecked.

4.5.5 'File' Ribbon Tab, 'Open Separate Spectra Files' Button

Allows you to select previously saved separate scans into a 3D graph.

4.5.6 'File' Ribbon Tab, 'Save Scans to Separate Files' Button

Allows you to save data in the 3D chart to separate files.

4.5.7 'File' Ribbon Tab, 'Open Single File Data (*.str)' Button

Loads multiple scans from a single file in Store To Ram format.

4.5.8 'File' Ribbon Tab, 'Save Single File Data (*.str)' Button

Saves the scans that are shown to a single Store To Ram file.

4.5.9 'File' Ribbon Tab, 'Export to Excel' Button

Exports the scans that are shown to an Excel sheet.

4.5.10 'File' Ribbon Tab, 'Export to Ascii' Button

Saves the scans that are shown to a single text file, in table form.

4.5.11 'File' Ribbon Tab, 'Save Graphs' Button

Saves the graph in Rich Text Format (*.rtf). Note that the .rtf format is a Microsoft format that will open in MS Word. The saved file holds a .png graph that you can extract from it if necessary.

4.5.12 'File' Ribbon Tab, 'Export 3D Graph' Button

Pull down menu:

- Bitmap (*.bmp)
- Windows Compressed bitmap (*.jpg)
- Portable Network Graphics (*.png)
- Acrobat Reader (*.pdf)

Saves the graph in one of several popular formats.

4.5.13 'Settings' Ribbon Tab, 'Input File Sort Order' Selection

Choose between 'Alphabetically' and 'File Date/Time' here. Since the Windows File Date/Time stamp has a limited resolution, it may be necessary to use Alphabetically ordered files.

4.6 Time Series

The Time Series application (or History Channel application) allows you to follow a number of functions or integrals against time. You can save the resulting values to disk or export them live to an Excel sheet. You can also drive both digital and analog outputs with the resulting values, comparing them with preset values.

4.6.1 'Function' Ribbon Tab, 'Start / Stop' Button

Used to start and stop recording. If you check the 'follow main' checkbox, you can start recording by pressing the Start button in the main AvaSoft windows, together with starting the spectrometers.

4.6.2 'Function' Ribbon Tab, 'New Function' Button

Use to prepare a new setup file for a time series

4.6.3 'Function' Ribbon Tab, 'Function' Selection

Use the drop down box to select time series settings that were saved in an earlier session.

4.6.4 'Function' Ribbon Tab, 'Device' Field

Shows the device that is used in the selected time series function.

4.6.5 ‘Function Entry’

- ‘Function’ ribbon tab, ‘Time Series Function’ Selection
- ‘Function’ ribbon tab, ‘Parameters’ Button

Both are used for entry of a time series function.

The functions are defined in a dialog, which can be reached by selecting a “Function Type” or by clicking the “Parameters” button. Select the function type by changing the radio button to one of the choices: Integral, User, Peak, Irradiance, Color or Script. Next press the ‘Parameters’ button.
A form will be opened, in which Measure Mode, Function Definition, Function Display Settings, Function output Settings and Function Digital or Analog Output can be set.

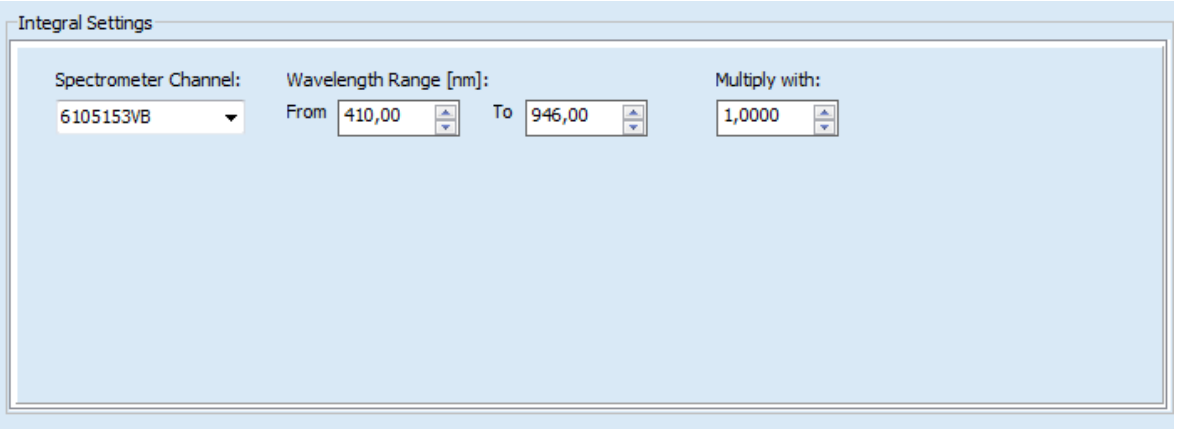
4.6.5.1 Measure Mode

The eight possible modes (Scope, Scope – Dark, Absorbance, Transmittance, Absolute Irradiance, Reflectance, Relative Irradiance or Temperature) are described in sections 4.4.4 to 4.4.10. Temperature mode can be used to display detector or board temperature against time in the user function type. Note that if the selected measure mode is Absorbance, Transmittance, Reflectance or Irradiance reference and dark spectra need to be saved or loaded before the Time Series Measurements can be started.

4.6.5.2 Function Definition

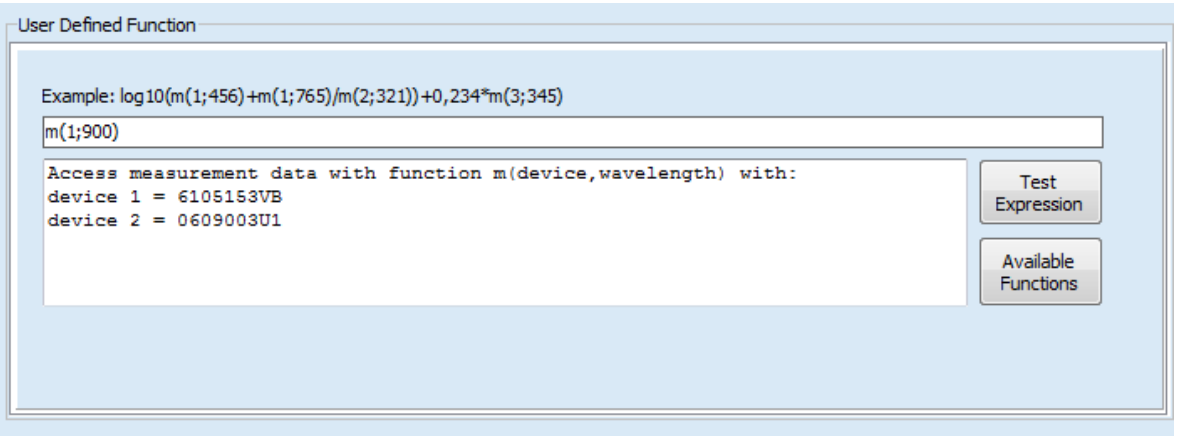
The parameters that need to be entered in the Function Definition Box depend on the Function Type that has been chosen: Integral, User Defined, Peak, Irradiance, Color or Script.

4.6.5.2.1 Function Definition: Integral Function



In case a function is defined to display the integral versus time, the following parameters can be set:
Spectrometer Channel. Select the channel in the drop down menu box.
The “from” and “to” edit boxes may be changed to specify the wavelength range in nanometer over which the integral needs to be calculated.
Finally, a multiplication factor can be entered. The value entered here is multiplied with the calculated integral.

4.6.5.2.2 Function Definition: User Defined Function



If you want to display the output of a self-defined function against time, a function needs to be defined first.

Input Functions:
A comprehensive example of an input function is given in the dialog, but it illustrates only a few of the functions AvaSoft can handle. A list of allowed operators and functions is given below:
Operators: *, /, +,-

Functions:

abs	arctan	cos	exp	frac	int	trunk	ln	pi
round	sin	sqr	sqrt	arccos	arcsin	arctan2	tan	cotan
hypot	cosh	sinh	tanh	arccosh	arcsinh	arctanh	lnxp1	log10
log2	logn	ceil	floor	log	dettemp	brdtemp	wavval	m

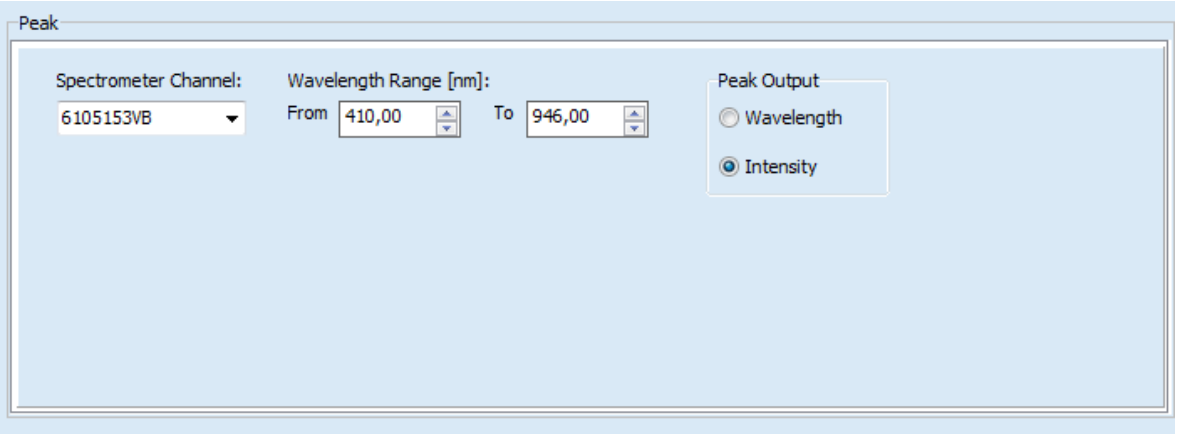
The list of functions includes a fairly complete collection of math functions, some functions have duplicate names for compatibility reasons (log, logn and ln, wavval and m)
Dettemp(1) will give the detector temperature of device 1
Brdtemp(1) will give the board temperature of device 1

Note that the syntax depends on your setting for decimal separator. If your decimal separator is a comma, you will need a semicolon between parameters. If your decimal separator is a point, then you need a comma between parameters.

In the US, the example line reads:
Example: `log10(m(1,456)+m(1,765)/m(2,321))+0.234*m(3,345)`

In Europe, it reads:
Example: `log10(m(1;456)+m(1;765)/m(2;321))+0,234*m(3;345)`

4.6.5.2.3 Function Definition: Peak Function

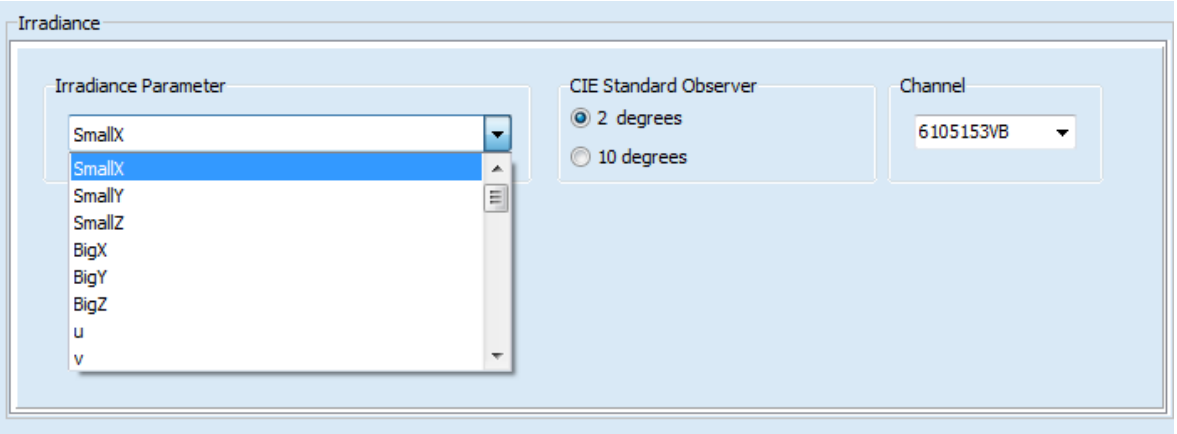


In case a function is defined to display a peak versus time, the following parameters can be set:
The Spectrometer Channel. Select the channel in the drop down menu box.

The “from” and “to” edit boxes may be changed to specify the wavelength range in nanometers, which will be evaluated in the peak search. Finally, a selection can be made to define the Peak Output: Wavelength or Intensity.

If both wavelength and intensity need to be followed against time, one of the time series can be used to follow the peak wavelength, and another one to follow the peak intensity.

4.6.5.2.4 Function Definition: Irradiance Function



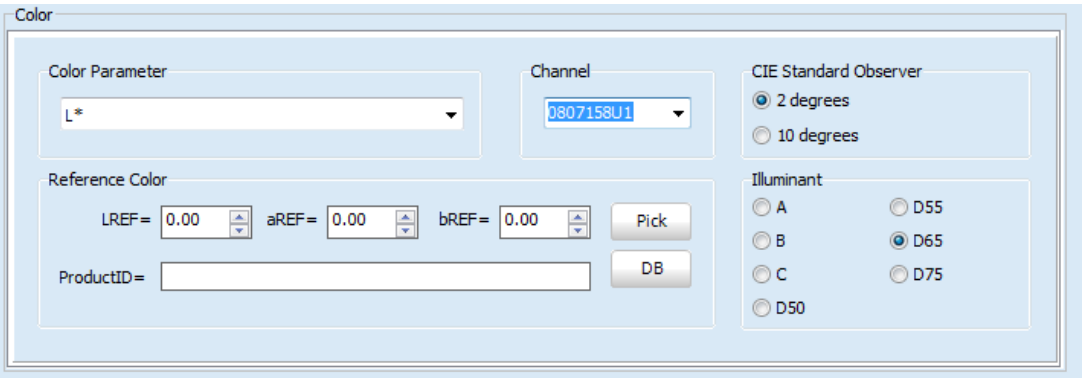
With time series irradiance measurements, radiometric parameters can be followed simultaneously in a graph against time. The following parameters can be set:

- Irradiance parameter: select the parameter from the drop down menu box.

Depending on choice of irradiance parameter, more parameters can be set:

- CIE Standard Observer. The original CIE standard observer functions x_λ, y_λ and z_λ were defined in 1931, and are known as the 2 degrees standard observer values. The 2 degrees corresponds with the angle of vision that was used in the experiments to determine these standard observer values. In 1964, the CIE recommended the use of different observer values for a higher correlation with visual perception for large samples. These are known as the 1964 supplementary standard observer, or 10 degrees observer values. Both standards are still in use, and in AvaSoft, the CIE standard observer can be selected by clicking one of the radio buttons. The default is 2 degrees.
- Spectrometer Channel: select the channel in the drop down menu box. Make sure white reference and dark spectra have been saved before for the selected spectrometer channel.
- Wavelength Range: The wavelength range is the spectral range over which the radiometric output will be integrated. For colorimetric parameters, this range is already set to 380 nm-780 nm, and cannot be changed.
- Emittance Parameters: If the source is not inside an integrating sphere, the radiant intensity (in µWatts/sr) and radiant energy (in µJoule/sr) can be calculated if the distance from source to diffuser surface has been specified. The radiant flux (µWatts emitted) and emitted energy (µJoule e.) can be calculated if the geometry of the lamp (in steradians) is specified.

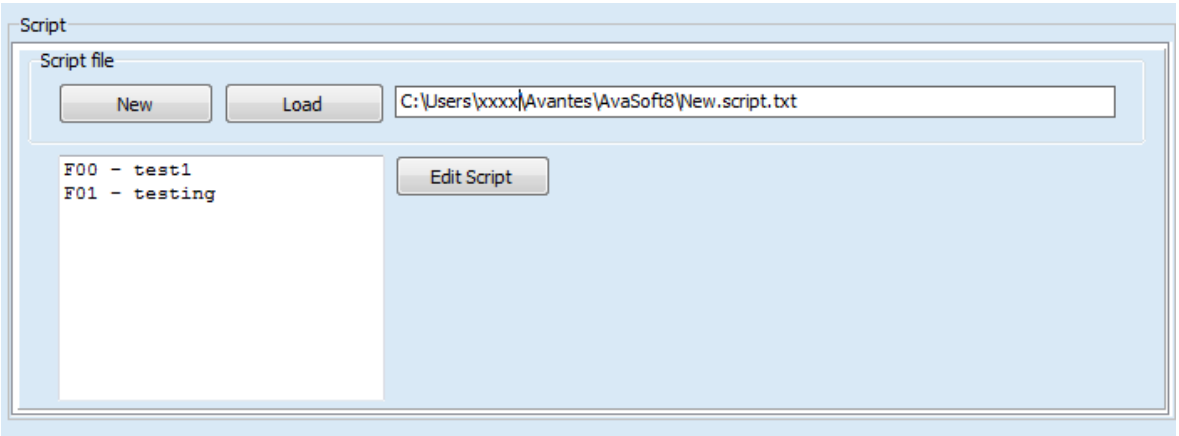
4.6.5.2.5 Function Definition: Color Function



With time series color measurements, color parameters or color differences can be followed simultaneously in a graph against time. The following parameters can be set:

- Color parameter: select the parameter from the drop down menu box.
- Spectrometer Channel: select the channel in the drop down menu box. Make sure white reference and dark spectra have been saved before for the selected spectrometer channel.
- CIE Standard Observer. The original CIE standard observer functions x_λ, y_λ and z_λ were defined in 1931, and are known as the 2 degrees standard observer values. The 2 degrees corresponds with the angle of vision that was used in the experiments to determine these standard observer values. In 1964, the CIE recommended the use of different observer values for a higher correlation with visual perception for large samples. These are known as the 1964 supplementary standard observer, or 10 degrees observer values. Both standards are still in use, and in AvaSoft, the CIE standard observer can be selected by clicking one of the radio buttons. The default is 2 degrees.
- Illuminant. The CIE Standard sources A, B or C or one of the illuminants D50, D55, D65 or D75 can be selected by clicking one of the radio buttons. The default is D65, which is the most widely used illuminant. It represents the power distribution of average daylight, with a correlated color temperature of 6500K. The D50, D55 and D75 have correlated color temperatures of 5000K, 5500K and 7500K. The CIE Standard sources A, B or C represent respectively: Incandescent light (2854K blackbody), Simulated noon sunlight and Simulated overcast sky daylight. Note that there is no relation between the illuminant chosen here and the light source that is used for measuring the color of an object. The selected illuminant is used in calculation of the color parameters. These color parameters will be different if for example A will be selected instead of D65, just as the color of an object will look different in average daylight or in incandescent light (2854K blackbody).
- Reference Color. If one of the color difference parameters (dL, da, db or dE) is selected, the reference color to which the measured color needs to be compared needs to be defined as well. You can enter L, a and b values and a product ID for your reference color. You can also select the reference values from a data base with the ‘Pick’ and ‘DB’ buttons.

4.6.5.2.6 Function Definition: Script Function



A scripting feature has been added to allow you to use more complicated calculations with many more mathematical and logical functions. Scripts will also allow you to combine the results of several time series.

AvaSoft uses the Microsoft VBScript language that comes with your copy of Windows. We have included a help file for VBScript for your reference. You can reach it from the main menu by selecting ‘Help’, ‘VBScript’. It lists among other things all available operators and functions.

The script references other time series results by their number. The available ones are listed in the box at the lower left part of the screen above. You must have defined other time series to use scripts.

You can start a new script by pressing the ‘New’ button, or load an existing one by pressing the ‘Load’ button. AvaSoft includes a simple script editor. The scripts are plain ASCII files, named name.script.txt.

An example of a script being edited is listed below.

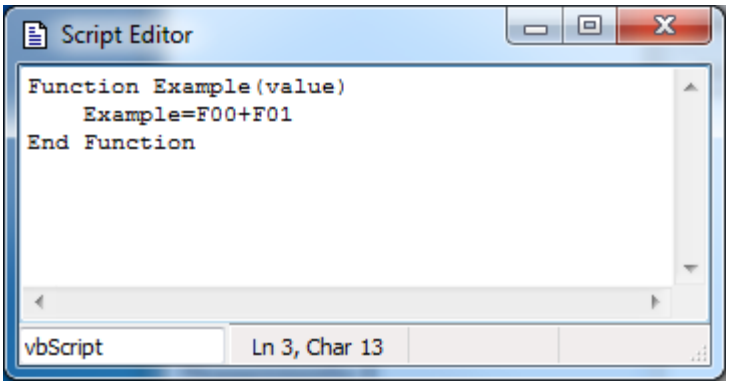
A starter script has the following contents:

```
Function Example(value)
      Example=0
End Function
```

You can elaborate on this function, as long as there is a value assigned to Example in the end. In this case, Example will be assigned the value 0.

You can refer to the other time series with the predefined variables F00 to F99. If you want to use data from the spectrometer, you will need to assign other time series to e.g. wavelength values or integrals. The following script defines the function value for Example as the sum of F00 and F01.

```
Function Example(value)
      Example=F00+F01
End Function
```



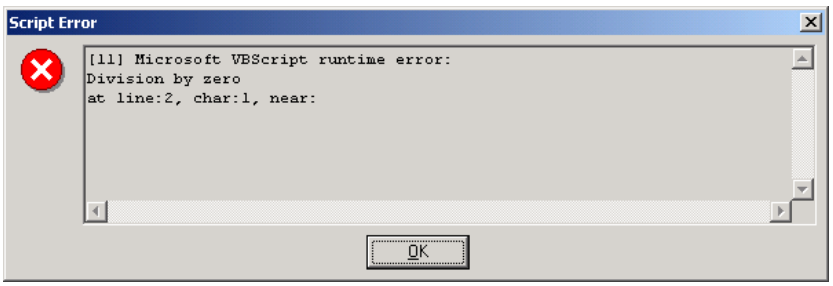
Please do not refer to the function value for the script itself, F02 in the case above. You can also not refer to other functions, if these are themselves assigned to a script. This will result in a scripting run-time error. If you want to use code from another script, please copy the necessary lines from that script into the one you’re working with.

Please understand that a script is executed by an interpreter, on a line by line basis. If you make a syntax error in your script, it will usually only show at the moment the line with the error is executed, as a run-time error.

Nothing will stop you, for instance, from entering the following script for function 3:

```
Function Error(value)
  Error=F1/0
End Function
```

Running this script will result in the run-time error at the right:

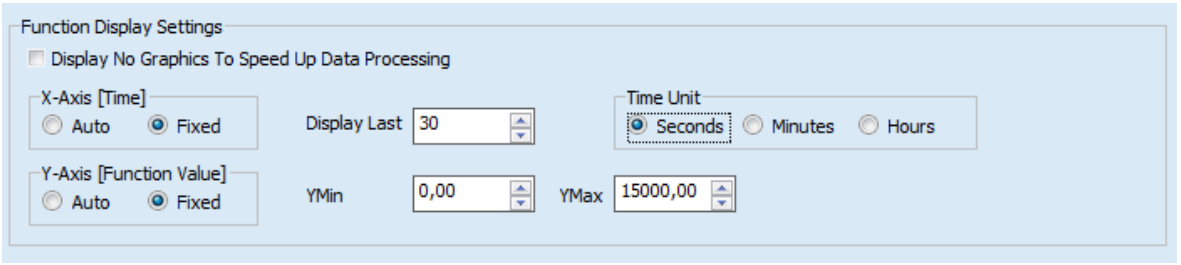


If you refer to channels that are undefined**,** they will be handled as uninitialized variables by VBScript, with value 0. This is the case for all uninitialized variables you might use in your scripts.

Finally, a small example to monitor the integral of a peak between 522 nm and 550 nm, in which an offset is subtracted. The offset area is the area below of the straight line between the output at 522 nm and the output at 550 nm.
F00 is defined as a user defined input function: m(1;522)
F01 is defined as a user defined input function: m(1;550)
F02 is defined as the zero-based integral between 522 nm and 550 nm.
The script for function Test can then be written as:

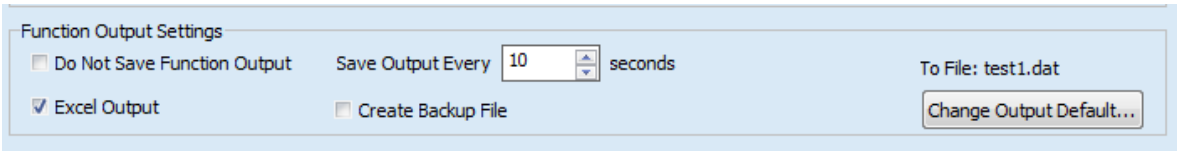
```
Function Test(value)
      If F00 > F01 Then
            offset = 28*(F01 + (0.5*(F00-F01)))
      Else
            offset = 28*(F00 + (0.5*(F01-F00)))
      End If
      Test = F02 - offset
End Function
```

4.6.5.3 Function Display Settings



Output is displayed graphically against time. The amount of time that will be displayed at the X-axis can be set manually by clicking the Fixed radio button. If set to Auto, the time axis will be set to 1 minute. The Y-Axis can also be set to Fixed or to Auto. The Auto option will set the Y-axis range to the minimum and maximum function values that are in the list of measured data points.
The 'Display No Graphics To Speed Up Data Processing' option is provided for situations, where an application requires fast data processing (e.g. more than 10 scans per second).

4.6.5.4 Function Output Settings



The results of a time series experiment will be saved to an ASCII-file except when the option "Do Not Save Function Output" has been checked. A number of seconds between saving can be entered for data reduction, in case measurements are carried out over long periods. Entering a value of zero results in saving every scan. The name of the file to which the data will be saved, can be changed after clicking the "Change Output Default…" button. You can enable or disable the possibility to create a backup file during the measurements with the 'Create Backup File' checkbox. If this option is enabled, AvaSoft will create a backup file with the same filename, but with the extension *.bak (also in ASCII). This backup file is updated every scan and can be used in case the filename that has been selected has failed to save the data, for instance because of a power failure during the measurements.

You can export the Data to Excel by enabling the 'Excel Output' option. The sheet will be called 'AvaSoft Data', each time series will use three columns that e.g. for the first time series will contain the following data:

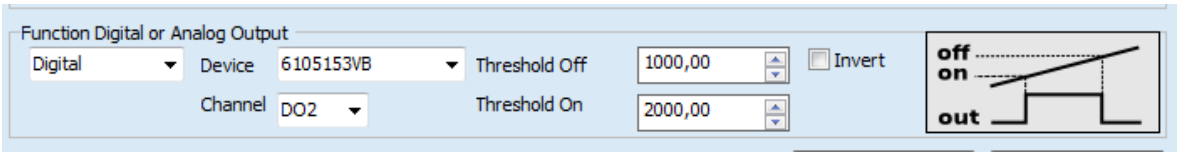
Column A contains a data/time value, formatted as 'dd:mm:yyyy hh:mm:ss'. This is a floating point value, in which the integer part is the day number, starting at January 1, 1900 with day 1. The fractional part represents a decimal time value, where 0.5 is 12:00 h. noon and 0.75 is 18:00 h.

This way, differences in date/time can be readily calculated by subtracting values, which would be much more difficult if this was a text representation.

Column B contains a time value, representing the elapsed milliseconds since midnight. This value does not have a one millisecond resolution. Remember that Windows is not a real-time operating system. It can, however, be used as a reasonably accurate indicator of the time that passes between scans.

Column C contains the time series values.

4.6.5.5 Function Digital or Analog Output



AvaSoft 8 lets you operate any available digital and analog output with every time series value. The output pins on the High Density 26-pole Sub-D connector which are used for this function are listed in the table below:

HD DB26 pins used by AvaSoft 8 Digital or Analog Output	
Signal Name	**Connector Pin[8]**
LED	11
DO2	2
DO3	20
SHUTTER	12
DO5	3
DO6	21
DO7	13
DO8	4
DO9	22
DO10	25
AO1	17
AO2	26
GND	8

The analog output signal is a 0-5V signal, with an 8 bit resolution (0.02V steps). To set minimum and maximum threshold values for the time series, values can be entered in the Threshold Off and On boxes. If 'Invert' is not selected, the corresponding output pin will be set high if the time series output

[8] Please note that pin numbers are valid for DB26 connectors on -USB2 and –EVO spectrometers

value lies between the minimum and maximum value. It will be set low if the time series output value exceeds the maximum value OR is smaller than the minimum value.

If 'Invert' is selected, the corresponding output pin will be set high if the time series output value exceeds the maximum value OR is smaller than the minimum value. It will be set low if the time series output value lies between the minimum and maximum value.

If you want to monitor both threshold values, you can assign two (identically configured) time series. To monitor a single level, set one threshold value to the desired level, and the other one to a value that is out of range, e.g. Min to –99999999 and Max to 1000, or Min to 2000 and Max to 99999999. That way, you will only need a single channel per threshold value.

To specify the time series function range(s) that should be converted into a 0-5V analog output signal, enter values in the 'Range Max' and 'Range Min' boxes.
For example, if you enter 100 and 50 for the ranges, the voltage will be calculated as follows:

`5.0*(x - 50.0)/(100.0 - 50.0)` where x is the output value of the time series.

4.6.6 'Graph' Ribbon Tab, 'Open' Button

Opens data from previous sessions and shows them in the graph.

4.6.7 'Graph' Ribbon Tab, 'Export' Button

Pull down menu:

- Windows Bitmap (*.bmp)
- Compressed bitmap (*.jpg)
- Portable Network Graphics (*.png)
- Acrobat Reader (*.pdf)

Saves the time series graph in one of several popular formats.

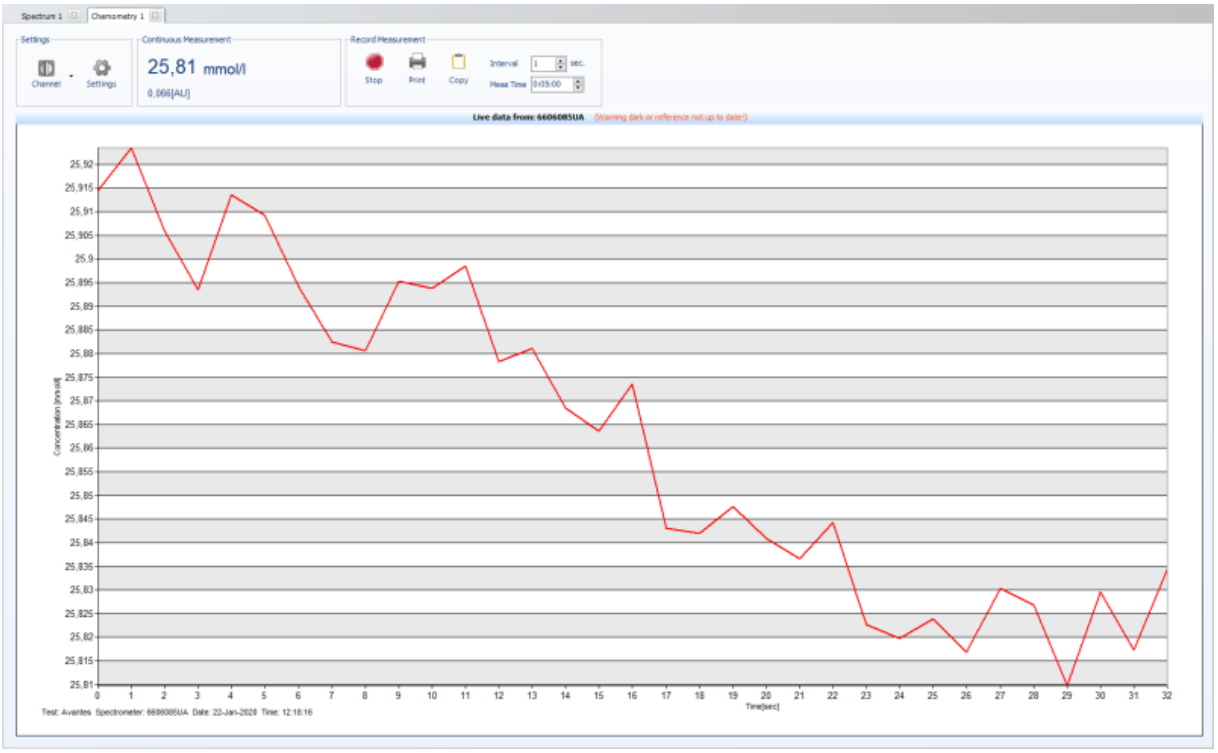
4.6.8 'Graph' Ribbon Tab, 'Copy' Button

Copies the time series graph to the clipboard.

4.6.9 'Graph' Ribbon Tab, 'Print' Button

Prints the time series graph.

4.7 Chemometry



The Chemometry application was developed to enable on-line concentration measurements with a spectrometer system.
According to Lambert-Beer's law, there is a linear relationship between absorbance and concentration.

A = ε*c*l

Where A is the absorbance (or extinction), ε is the extinction coefficient of the compound to be measured, c is the concentration and l is the optical path length.
In practice, this relationship is only linear at reasonably low absorbance levels (say less than 2). The wavelength at which the absorbance is measured must of course be kept constant.

To take concentration measurements, you will need a spectrometer with either a cuvette-holder or a dip-probe and a suitable light source.
If you use cuvettes, remember that glass cuvettes will absorb UV light. If your wavelength is in the UV range, use quartz or polystyrene ones instead.

AvaSoft-Chem can display and save the calculated concentration in two ways:

- The concentration can be displayed and saved on-line in a separate display window.
- You can display and save concentration values against time.

4.7.1 Measurement screen

In the measurement screen the readings will be shown continuously if the application is in run mode. Measurements can also be recorded by pressing the start button. The time interval and measurement time can be set. The time interval is the interval between consecutive readings. The measurement

time is the total time of the measurement. Recording will stop after this period has elapsed. The recorded graph can be printed or copied to the clipboard. The graph is automatically annotated with the setup name, spectrometer and date/time stamp.

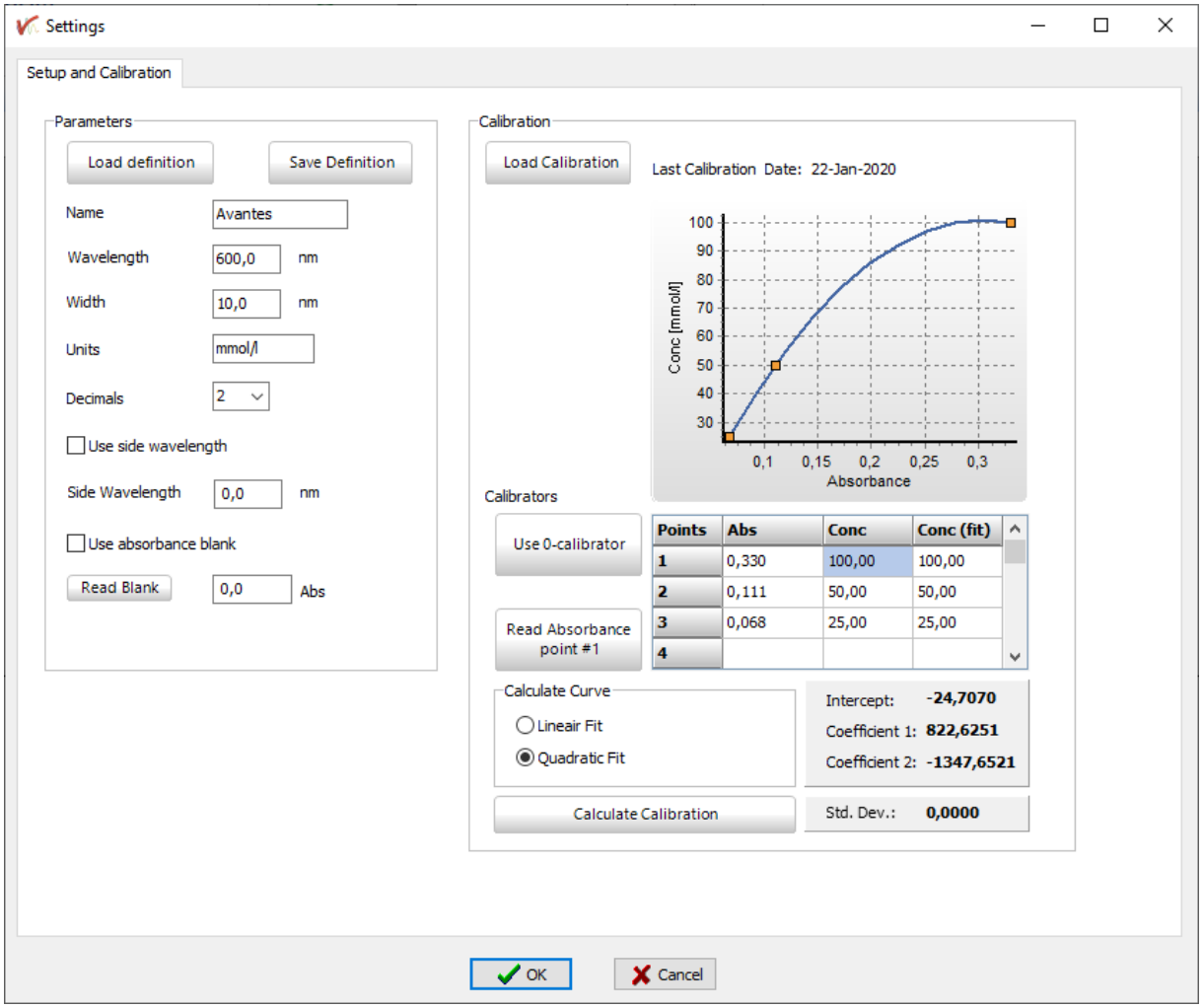
4.7.1.1 Spectrometer selection

If the spectrometer system contains one or more slave spectrometer channels, the spectrometer channel on which the chemometry will be measured can be selected from the drop down box that will appear after pressing this button.

4.7.2 Quick Start: Measuring Concentrations with the Chemometry Application

1. Start the AvaSoft software and click the Start button in the main window.
2. Set up the absorbance experiment with a cuvette holder or a dip-probe measuring the sample with the lowest concentration, usually your reference. Switch on the light source.
3. Adjust the integration time to get a good reference signal with a maximum around 58000 counts. The easiest way to do this is by using the AutoConfigure button in spectrometer window.
4. Adjust the number of averages. The higher the better, however the time for a single absorbance reading must remain practical. If you want to change it, click the Averaging value in the spectrometer window.
5. Switch off the light source and save a dark spectrum, switch it back on and save a reference.
6. Change to Absorbance mode by clicking the ‘A’ button in the ribbon. Measure the absorbance of a sample with a high concentration to find the wavelength and bandwidth of an absorbance peak to use (most of the time, the wavelength with the highest absorbance is used.
7. Open a Chemometry window by pressing the icon in the Applications section of the Home menu in the main window.
8. Click on the ‘Settings’ button and calibrate your absorbance readings in the ‘Setup and Calibration’ form. You can also just use a previous calibration line, as it can be saved to disk under a user defined filename and reloaded at the start of the application.
9. Close the settings screen to see the concentration readings. Press the Start button to record the readings.

4.7.3 Setup and Calibration Form



You need to measure a number of samples with known concentration to create your own calibration file(s). Once a calibration has been saved, it can be loaded later on and modified if needed.

4.7.3.1 Parameters

Load / Save Definition buttons
Setup definitions can be loaded and saved with these buttons. The definitions are stored in xml format with the extension .tdf.xml. If a definition is loaded, the plugin will also check for a calibration definition file (extension cal.tdf) with a filename equal to the loaded setup name. Note that this is not necessarily the setup definition file name. All files are stored under the subdirectory '\chem' in the current experiment directory.

Name
This is the ID for the current setup, this name is also used for referencing the calibration data.

Wavelength
This is the primary wavelength for the measurement.

Width

The bandwidth for the measurement. The program will integrate the absorbance values from “Wavelength minus Width” to “Wavelength plus Width” and uses this integral as the absorbance value in the concentration calculations.

Units
The concentration units for the measurement. The raw absorbance values will be converted to concentrations with this unit.

Decimals
The number of decimals for the concentration result. Absorbance values have a fixed number of 3 decimals.

Use side wavelength
This option allows for dichromatic measurements, measurements in relation to another wavelength. The correction will be done on absorbance level, before converting to concentration:

$$Abs = Abs_{primary-}\ Abs_{side}$$

The side wavelength will use the same width as the primary wavelength.

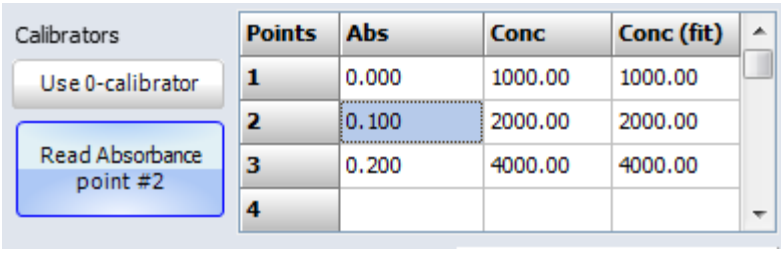
Use absorbance blank
A blank value can be subtracted to remove static offset. The value is subtracted on absorbance level:

$$Abs = Abs_{primary-}\ Abs_{side-}\ Abs_{blank}$$

Read Blank button
This will fill in the absorbance blank value.

4.7.3.2 Calibration

Calibrating is done to determine the relation between Absorbance and Concentration. This relation is a function of the first or second order. The calibration is performed by reading the absorbance values of fixed concentrations. These fixed concentrations are called concentration points or calibrators. The calibrators should be entered in the calibration grid under the column ‘Conc’. A calibrator measurement can be done by selecting the ‘Abs’ cell and pressing the ‘Read Absorbance #n’ button.



Use 0-Calibrator button
Pressing the Use 0-calibrator button will enter the value to 0.000 Abs.

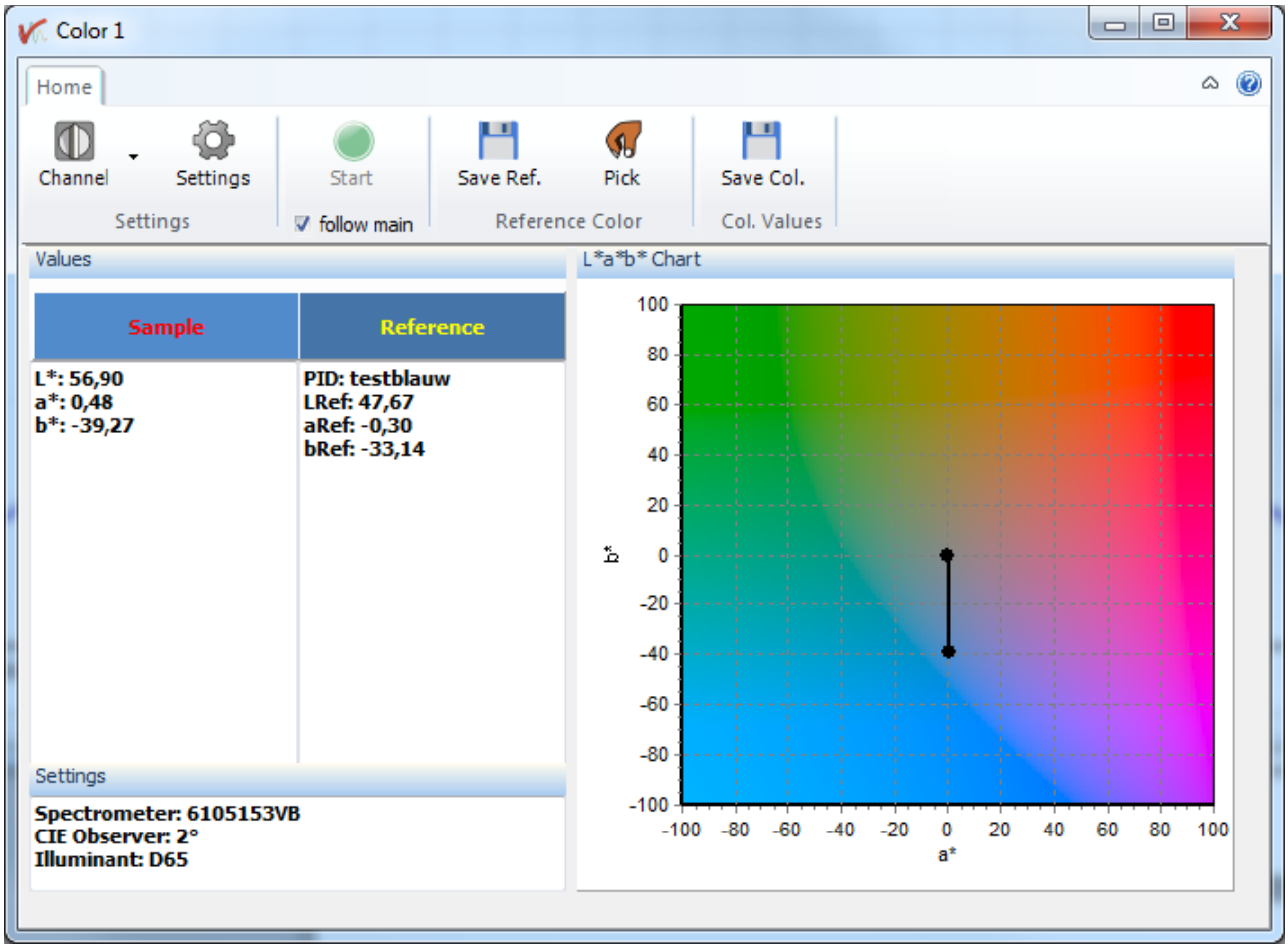
Calculate Curve options
Select either a Linear (first order) or a Quadratic (second order) fit.

Calculate Calibration button
After all calibrators are measured, the curve can be calculated by pressing the Calculate Calibration button. A linear (1st order) or quadratic curve (2nd order) can be calculated. After pressing the

Calculate Calibration button the calibration result must be accepted by the operator. If this is accepted the calibration is stored under the current setup name and the calibration date is set.
The polynomial and standard deviation are displayed. A graphic presentation of the relation between Absorbance and concentration will also be shown.

Load Calibration button
Other calibrations can be loaded. Note that the values of a loaded concentration are stored under the current setup name if the calculation curve is recalculated.

4.8 Color



The AvaSoft Color Application has been developed to perform on-line color measurements with a spectrometer system. It can be used for reflective color measurements, in earlier versions of AvaSoft called “color of object measurements”. The CIE 1976 L*a*b* color parameters are calculated, as well as other frequently used parameters, like Hue, Chroma and X, Y, Z.

These parameters can be displayed in a CIELAB chart or in a graph versus time. It is also possible to save the measured L*a*b* values online to a database and use one of the products from the database as a reference color. By comparing the measured L*a*b* values to the stored database values, color differences (ΔELab, ΔL*, Δa*, or Δb*) can be measured as well.

Emissive color measurements can be done to measure the color of a light source (e.g. LED's). These measurements require an irradiance spectrum to calculate the color parameters x, y and z. With Irradiance application of AvaSoft, it is possible to perform irradiance measurements with a lot higher accuracy than when using the relative irradiance mode (which assumes a perfect blackbody light source with known color temperature). For this reason the emissive color or "color of light" calculation is one of the features in the Irradiance Application.

4.8.1 Color of an Object - Background

The color of an object can be expressed by the CIE 1976 (L*a*b*) color space. L* describes the lightness of the color. A positive value of a* describes the redness of the color, a negative a* the greenness. Similarly, yellowness or blueness is expressed by coordinate b*, which is positive for yellow and negative for blue. The L*a*b* values are derived from the CIE tristimulus values X, Y and Z of the sample (object) and the standard illuminant tristimulus values X_n, Y_n and Z_n.

The standard illuminant tristimulus values for X_n, Y_n, and Z_n are constant and depend only on the type of standard illuminant that has been chosen.

The CIE tristimulus values X, Y and Z of the color of an object are obtained by multiplying the relative power P of a standard illuminant, the reflectance R (or the transmittance) of the object, and the CIE standard observer functions x_λ, y_λ and z_λ (2 degrees or 10 degrees angle). The integral of these products over all the wavelengths in the visible spectrum (380 to 780 nm with a 5 nm interval) gives the tristimulus values.

The chromaticity coordinates x, y and z are obtained by taking the ratios of the tristimulus values (X, Y and Z) to their sum:

$$x = \frac{X}{(X+Y+Z)} \qquad y = \frac{Y}{(X+Y+Z)} \qquad z = \frac{Z}{(X+Y+Z)}$$

Another well-known way to present the color parameters a* and b* is by their hue angle (h*) and Chroma (C*).

Hue angle is measured in degrees starting with h*=0 in the red direction (+a*) and increasing counterclockwise:

$$h^* = \arctan\frac{b^*}{a^*}$$

Chroma is defined as the length of the line from the point a*=b*=0 to the sample point:

$$C^* = \sqrt{a^{*2} + b^{*2}}$$

To describe color differences, a well-known parameter is ΔE_{Lab}, which is defined as:

$$\Delta E_{Lab} = \sqrt{(\Delta L^*)^2 + (\Delta a^*)^2 + (\Delta b^*)^2}$$

In which,
ΔL*, Δa* and Δb* represent the difference in L*a*b* values between the reference color and the actual measured L*a*b* values.

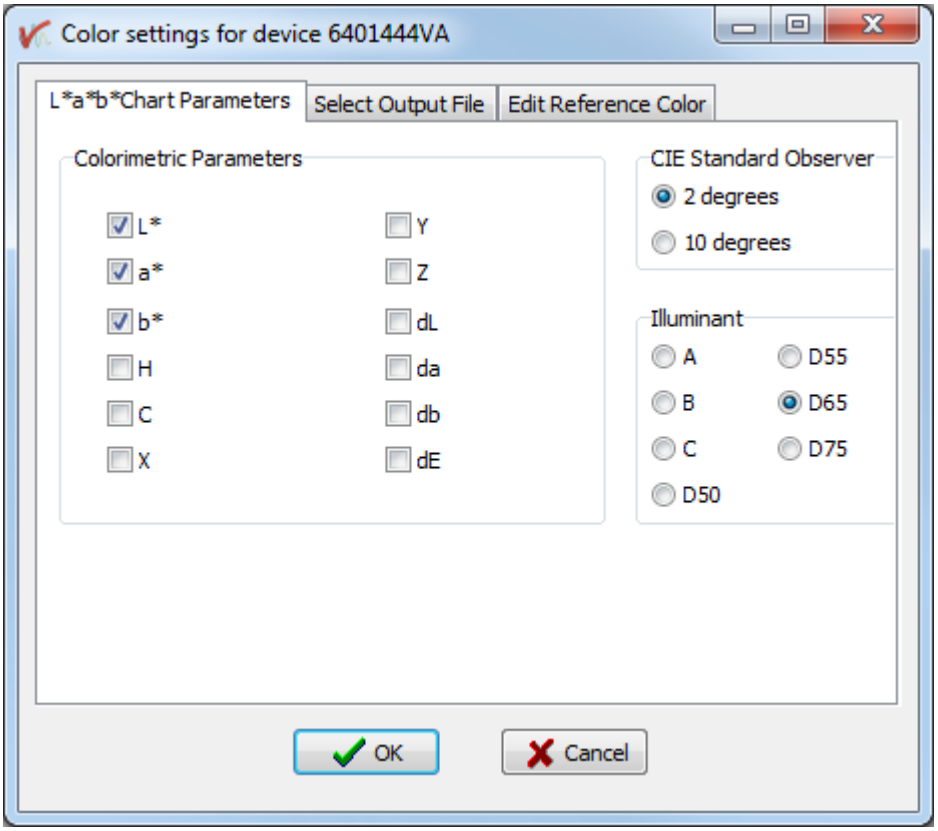
4.8.2 'Home' Ribbon Tab, 'Channel' Button

If the spectrometer system contains one or more slave spectrometer channels, the spectrometer channel on which the color will be measured can be selected from the drop down box that will appear after pressing this button. Make sure white reference and dark spectra have been saved before for the selected spectrometer channel.

4.8.3 'Home' Ribbon Tab, 'Settings' Button

After selecting the 'Settings' button a form is displayed in which the input parameters can be set. The dialog shows three tabbed pages: one is called "L*a*b*Chart Parameters" and shows the input parameters for displaying the color measurements in a color chart; the second one is called 'Select Output File', and the third one is called 'Edit Reference Color'.

4.8.3.1 L*a*b*Chart Parameters



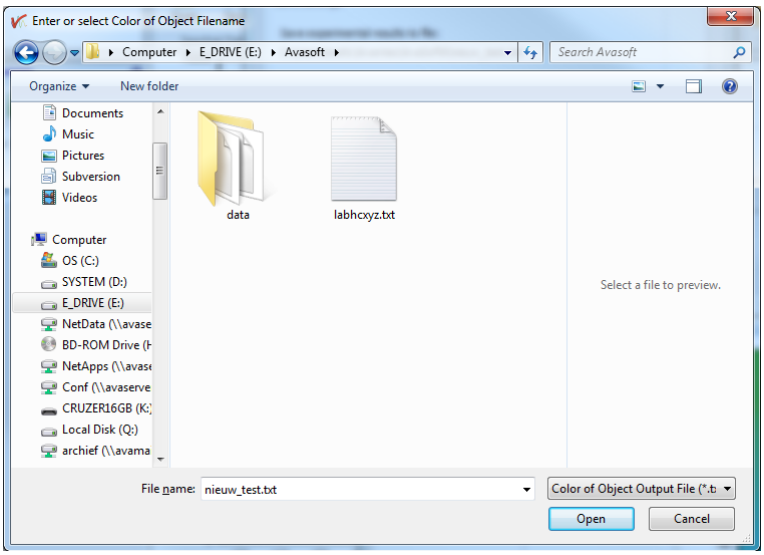
The following parameters can be set before the measurements are started:

- **Colorimetric Parameters**; select which parameters are to be calculated and shown in the measurement.
- **CIE Standard Observer**; the original CIE standard observer functions x_λ, y_λ and z_λ were defined in 1931, and are known as the 2 degrees standard observer values. The 2 degrees corresponds with the angle of vision that was used in the experiments to determine these standard observer values. In 1964, the CIE recommended the use of different observer values for a higher correlation with visual perception for large samples. These are known as the 1964 supplementary standard observer, or 10 degrees observer values. Both standards are still in use, and in AvaSoft, the CIE standard observer can be selected by clicking one of the radio buttons. The default is 2 degrees.
- **Illuminant**; the CIE Standard sources A, B or C or one of the illuminants D50, D55, D65 or D75 can be selected by clicking one of the radio buttons. The default is D65, which is the most widely used illuminant. It represents the power distribution of average daylight, with a correlated color temperature of 6500K. The D50, D55 and D75 have correlated color temperatures of 5000K, 5500K and 7500K. The CIE Standard sources A, B or C represent respectively: Incandescent light (2854K blackbody), Simulated noon sunlight and Simulated

overcast sky daylight. Note that there is no relation between the illuminant chosen here and the light source that is used for measuring the color of an object. The selected illuminant is used in calculation of the color parameters. These color parameters will be different if for example A will be selected instead of D65, just as the color of an object will look different in average daylight or in incandescent light (2854K blackbody).

4.8.3.2 Select Output File

The color parameters can be saved to an ASCII file during the measurements. The current name and location of this ASCII file is shown under the 'Select Output File' tab. This filename (and path) can be changed by clicking the "Change Output File" button. The next dialog will be displayed:

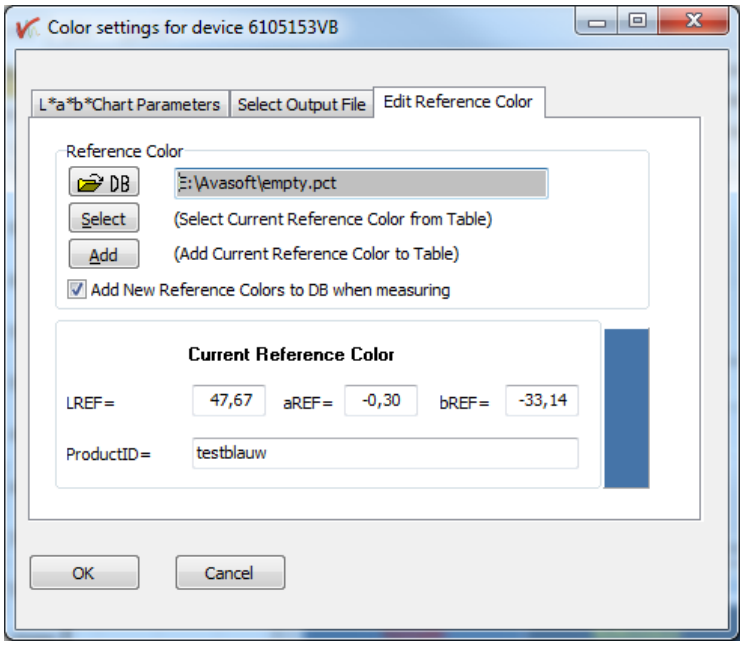


To start a new file for saving the color parameters, enter a filename that does not already exists (AvaSoft will add the .txt extension), and click Open.

If an existing file is selected, the color parameters that will be saved are appended to this file. This way experiments that were saved before can be proceeded, using the same output file.

You can also export the current output file to a comma-separated values (CSV) file, or to Excel. Both the .csv file and the .xlsx file will be saved in the same directory as the current output file, and these files will have a date/time stamp in their filename. Note that Excel must be present on the PC if you want to use the export to Excel feature. Excel will not be closed automatically after the conversion.

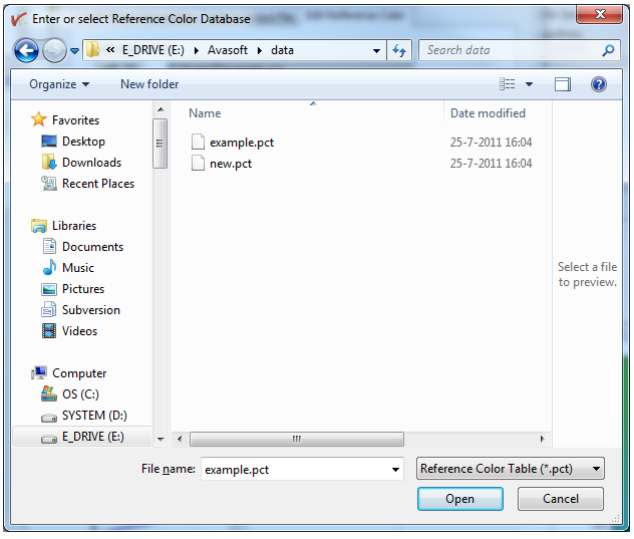
4.8.3.3 Edit Reference Color



The reference color can be set to compare the L*, a* and b* color parameters during the online measurements with the LREF, aREF and bREF of the reference color. The color differences can be shown during the measurements by dL (=L*-LREF), da (=a*-aREF), db (=b*-bREF) and/or dE (=√(dL2+da2+db2)).

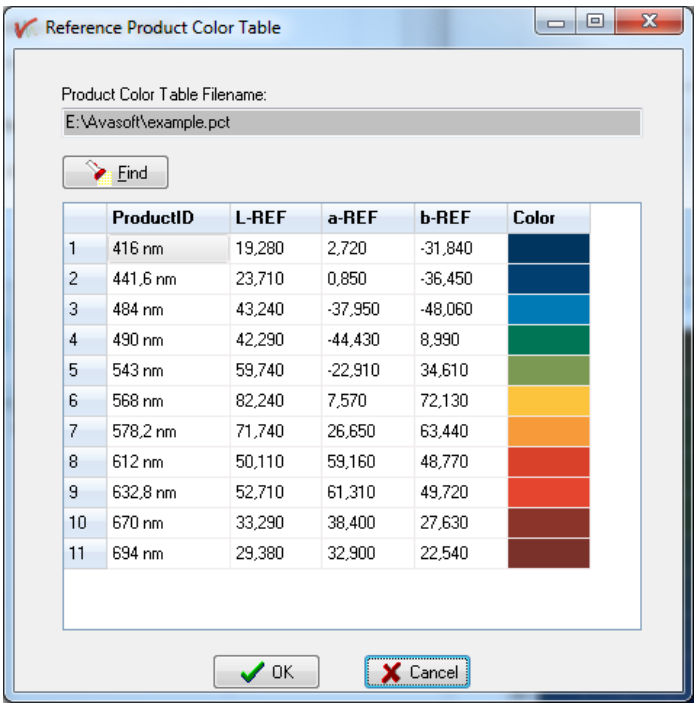
The reference color can be entered manually under “Current Reference Color” in the figure above, or it can be selected from a database file. The database file is a list of reference colors that were saved before to this file, all with a unique ProductID. By default the name of the database file is “empty.pct”. By clicking the DB button, a different database file can be selected, or a new file can be created.

To start a new database file for saving reference colors, enter a filename that does not already exists (AvaSoft will add the .pct extension), and click Open.



To open an existing file simply double click on the filename, or select it and click the Open button. The file example.pct can be found in AvaSoft main directory and contains a few measured reference colors.

To select a reference color from the database file, click the select button, below of the DB button. The contents of the database file will be displayed as shown in the figure below:



	ProductID	L-REF	a-REF	b-REF	Color
1	416 nm	19,280	2,720	-31,840	
2	441,6 nm	23,710	0,850	-36,450	
3	484 nm	43,240	-37,950	-48,060	
4	490 nm	42,290	-44,430	8,990	
5	543 nm	59,740	-22,910	34,610	
6	568 nm	82,240	7,570	72,130	
7	578,2 nm	71,740	26,650	63,440	
8	612 nm	50,110	59,160	48,770	
9	632,8 nm	52,710	61,310	49,720	
10	670 nm	33,290	38,400	27,630	
11	694 nm	29,380	32,900	22,540	

To select one of the products from the list, click on one of the numbers (1..11) in the first (gray) column.

To delete a product from the list, select it and click the delete key on the keyboard. To search for a certain productID or number, click the Find button. To sort the records by ProductID, L-REF, a-REF or b-REF, click on the corresponding column header. A yellow marked '1' will be shown in the column header. By clicking again at the header which is already marked, the sorting direction will be converted.

By clicking the Cancel button, the selected product will not be moved to the current reference color in the LABChart settings dialog, and changes (e.g. deleting a product from the list) will be ignored.
By clicking the OK button, the current reference color in the LABChart settings dialog is changed to the color which has been selected.

To add the current reference color (specified in the LABChart settings dialog) to the database file, the Add button (below of the select button) can be clicked. If the ProductID already exists, a dialog will be shown in which the choice can be made to overwrite the old color parameters with the new ones, or to keep the old values for this productID. As an alternative, a reference color can be added to the database during the online measurements. This can be done only if in the LABChart settings dialog, the option "Add new reference colors to DB when measuring" is enabled.

The color measurements are started by clicking the OK button. AvaSoft returns to the main window if the Cancel button is clicked.

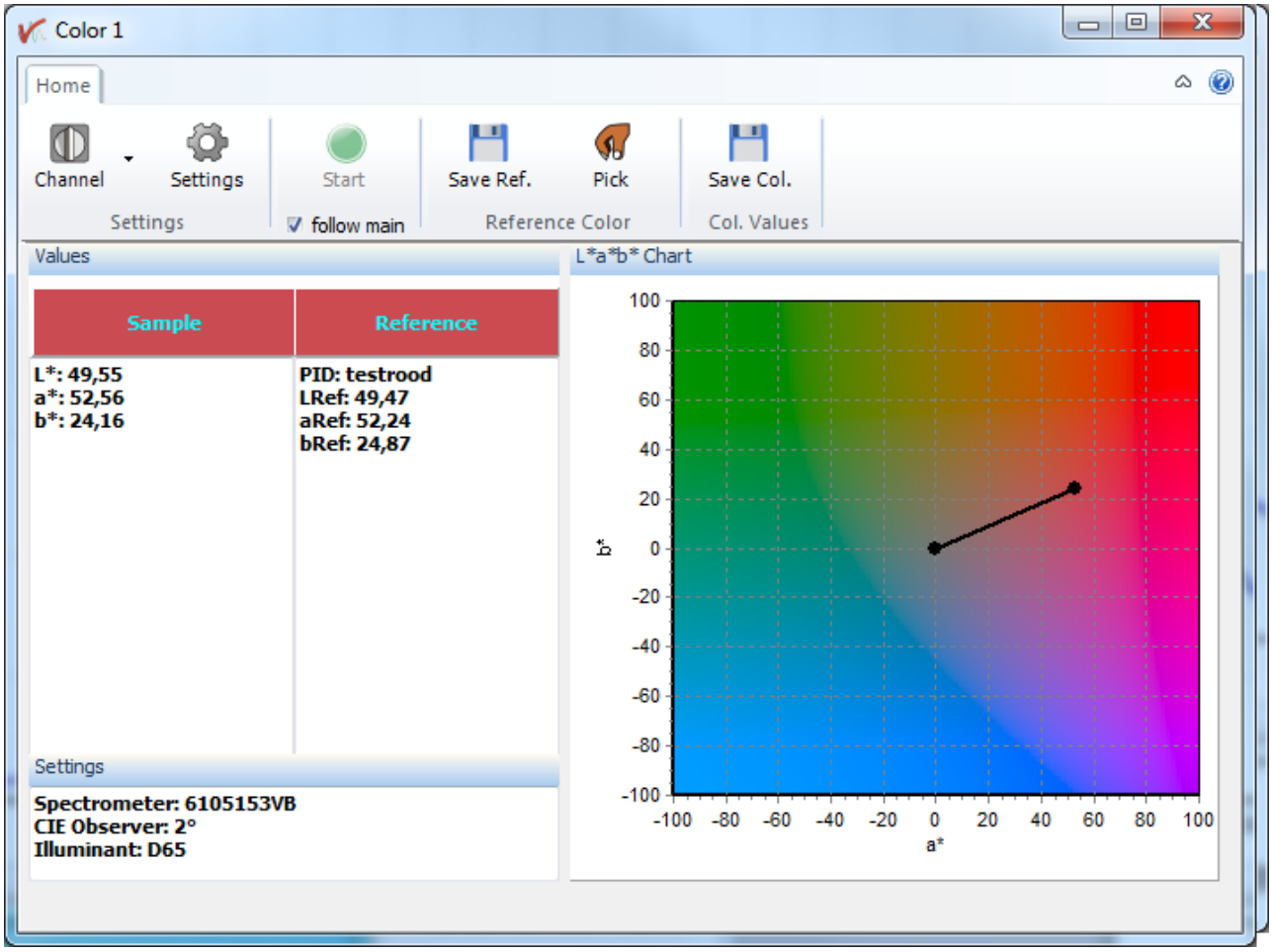
4.8.4 'Home' Ribbon Tab, 'Start/Stop' Button

After all settings are filled in correctly the measurements can be started by clicking the 'Start' button. It might be easier to check the 'follow main' checkbox, in which case starting the spectrometer measurements will also start the color measurements.

The figure below shows a measurement in progress.

The 'Values' panel shows a sample and reference color panel. Note that the displayed colors on the monitor may not match the color of the object exactly (depends on monitor), but it will give a good impression. Under the panels are tables of the values for measured color parameters and the reference color values.

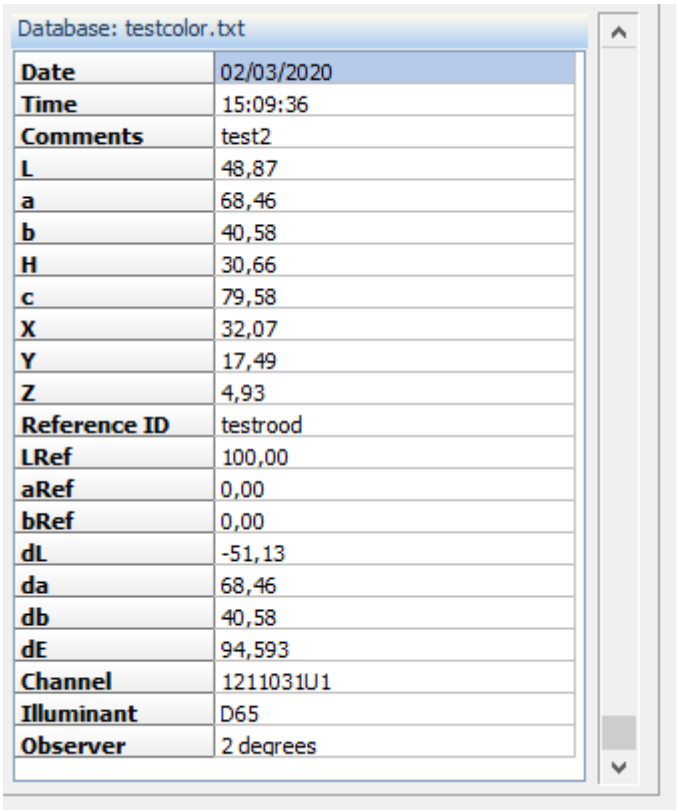
The 'Settings' panel shows the parameters that were set for this measurement.
The L*a*b*Chart panel shows a* and b* by a moving dot in a CIELAB graph.



The measurements in the figure are performed with the spectrometer nr. 6105153VB channel and illuminant D65 has been selected. The color parameters are calculated with the 2 degrees CIE standard observer values.

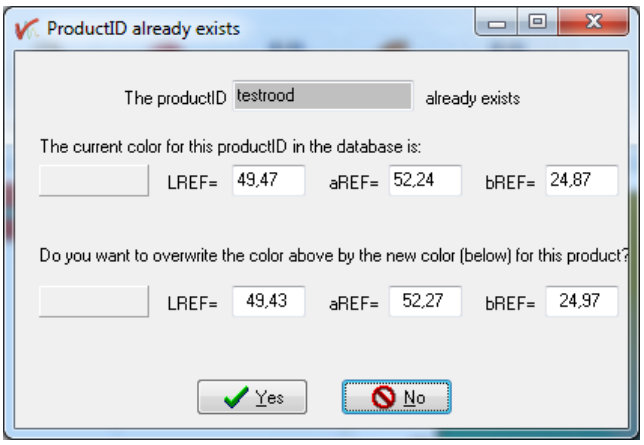
The 'Stop' button is clicked to stop the color measurements.

You can view the measurements in the output file in the right section of the screen. All fields that are saved in the output file are shown. Use the scrollbar to scroll through the measurements.



4.8.5 'Home' Ribbon Tab, 'Save Reference Color' Button

The "Save Reference Color" button is used to update the current reference color. After clicking this button, a dialog is displayed in which a name for the ProductID needs to be entered. If the productID already exists in the database file and if the option "Add new reference colors to DB when measuring" is enabled in the LABChart settings dialog, then a dialog will be shown in which the choice can be made to overwrite the old color parameters with the new ones, or to keep the old values for this productID (see the next figure).



4.8.6 'Home' Ribbon Tab, 'Pick Reference Color' Button

The 'Pick' button can be used to select a new reference color from the database, as described in detail on the previous page.

4.8.7 'Home' Ribbon Tab, 'Save Col. Values' Button

Each time the 'Save Col. Values" button is clicked, a new record is added to the Filename in the lower left corner. One record contains the following fields: Date, Time, Comments, L, a, b, h, c, X, Y, Z, RefProductID, Lref, aRef, bRef, dL, da, db, dE, Channel, Illuminant and Observer. The Comments field contains the text that is entered in the dialog that is shown after clicking the Save button.

4.9 Irradiance

AvaSoft-IRRAD has been developed to perform on-line absolute irradiance measurements with an Avantes spectrometer system. A calibrated light source AvaLight-HAL-CAL or AvaLight-DH-CAL with known energy output (in µWatt/cm^2/nm) is used as a reference. Also the calibration of an Avantes spectrometer system can be done in our calibration lab, after which this calibration can be loaded. Color of light parameters can be expressed by the chromaticity coordinated x, y and z. These chromaticity coordinates are obtained by taking the ratios of the tristimulus values (X, Y and Z) to their sum. The tristimulus values X, Y and Z and the spectral irradiance are computed in a wavelength range from 380 nm to 780 nm, using a 1 nm interval. These parameters, as well as the coordinates u, v and the color temperature of an external light source can be calculated and displayed in real-time. For LED measurements, the Dominant Wavelength and Purity are interesting parameters, which can be calculated as well. The Color Rendering Index (CRI) is a measure of the color rendering properties of a light source.
The same experimental set up (spectrometer with fiber optics and cosine corrector or integrating sphere) is used to calculate the photometric and/or radiometric parameters of the light to be measured. The calculated output can be displayed and saved in three ways:

- In a Spectrum application window the data can be displayed as spectral irradiance in µWatt/cm^2/nm versus wavelength.
- The measurement results can also be displayed in an Irradiance application window (figure above), which shows the chromaticity diagram and many parameters for colorimetry, photometry, radiometry and peak measurements. Up to 10 different radiometric parameters and/or wavelength ranges can be selected for which the output will be displayed.
- In a Time series application window, a function can be displayed simultaneously against time. For each window, a different radiometric, photometric, color coordinate or peak output parameter and/or wavelength range may be selected, as well as a different spectrometer channel.

4.9.1 Background

Before irradiance measurements can be done, an intensity calibration is required. The intensity calibration contains the data transfer function for each pixel. The data transfer function is used to convert the scope data (A/D Counts) into irradiance data (in µWatt/cm^2). To be able to calculate the transfer function, a calibrated light source, with known output (in µWatt/cm^2/nm) needs to be available.

When saving the A/D Counts with the reference light source on and off, we know the relation between the A/D Counts and µWatt/cm^2:

$$\left(\frac{Caldata_n}{refcal_n - darkcal_n}\right)$$

$Caldata_n$ = Intensity of the calibrated light source at pixel n (in µWatt/cm^2) from lamp file
$refcal_n$ = A/D Counts at pixel n that were saved with the reference light source on
$darkcal_n$ = A/D Counts at pixel n that were saved with the reference light source off

When measuring the A/D counts received from a light source different from the calibrated light source (but of course with the same fiber optic cable and diffuser), this relation can be used to measure the intensity at every pixel n (in µWatt/cm^2). If $sample_n$ is the measured A/D counts at pixel n when looking at the sample light source, and $dark_n$ is the measured A/D Counts with the sample light source off, then the equation for intensity I_n (in µWatt/cm^2) becomes:

$$I_n = Caldata_n * \left(\frac{sample_n - dark_n}{refcal_n - darkcal_n}\right)$$

If during the intensity calibration an integration time was used (e.g. 100ms) that differs from the integration time during the sample measurements (e.g. 2 ms), a factor needs to be added to the equation to compensate for the difference. In the example the factor is 100/2 = 50.

Calculating the intensity (in µWatt/cm^2) from the measured sample spectrum (in A/D Counts) can therefore be done by the following equation:

$$I_n = Caldata_n * \left(\frac{sample_n - dark_n}{refcal_n - darkcal_n}\right) * factor$$

From the irradiance spectrum (in µWatt/cm^2), a lot of light output parameters can be calculated: colorimetric, photometric and radiometric.

Below, short background information is given about the colorimetric, radiometric and photometric parameters. We also describe the definition of the peak parameters that can be measured as well.

Colorimetry
The color of light can be expressed by the chromaticity coordinates x, y and z. These chromaticity coordinates are obtained by taking the ratios of the tristimulus values (X, Y and Z) to their sum:

$$x = \frac{X}{(X+Y+Z)} \qquad y = \frac{Y}{(X+Y+Z)} \qquad z = \frac{Z}{(X+Y+Z)}$$

The tristimulus values X, Y and Z are computed by:

$$X = k * \sum I_\lambda * x_\lambda \qquad Y = k * \sum I_\lambda * y_\lambda \qquad Z = k * \sum I_\lambda * z_\lambda$$

where:
k = Constant (= $1/(\Sigma y_\lambda)$ = 0.00934
$I\lambda$ = Spectral irradiance at wavelength λ
$x\lambda$, $y\lambda$, $z\lambda$ = CIE 1931 or 1964 Standard Observer value (2 or 10 degrees angle) at wavelength λ

The tristimulus values X, Y and Z and the spectral irradiance are computed in a wavelength range from 380 nm to 780 nm, using a 1 nm interval.
The CIE1960 UCS color coordinates u and v are calculated by:

$$u = \frac{4x}{(-2x+12y+3)} \qquad v = \frac{6y}{(-2x+12y+3)}$$

The equation that is used for calculating the color temperature is empirical and assumes a black body radiator:

$$p = ((x-0.332)/(y-0.1858))$$
$$\text{Color Temp} = 5520.33-(6823.3*p)+(3525*p^2)-(449*p^3)$$

The **Color Rendering Index (CRI)** is a measure of the color rendering properties of a light source. The CIE has defined 14 standard color samples and the CRI Ra is defined as the mean value of the color rendering values of the first 8 R values of these standard CIE samples.

A CRI Ra of 100 indicates that the sample sources have identical color coordinates under the light source to be tested and the reference light source. A CRI Ra value of 50 is assigned to the CIE standard warm white fluorescent lamp. The CRI calculation method used is based on the CIE 13.3-1995 standard.

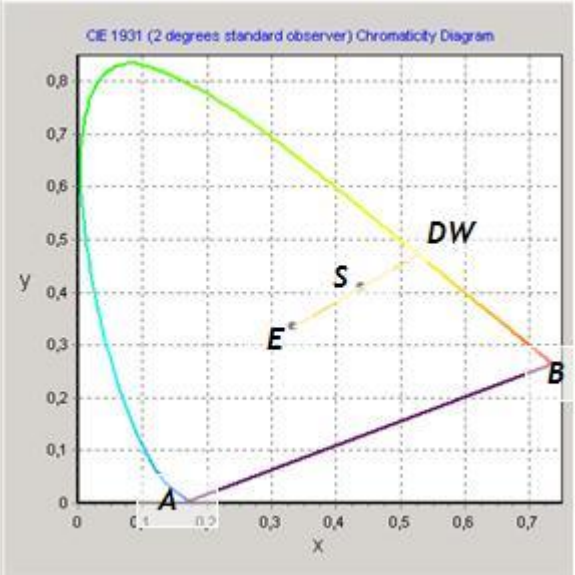
A reference light source is calculated on the basis of the color temperature of the light source to be tested. The color temperature calculation is done with the McCamy algorithm described above.
For color temperatures under 5000K, a standard Planckian radiator is calculated with a color temperature that equals the color temperature of the sample light source. For color temperatures between 5000K and 25000K, a standard daylight distribution is calculated, again with an identical color temperature.

The 14 standard CIE samples are then 'illuminated' with both light sources, and from the difference in chromaticity values the 14 Special Rendering Indices are calculated, the first 8 of which yield the CRI. You can calculate either the general Ra, or any one of the 14 separate R values.

A more recent development is the **Color Quality Scale (CQS)**, proposed by the NIST. It addresses some of the limitations that are present in the CRI, e.g. by using a larger set of samples, all of high chroma, by using a better chromatic adaptation transform and by avoiding negative score values.
The version of the CQS that is implemented in AvaSoft is version 9.0.1.
The 15 standard CQS samples are again 'illuminated' with the light source to be tested and a calculated reference light source. An rms calculation on all 15 samples yields the general CQS Qa value. You can choose to calculate either the general Qa, or any one of the 15 separate Q values.

In LED measurements, the Dominant Wavelength and Purity (also known as Helmholtz coordinates) are often used to describe a color. The Dominant Wavelength can be calculated for a measured sample point S with chromaticity coordinates (Sx,Sy) by drawing a straight line from the midpoint in the chromaticity diagram (E with x=y=0.333) through S towards the edge of the Chromaticity Diagram (spectrum locus). The points at the spectrum locus correspond with a wavelength and the interception of the straight line through E and S with the locus is called the Dominant Wavelength. Purity, is the distance from the midpoint (E) to the sample point (S), divided by that from the midpoint (E) to the spectrum locus (DW):

Purity = (E-S) / (E-DW)
The method described above is used for all colors with a Dominant Wavelength from 380 to 699 nanometres. If the x,y coordinates are in the triangle area encompassed by the 3 points E, A and B, then the Dominant Wavelength cannot be calculated because the interception point through E and S with the spectrum locus (between A and B) does not correspond with a wavelength. In that case the Complementary Dominant Wavelength (CDW) is used. The line from E through S is extended backward in order to determine the Complementary Dominant Wavelength (CDW).



Radiometry
The radiometric parameters can be grouped into three categories:

- Radiant Flux [µWatt]: The radiant flux is the total optical power emitted from a source in all directions. The best way to measure the power emitted by a source is to measure the source inside an integrating sphere. This is often done when measuring LED's. It is also possible to calculate the flux of a source by measuring the irradiance at the surface of the diffuser (cosine corrector or integrating sphere sample port) at a certain distance from a light source. An important assumption in this calculation is that the source should be isotropic and the distance between diffuser and source should be greater than five times the largest dimension of the source (approximation of point source).
- Radiant Intensity [µWatt/sr]: The radiant intensity is the optical power per unit solid angle. It is used to quantify the optical power that is emitted by a source into a certain direction. Radiant intensity is calculated from the measured irradiance by multiplication with the square of the distance between source and diffuser surface. It is assumed that the source is a point source.
- Irradiance [µWatt/cm^2]: Irradiance is used to measure the power that is received by a surface.

Radiometric measurement can be done in different setups, like with fiber optic cosine corrector or integrating sphere. Both setups can be used to measure the irradiance spectrum received at the surface of the diffuser (cosine corrector or integrating sphere sample port) at a certain distance from a light source. When measuring at a certain distance from the source, the radiant intensity and flux can be calculated as described above. When measuring a light source inside an integrating sphere, the radiant flux can be measured, but radiant intensity and irradiance parameters cannot be measured.

<u>Radiometric parameters calculated from the power distribution</u>
The power distribution can be easily converted in an **energy distribution** by multiplying the power with the integration time. The result is the amount of energy that has been emitted or received during one integration time cycle.

Another radiometric parameter that can be calculated from the irradiance spectrum, is the **number of photons** that is received by a surface. Since the number of photons per nanometer is a huge number (even with very low light intensity), the number of Avogadro is used to express the number of photons in mols, or as in our application in µmols. The number of photons per nanometer can be calculated from the wavelength dependent photon energy, and the absolute light energy that is measured. A detailed description how this is done can be found at the next page.

The photon count distribution [µMol/(s.m^2.nm)] shows the photon flux received per square meter. Other photon count units that can be calculated from this are:

- [µMol/(s.nm)] photon flux received at diffuser surface
- [µMol/(m^2.nm)] photons received per square meter during one integration cycle
- [µMol/nm] photons received at diffuser surface during one integration cycle

How to convert a power distribution [µWatt/(cm^2.nm)] into a photon count distribution [µMol/(s.m^2.nm)]

Photon energy $E(\lambda) = h.c/\lambda$ e

Where:
h = Planck´s constant 6,626 068 76 x10^{-34}
c = velocity of light 2,998 x10^8 m/s
λ = wavelength in meters

For example, the photon energy at 250 nm and at 1000 nm is:
E(250) = (6,626 x 10^{-34}. 2,998 x 10$^{8)}$/ 250.10^{-9} = 7,946 x10^{-19} (Joule/photon) (1)
E(1000)= (6,626 x 10^{-34}. 2,998 x 10$^{8)}$/ 1000.10^{-9} = 1,986 x10^{-19} (Joule/photon) (2)

1eV = 1,60207 x 10^{-19} Joule, so the photon energy expressed in eV/photon becomes:
E(250) = 7,946 x10^{-19} /1,60207 x 10^{-19} = 4,9592 (eV/photon) (3)
E(1000)= 1,986 x10^{-19} /1,60207 x 10^{-19} = 1,2398 (eV/photon) (4)

Suppose we measure 20 µWatt/cm^2 at a certain wavelength

20 µWatt/cm^2 = 20 µJoule/s/cm^2 = 0.2 Joule/s/m^2
= 0.2/(1,60207 x 10^{-19}) eV/s/m^2
= 1,248 . 10^{18} eV/s/m^2 (5)

Knowing the photon energy at 250 nm and at 1000 nm from (3) and (4), the number of photons that correspond with 20 µWatt/cm^2 at 250 nm and at 1000 nm can be calculated from (5) by:

for 250 nm : #photons = 1,248 . 10^{18} / 4,9592 = 2,517 . 10^{17} photons/s/m^2
for 1000 nm : #photons = 1,248 . 10^{18} / 1,2398 = 1,007 . 10^{18} photons/s/m^2

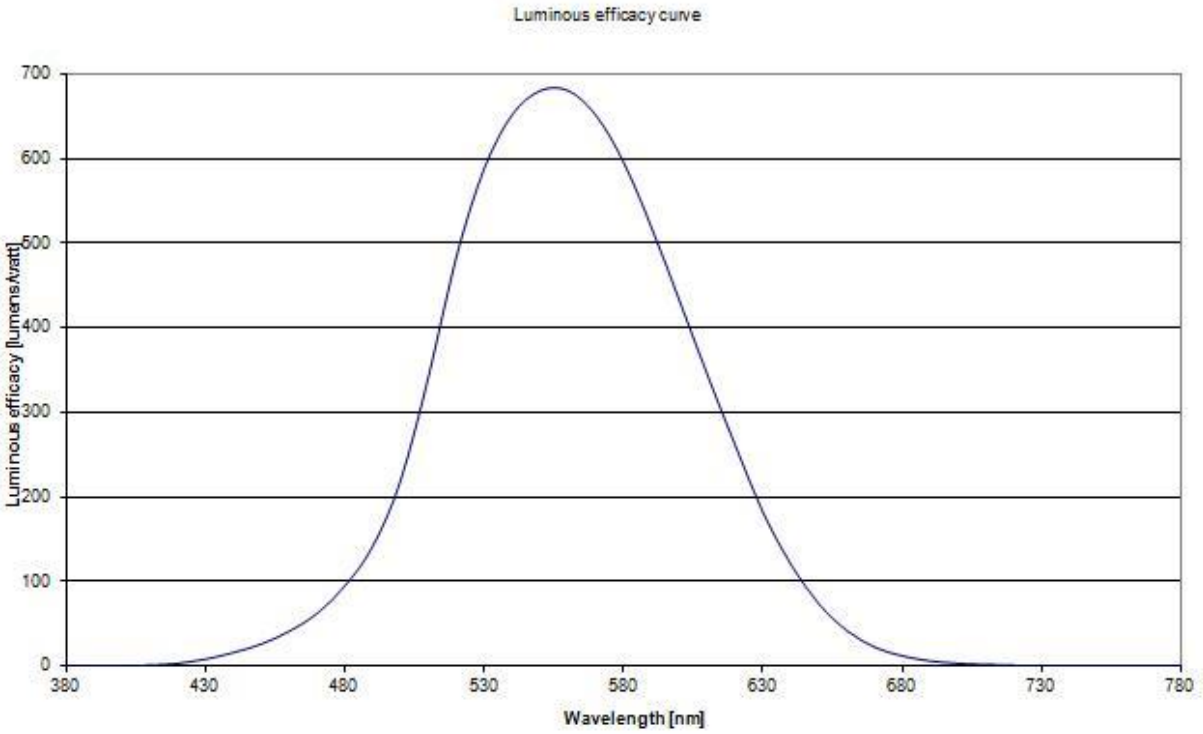
With 1 mol = 6,02308 x10^{23} (Number of Avogadro)
1 µmol = 6,02308 x10^{17}

So, the number of photons, expressed in µmol/s/m^2, when measuring 20 µWatt/cm^2 at wavelength 250 nm and also 20 µWatt/cm^2 at 1000 nm becomes:
for 250 nm : 2,517 . 10^{17} / 6,02308 .10^{17} = 0,418 µmol/s/m^2
for 1000 nm : 1,007 . 10^{18} / 6,02308 .10^{17} = 1,672 µmol/s/m^2

In the table below, the radiometric parameters that can be measured in AvaSoft are listed. Note that a wavelength range needs to be specified over which the parameter spectral output will be integrated. In the first column (Hardware setup), “inside sphere” refers to measurements that are done with the light source inside an integrating sphere, while “outside sphere or cc” refers to measurements that are done with a light source at a certain distance from the sphere or with a cosine corrector

Hardware Setup	Parameter	Unit	Description
inside sphere	Radiant Flux	µWatt	Total optical power emitted from a source

	(Power emitted)		
inside sphere	Energy emitted	µJoule	Total optical energy emitted from a source, calculated by multiplication of the power with the integration time
outside sphere or cc	Radiant Flux (Power emitted)	µWatt	Total optical power emitted from a source, calculated by multiplication of radiant intensity with the solid angle of the light source
outside sphere or cc	Energy emitted	µJoule	Total optical energy emitted from a source, calculated by multiplication of the power with the integration time
outside sphere or cc	Radiant Intensity	µWatt/sr	Optical power per unit solid angle, calculated by multiplication of irradiance with the square distance between point source and diffuser surface
outside sphere or cc	Radiant Energy	µJoule/sr	Total optical energy emitted from a source, calculated by multiplication of the radiant intensity with the integration time
outside sphere or cc	Power received	µWatt	Power received at diffuser surface
outside sphere or cc	Energy received	µJoule	Energy received at diffuser surface, calculated by multiplication of the power with the integration time
outside sphere or cc	Irradiance	µWatt/cm^2	Power received per square centimeter
outside sphere or cc	Energy/cm^2	µJoule/cm^2	Energy received per square centimeter, calculated by multiplication of irradiance with the integration time
outside sphere or cc	Photon Flux/m^2	µMol/(s.m^2)	Photons received per second and per square meter, see for calculation previous page
outside sphere or cc	Photon Flux	µMol/s	Photons received per second at diffuser surface
outside sphere or cc	Photons/m^2	µMol/m^2	Photons received per square meter during one integration time cycle
outside sphere or cc	Photons	µMol	Photons received at diffuser surface during one integration time cycle



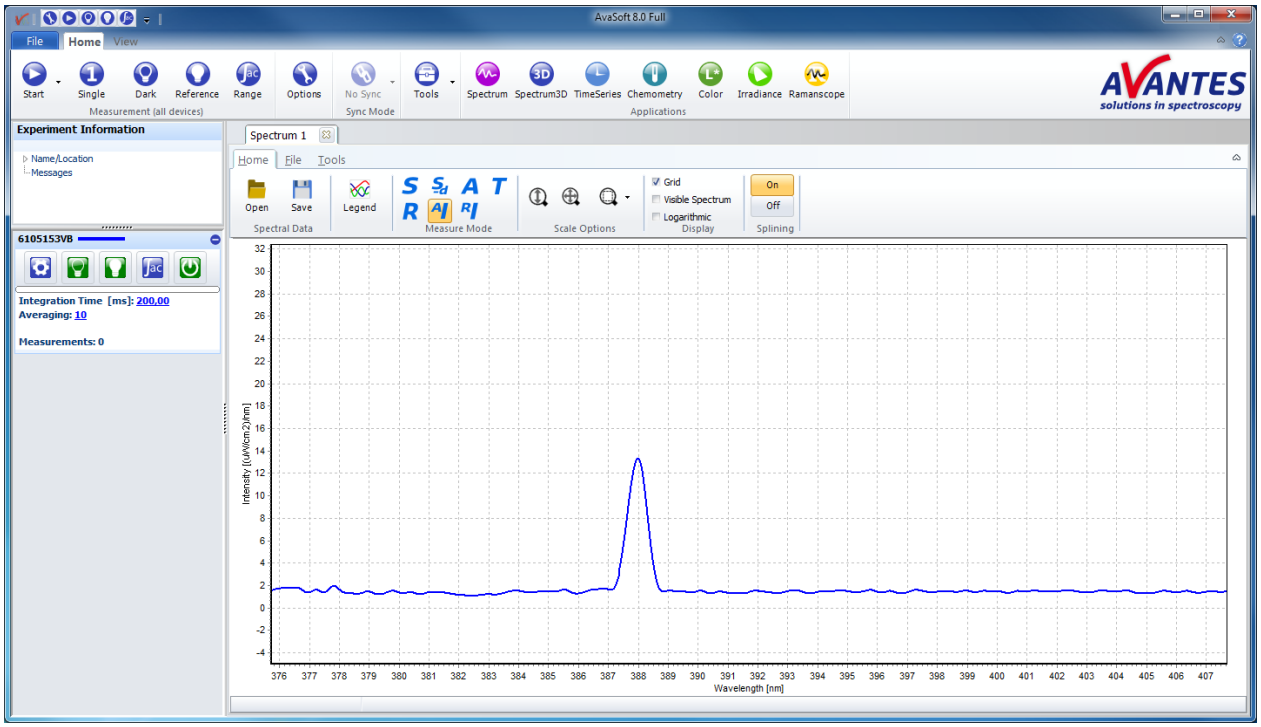
Photometry
Photometry is the measurement of visible light. Unlike radiometry, it is not a purely physical measurement and is calculated considering a 'standard' human visual perception. This is attained by multiplying the radiometric data by the luminous efficacy curve (see figure above) and integrating the product over the visible range (380 – 780 nm).

The three categories that were defined for the radiometric parameters can also be used for the photometric parameters.
The photometric equivalent for the Radiant Flux [µWatt] is the Luminous Flux, expressed in Lumens.
The photometric equivalent for the Radiant Intensity [µWatt/sr] is the Luminous Intensity, expressed in Lumens/sr. This unit is equal to Candela.
The photometric equivalent for Irradiance [µWatt/cm^2] is called Illuminance, expressed in Lumens/m^2. This unit is equal to Lux.

Since the geometry of the three categories is the same for radiometry and photometry, the same can be written about the hardware setup: luminous flux can be measured inside an integrating sphere. When measuring a source at a certain distance from the integrating sphere or cosine corrector, the luminous flux can be calculated, assuming that the source is an isotropic point source. The Luminous Intensity [Candela] and Illuminance [Lux] of a sphere can be measured outside the integrating sphere or with a cosine corrector.

Peak Measurements

A peak from a fluorescent lamp is shown in the figure below. A number of peak parameters can be calculated from this spectrum:



FWHM and Center Wavelength

The Full Width Half Maximum of a peak is the bandwidth (in nanometers) for which the intensity is higher than half of the maximum intensity of that peak. The Center Wavelength is the wavelength halfway between the left and right wavelength where the intensity is half of the maximum intensity.

Peak Wavelength

Wavelength at the maximum spectral power

Centroid Wavelength

The total spectral power left and right from the centroid wavelength (integral) is the same.

4.9.2 Quick Start

Quick Start (1): Perform absolute irradiance measurements using a calibrated lamp

Start the AvaSoft software, and click the Start button in the main window. Connect a fiber to the Spectrometer input port. Click the “Settings” button in the correct spectrometer window and select the “Irradiance” tab. Click the “Perform Intensity Calibration” button. Select the calibration lamp file and enter the diameter of the fiber/cosine corrector or integrating sphere sample port that is used, as described in section 4.9.4.

Turn on the reference light source (e.g. AvaLight-HAL-CAL or AvaLight-HAL-CAL-ISP). If a cosine corrector is used at the end of the fiber, mount it directly on the reference light source. If an integrating sphere is used at the end of the fiber, put the integrating sphere sample port over the light output port. Verify that the calibration lamp is ON for at least 15 minutes, and click the “Start Intensity Calibration” button. Try to adjust the integration time while looking at the reference light, such that the maximum count over the wavelength range is around 90% of the full ADC scale, which is 59000 counts for the 16bit ADC. It’s also possible to let AvaSoft search for an optimal integration time by clicking the ‘∫AC’ button.

Adjust the Smoothing Parameter to optimize smoothing for the Fiber/Slit diameter that is used. If a good reference signal is displayed, click the bright lightbulb “Save Reference” button. A white line will mark the reference spectrum. Then switch off the calibration lamp, wait until the spectrum becomes flat, near the bottom of the scale, and click the dark lightbulb button to save a dark spectrum. A black line will mark the dark spectrum.

Click the “Save Intensity Calibration” button. A dialog shows up in which the current settings in this intensity calibration are shown. If the calibration has been performed with diffuser, the intensity calibration data will be saved to an ASCII file with extension *.dfr, with bare fiber this extension will be *.fbr. The name of the intensity calibration file can be entered after clicking the “Save As” button. With USB2 spectrometers, the intensity calibration can also be saved to EEPROM by clicking the “Save to EEPROM” button. Click the Close button to Close the dialog.

Open an Irradiance application window to select the colorimetric, radiometric, photometric and/or peak parameters of interest (see section 4.9.5). Then click OK. Measure the output parameters in the experiment. If needed, change the integration time, such that the maximum in Scope Mode is around 90% of the full ADC scale, which is 59000 counts for the 16bit ADC). Block the light path to the spectrometer, and save a dark spectrum. If the (ir)radiance of the light to be measured needs to be displayed against time, open a Time series application window and select an Irradiance function as described in section 4.6.

The intensity calibration as performed under point 9 can be loaded in future experiments by selecting the option “Load Intensity Calibration”, as described below under Quick Start (2). For the USB2 spectrometers, the intensity calibration that has been stored in the EEPROM is loaded automatically during the initialization of AvaSoft. After loading an intensity calibration, a dark spectrum needs to be saved before switching to Irradiance mode.

Quick Start (2): Perform absolute irradiance measurements by loading an intensity calibration

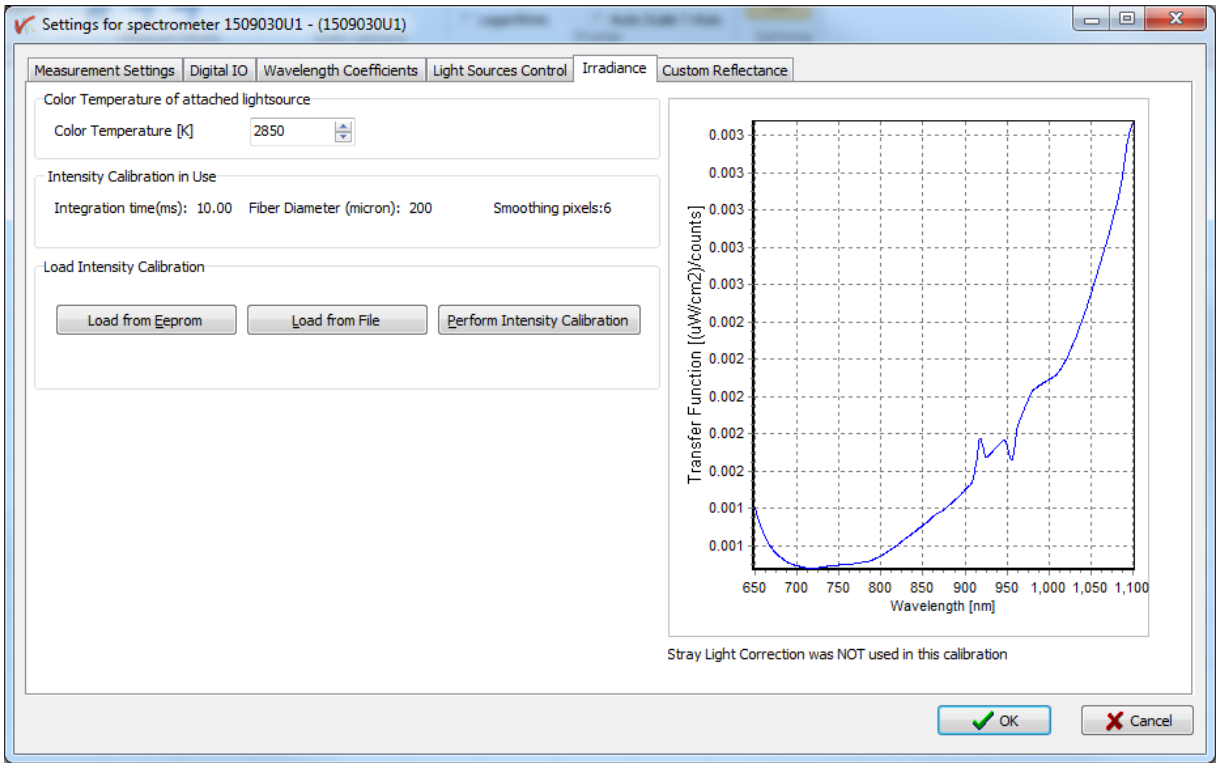
Start the AvaSoft software, and click the Start button in the main window. Connect the same fiber (and diffuser or integrating sphere) that was used during the intensity calibration that will be loaded to the Spectrometer input port.

Click the “Settings” button in the correct spectrometer window and select the “Irradiance” tab. If an intensity calibration has been stored in EEPROM before, this will be autoloaded at AvaSoft program initialization. Click the “Load from File” button. A dialog shows up in which the intensity calibration file can be selected. Select the file and click the open button.

Open an Irradiance application window and select the colorimetric, radiometric, photometric and/or peak parameters of interest (see section 4.9.5.2). Then click OK. Measure the output parameters in the experiment. If needed, change the integration time, such that the maximum in Scope Mode is around 90% of the full ADC scale (59000 counts for the 16bit ADC). Block the light path to the spectrometer, and save a dark spectrum. If the (ir)radiance of the light to be measured needs to be displayed against time, open a Time series application window and select an Irradiance function as described in section 4.6.

4.9.3 Load Intensity Calibration

By selecting the Spectrometer Settings button in the spectrometer windows, and then selecting the Irradiance tab, a window is shown in which the intensity calibration that was saved before can be loaded by clicking the “Load from File” button.

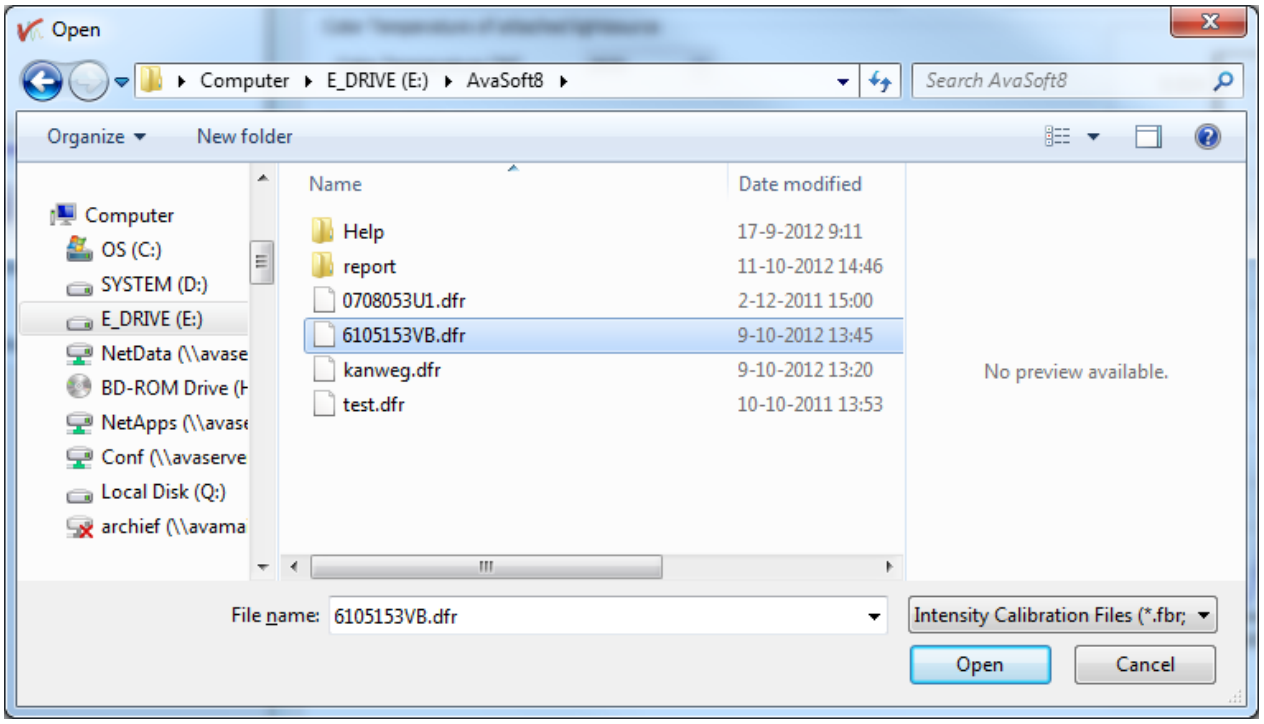


An intensity calibration file contains the data which is necessary to convert the Scope data to Irradiance data. If the spectrometer system has one or more slave channels, it is important to know that the calibration data for each spectrometer channel are saved in a separate file. To measure irradiance data at more spectrometer channels simultaneously, the calibration files for each spectrometer channels need to be loaded first. After loading an intensity calibration file, a graph is displayed which shows the data transfer function for the loaded channel. The irradiance spectrum is calculated by multiplying the measured scope data (from which a saved dark spectrum is subtracted) with this data transfer function.

The intensity calibration is loaded from EEPROM by default. However, if multiple calibrations are available for a spectrometer, the EEPROM calibration can be overruled by loading a calibration from file. The filename that holds the intensity calibration needs to include the serial number of the spectrometer channel.

Please note that you must match the setting of the Stray Light Correction of your irradiance measurements with that of the irradiance calibration. Do not use a calibration that was recorded with

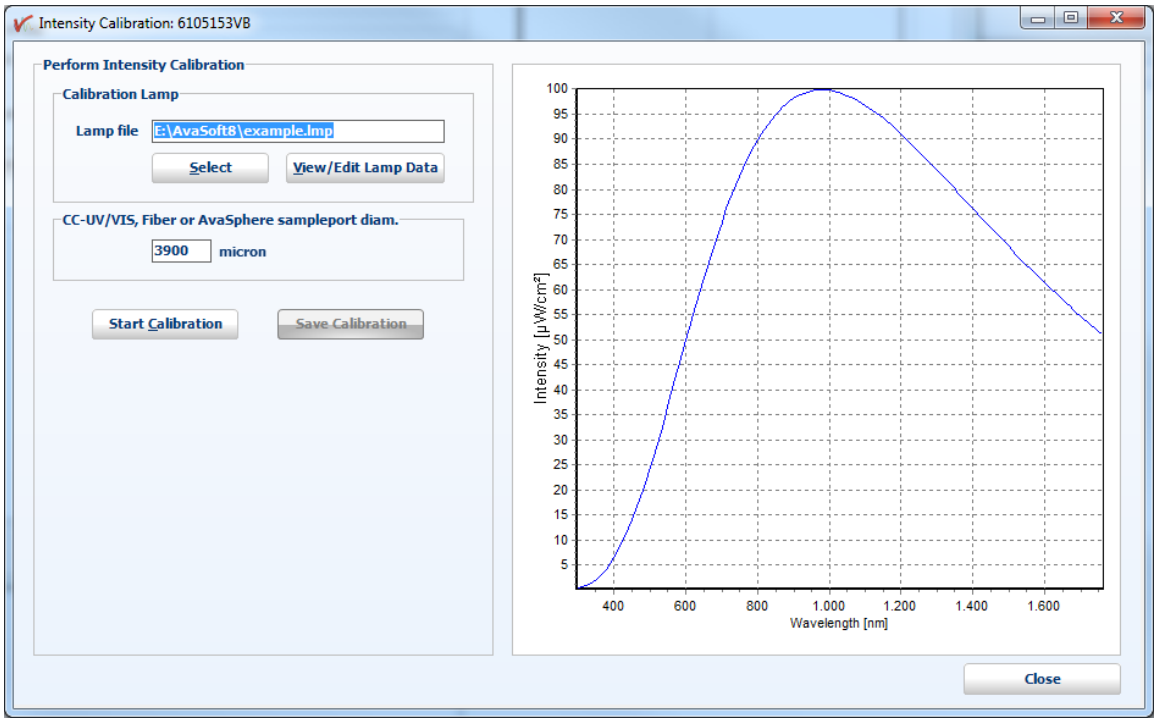
Stray Light Correction, when this feature has been turned off, or vice versa. A mismatch will result in a warning when loading the calibration. After loading an intensity calibration from file or EEPROM, a line will be displayed under the data transfer function, indicating if the intensity calibration has been performed with or without straylight correction.



4.9.4 Perform Intensity Calibration

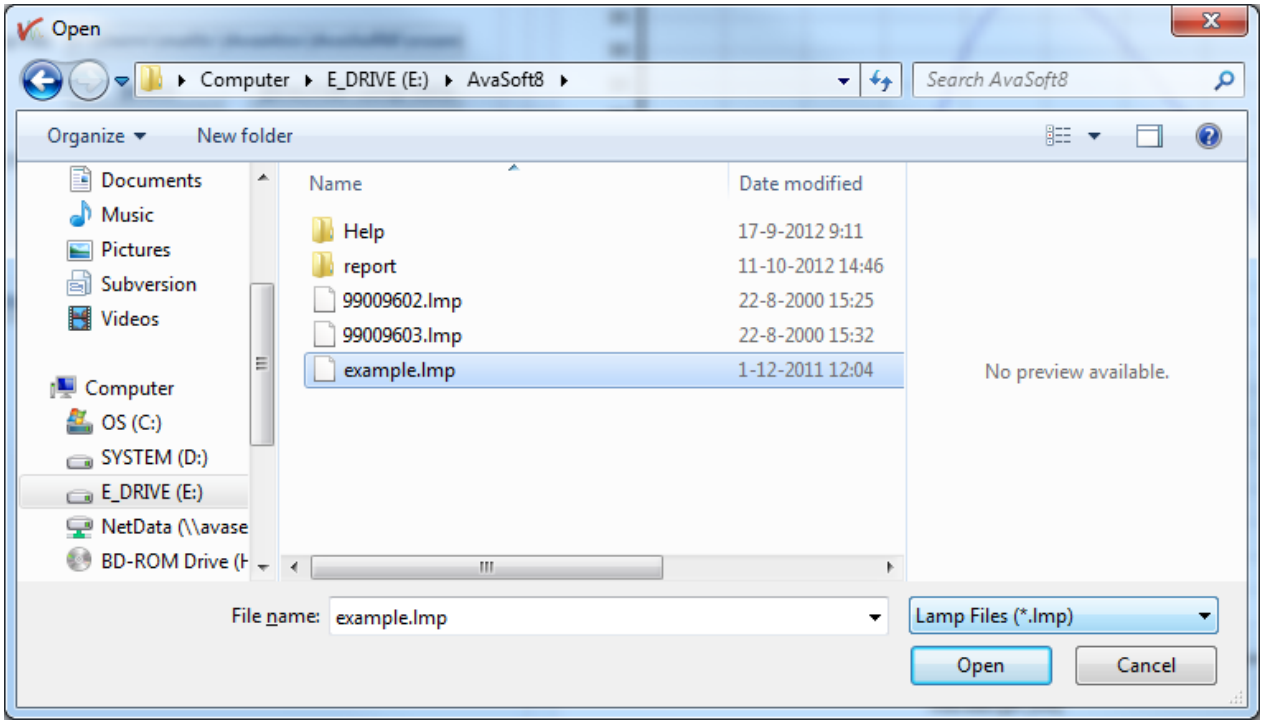
If a calibrated light source such as the AvaLight-HAL-CAL or AvaLight-DH-CAL is available, an intensity calibration can be performed. The Irradiance tab contains a “Perform Intensity Calibration” field. The following settings need to be entered before starting the intensity calibration:

- Calibration Lamp file
- CC-UV/VIS, Fiber or AvaSphere sample port diameter



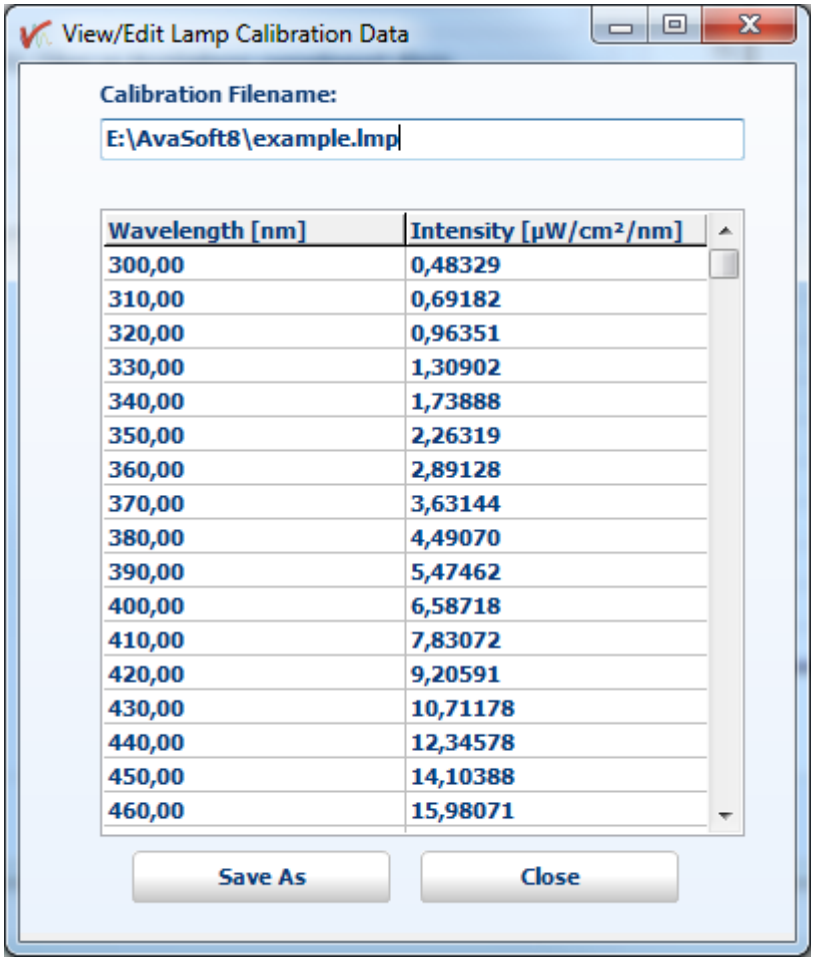
Calibration Lamp

The energy output (in µWatt/cm^2/nm) for the calibration lamp that will be used can be found in a file with the extension *.lmp. This file needs to be selected by clicking the “Select” button.



After the calibration file has been selected, the data can be viewed, edited and/or saved under a different filename by clicking the “View/Edit Lamp Calibration Data” button.

A dialog with the intensity versus wavelength values for the selected calibration light source is shown, as well as a graph in which the intensity is displayed versus wavelength:



If needed, the data can be edited and saved under another filename by clicking the Save As… button. Before the changed data takes effect, the new filename needs to be loaded with the Select lamp option described above.

CC-UV/VIS, Fiber or AvaSphere sample port diameter

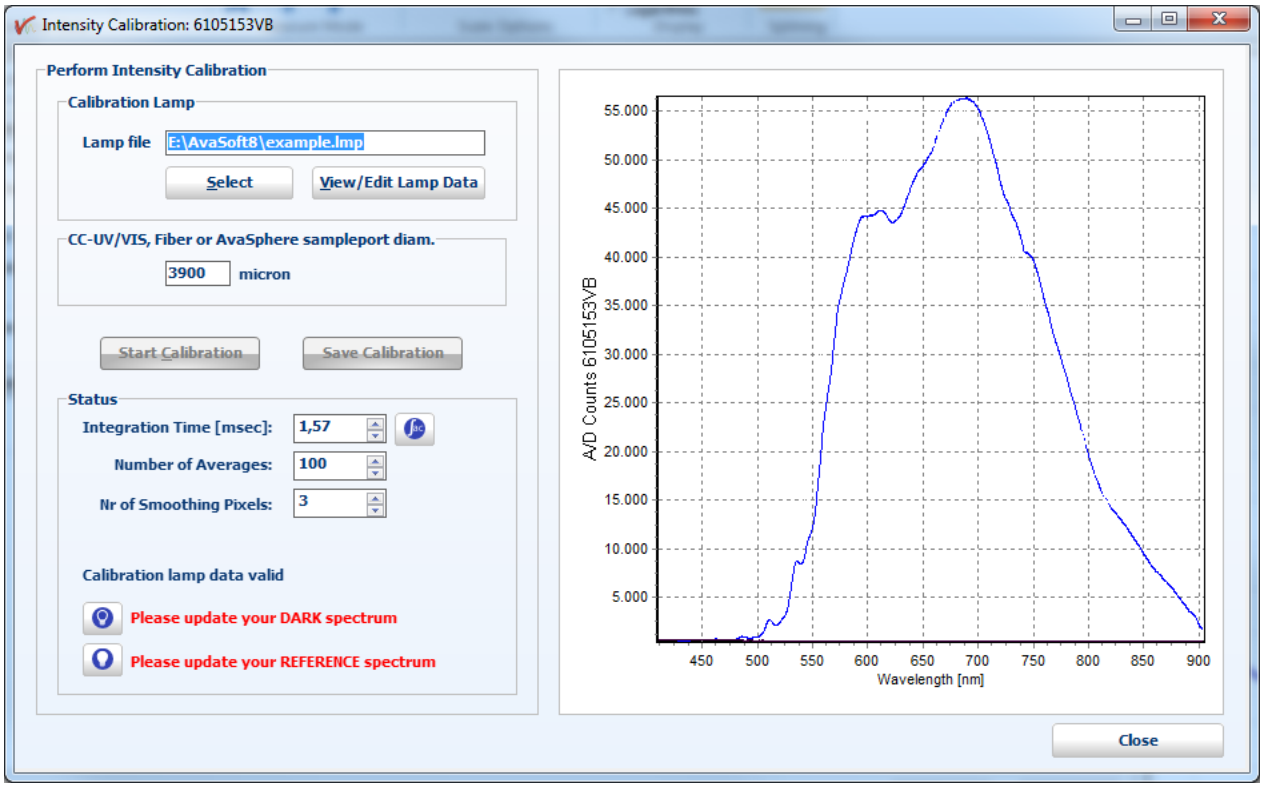
The hardware setup for which the calibration lamp has been calibrated (CC-UV/VIS cosine corrector, bare fiber or integrating sphere), should match the hardware setup that is used during the intensity calibration. The diameter of the cosine corrector (3900 micron), bare fiber, or AvaSphere (6000, 10000 or 15000 micron for respectively AvaSphere-30, AvaSphere-50 and AvaSphere-80) needs to be entered in micron.

It is important that the hardware setup that is used during the calibration, is the same as the hardware setup in the (ir)radiance measurements.

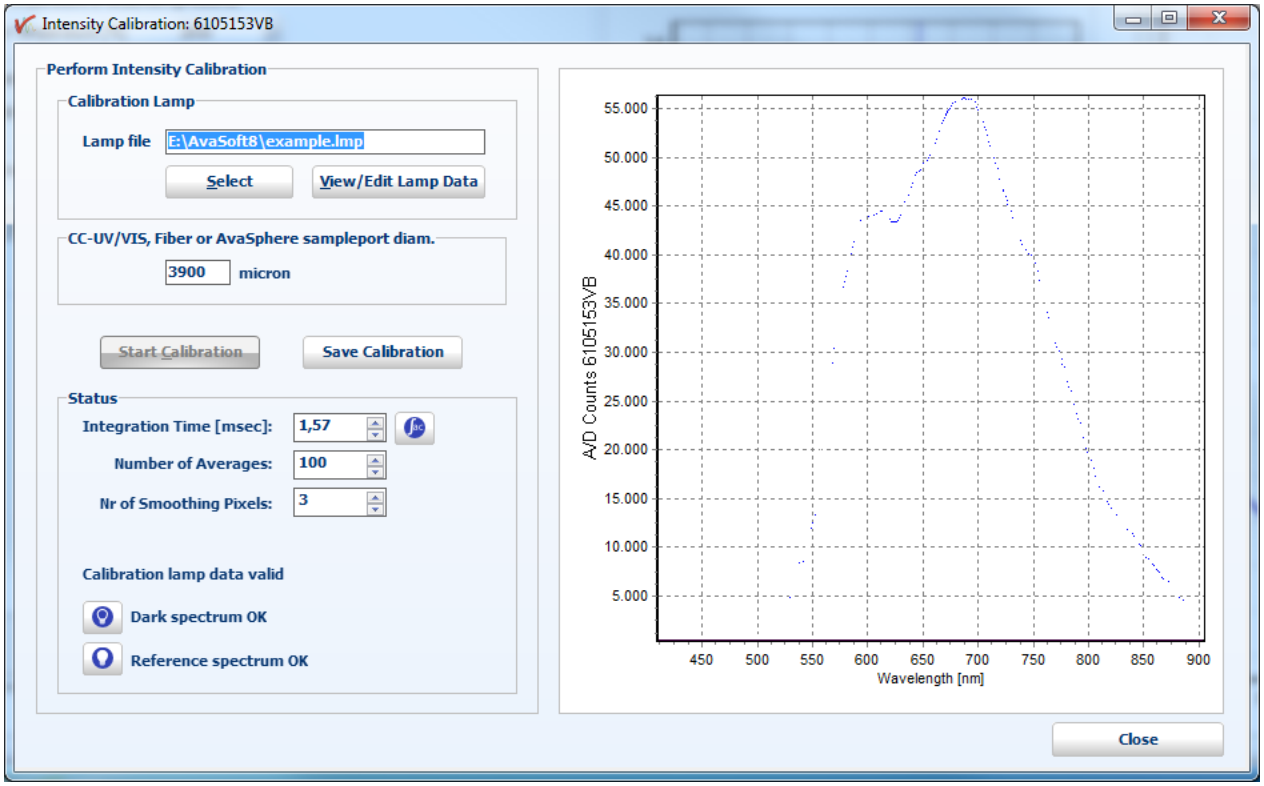
4.9.4.1 Start Intensity Calibration

Verify that the calibration is ON for at least 15 minutes, and that the hardware has been setup correctly. Then click the button “Start Calibration”. As a result, the Scope data (A/D Counts) for the selected spectrometer channel will be displayed graphically. Set the smoothing parameter to optimize smoothing for the fiber/slit diameter used (see also section 4.3.4.1, Measurements Settings).

Set the integration time such that a good reference signal is measured (maximum around 90% of the full ADC scale, which is 59000 counts for the 16bit ADC). It’s also possible to let AvaSoft search for an optimal integration time by clicking the AutoConfigure Integration time (‘∫AC’) button.

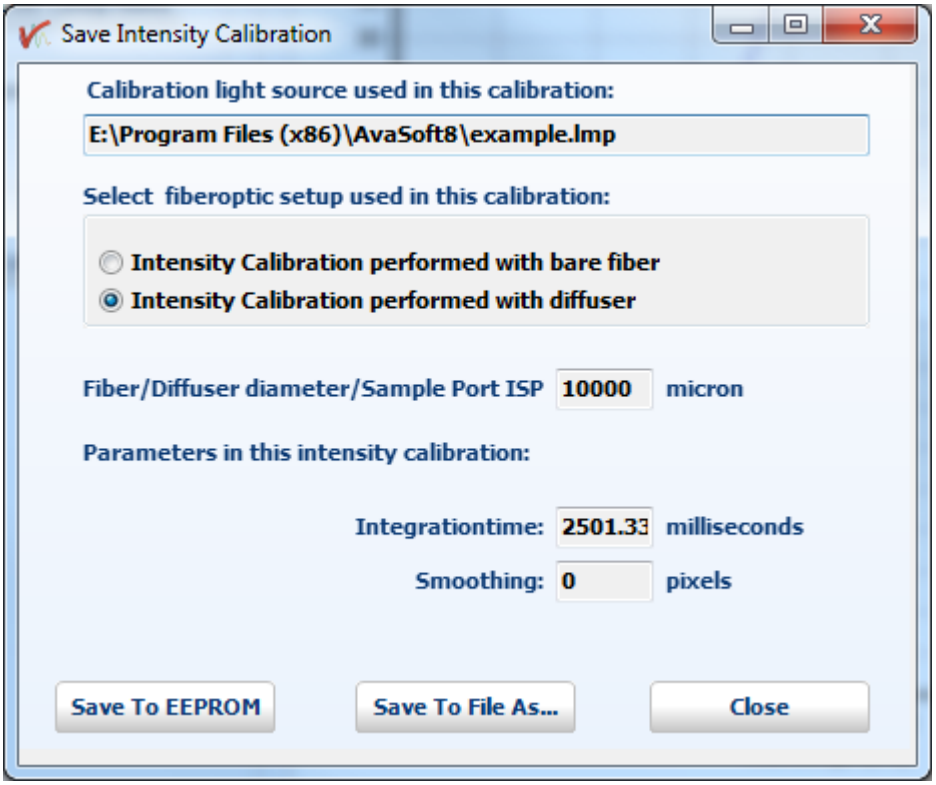


Set the Number of Averages to a high number to reduce the noise during the intensity calibration.
If a good reference signal is displayed, click the bright bulb button in the dialog above. A white line will mark the reference spectrum. Then switch off the calibration lamp, wait until the spectrum becomes flat, near the bottom of the scale, and click the dark bulb button to save a dark spectrum. A black line will mark the dark spectrum.



4.9.4.2 Save Intensity Calibration

If reference and dark data have been saved in the figure above, the intensity calibration can be saved by clicking the “Save Calibration” button.



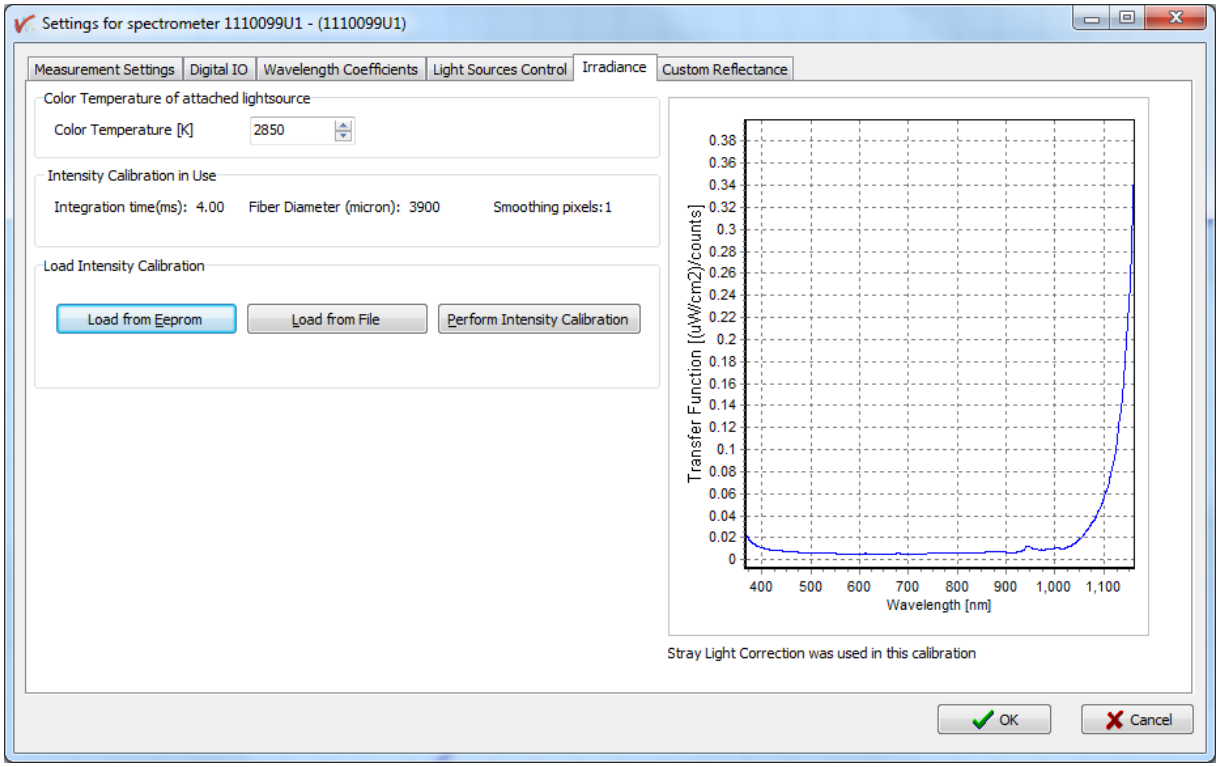
A dialog shows up in which the current settings in this intensity calibration are shown. If the calibration has been performed with diffuser, the intensity calibration data will be saved to an ASCII file with extension *.dfr, with bare fiber this extension will be *.fbr. The name of the intensity calibration file can be entered after clicking the “Save To File As…” button. When saving an intensity calibration to file, make sure to include the serial number in the filename.

The following data will be saved to the intensity calibration file:

- The name of light source calibration file (*.lmp)
- The number of pixels
- The integration time in milliseconds
- The diameter of diffuser surface in microns
- A value per pixel, which represent the dynamic range (reference minus dark data) at each pixel during the intensity calibration, divided by the intensity of the calibrated light source that was used.
- The setting for the Smoothing parameter during the intensity calibration.
- The setting for Stray Light Correction (0=off, 1= on)

By pressing the “Save to EEPROM” button, the calibration will be saved to the AvaSpec itself.

After an intensity calibration has been performed, a graph is displayed which shows the data transfer function for the spectrometer channel. The irradiance spectrum is calculated by multiplying the measured scope data (from which a saved dark spectrum is subtracted) with this data transfer function.



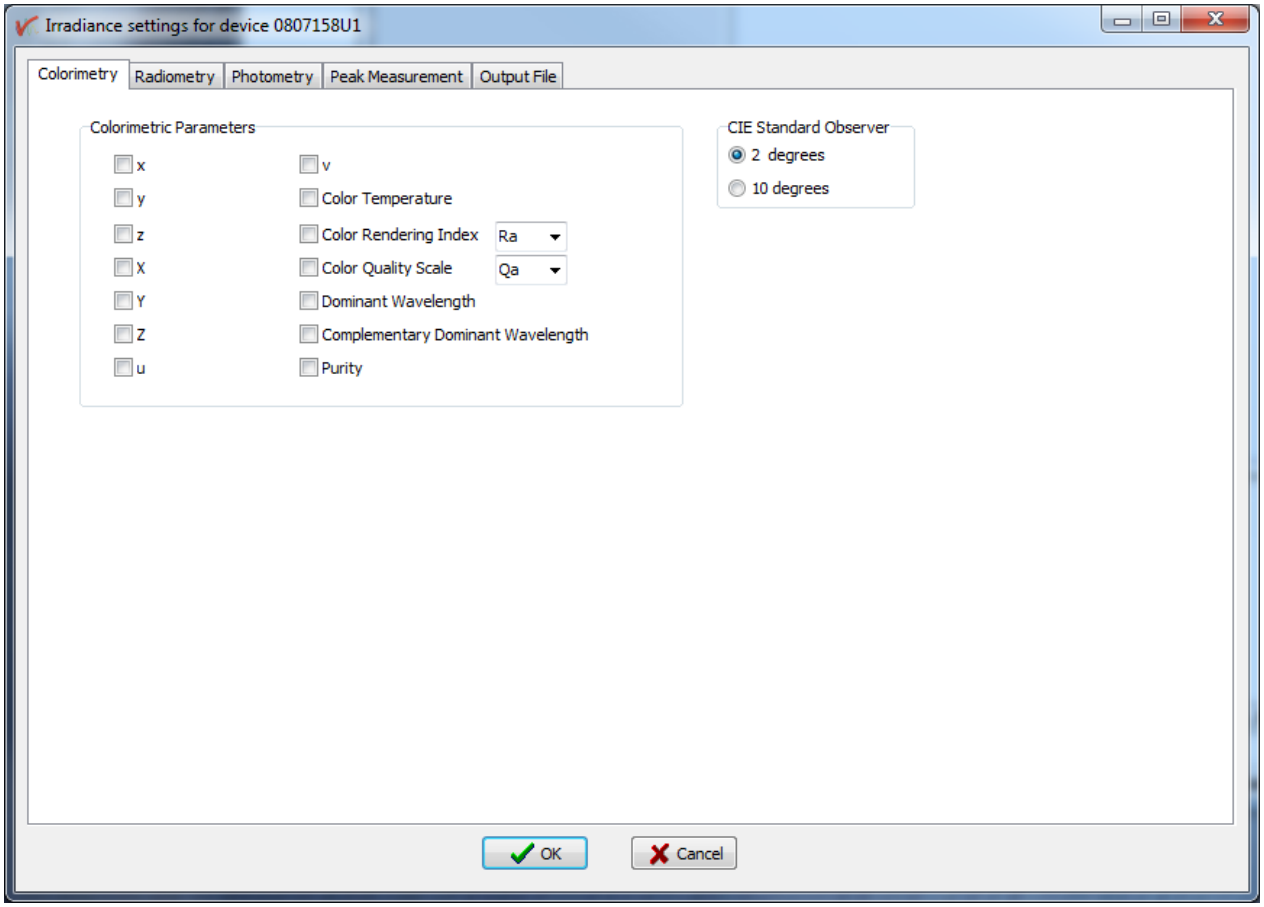
4.9.5 Irradiance Application Window

4.9.5.1 'Home' ribbon tab, 'Channel' Button

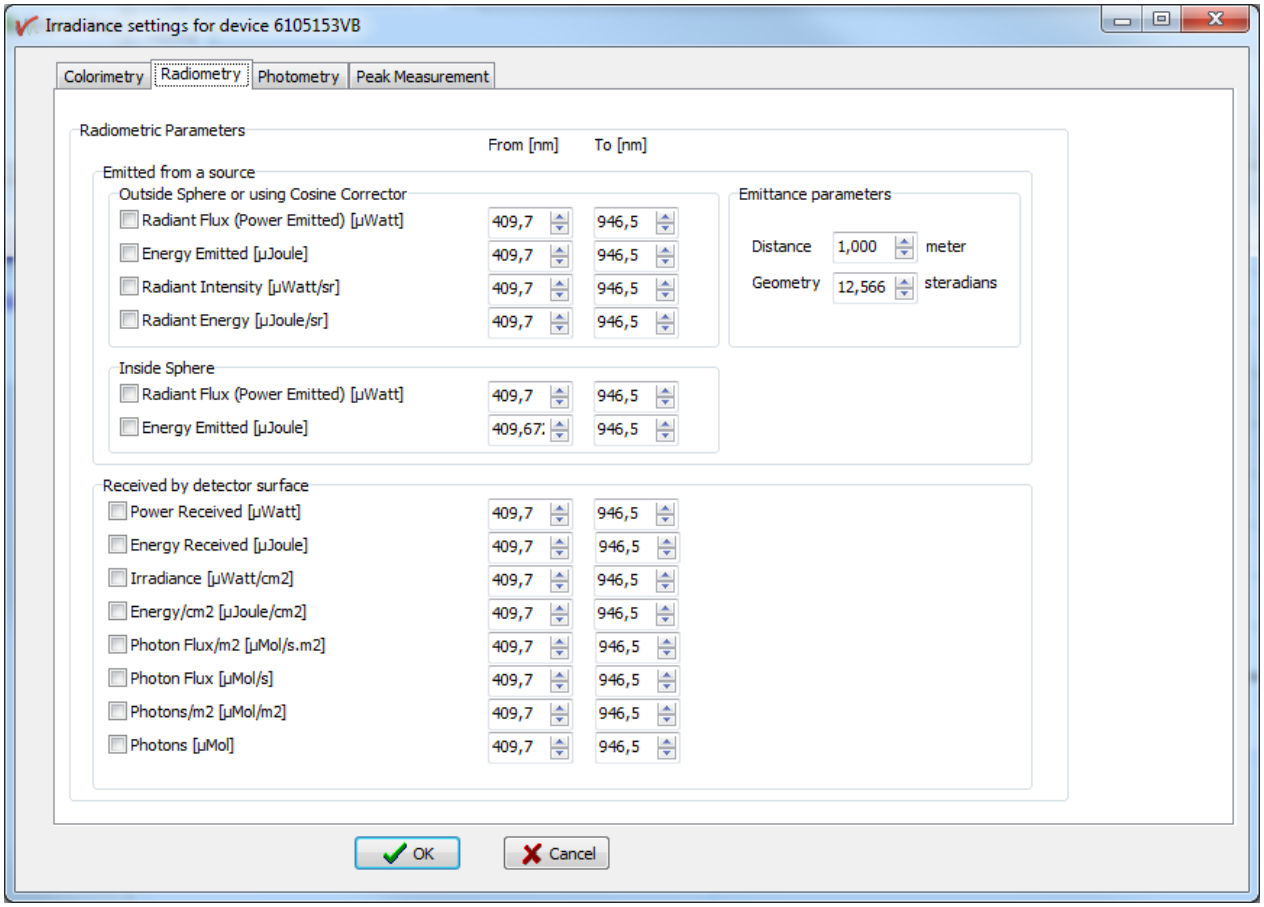
4.9.5.2 'Home' ribbon tab, 'Settings' Button

After clicking the 'Settings' button, you can select the parameters that will be shown in the irradiance chart. They are distributed over 4 tab sheets, one for each kind of measurement. A description of these parameters and how they are calculated can be found in section 4.9.1, Background.

Colorimetric parameters

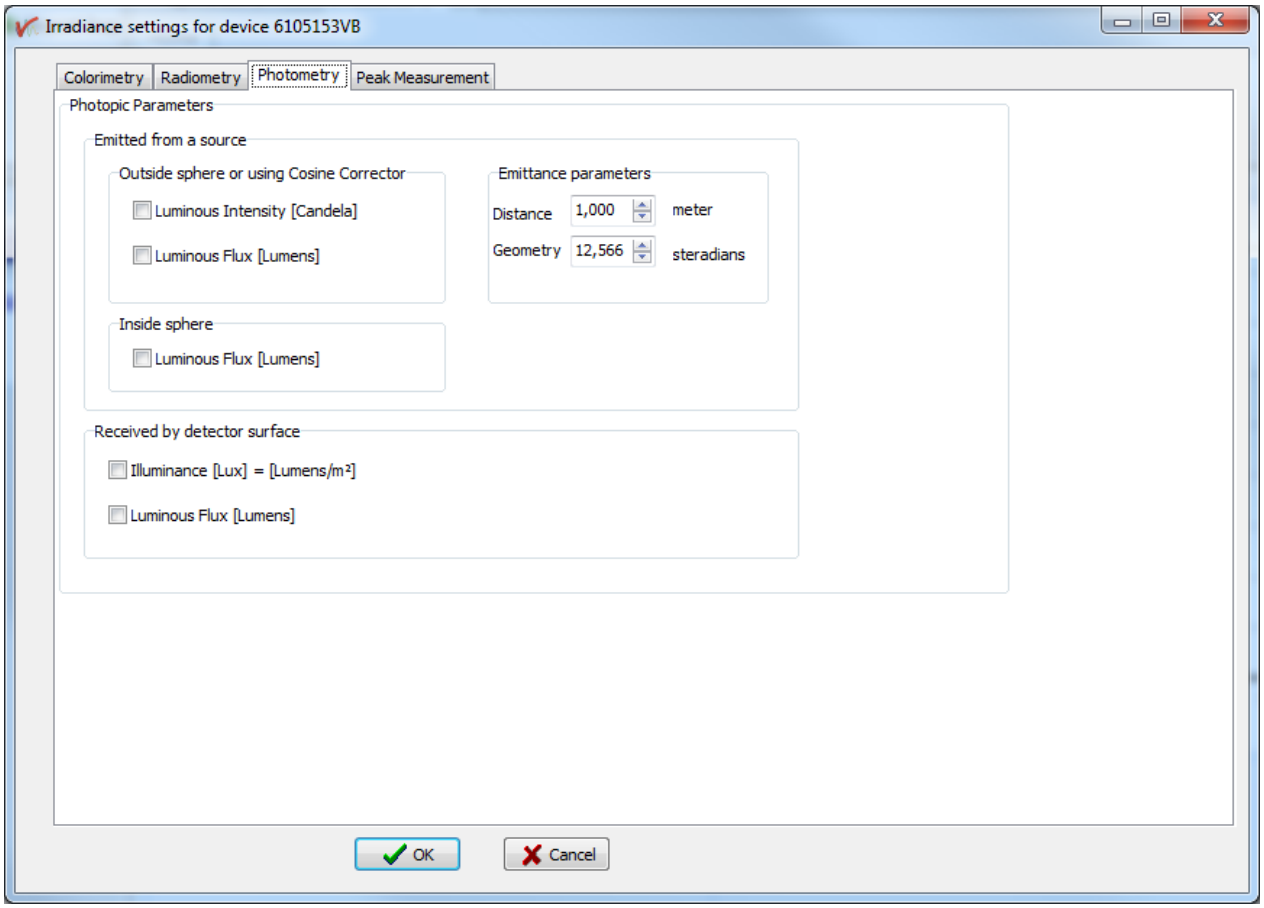


Radiometric parameters



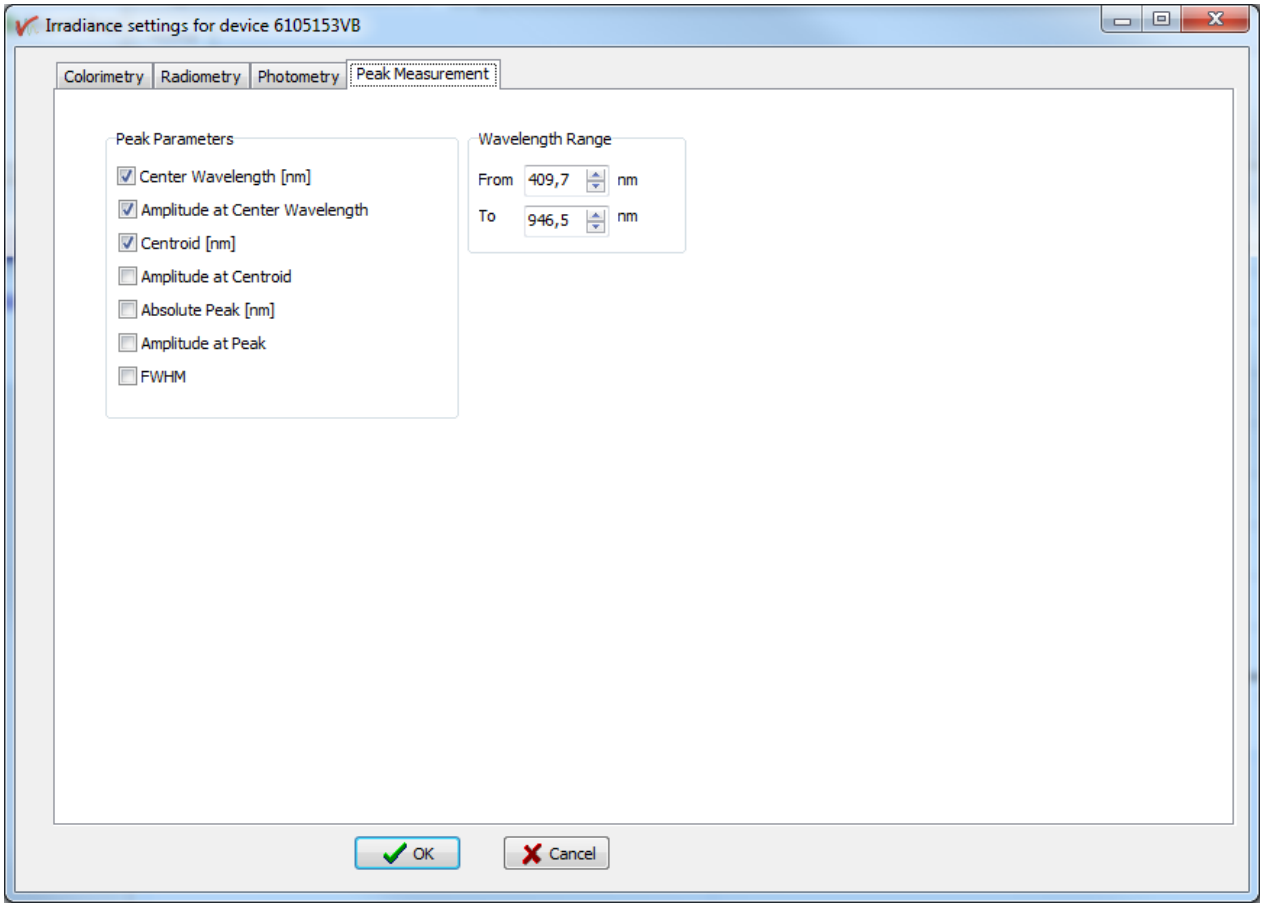
An important assumption when calculating the emitted power or energy is that the source should be an isotropic point source.

Photometric parameters



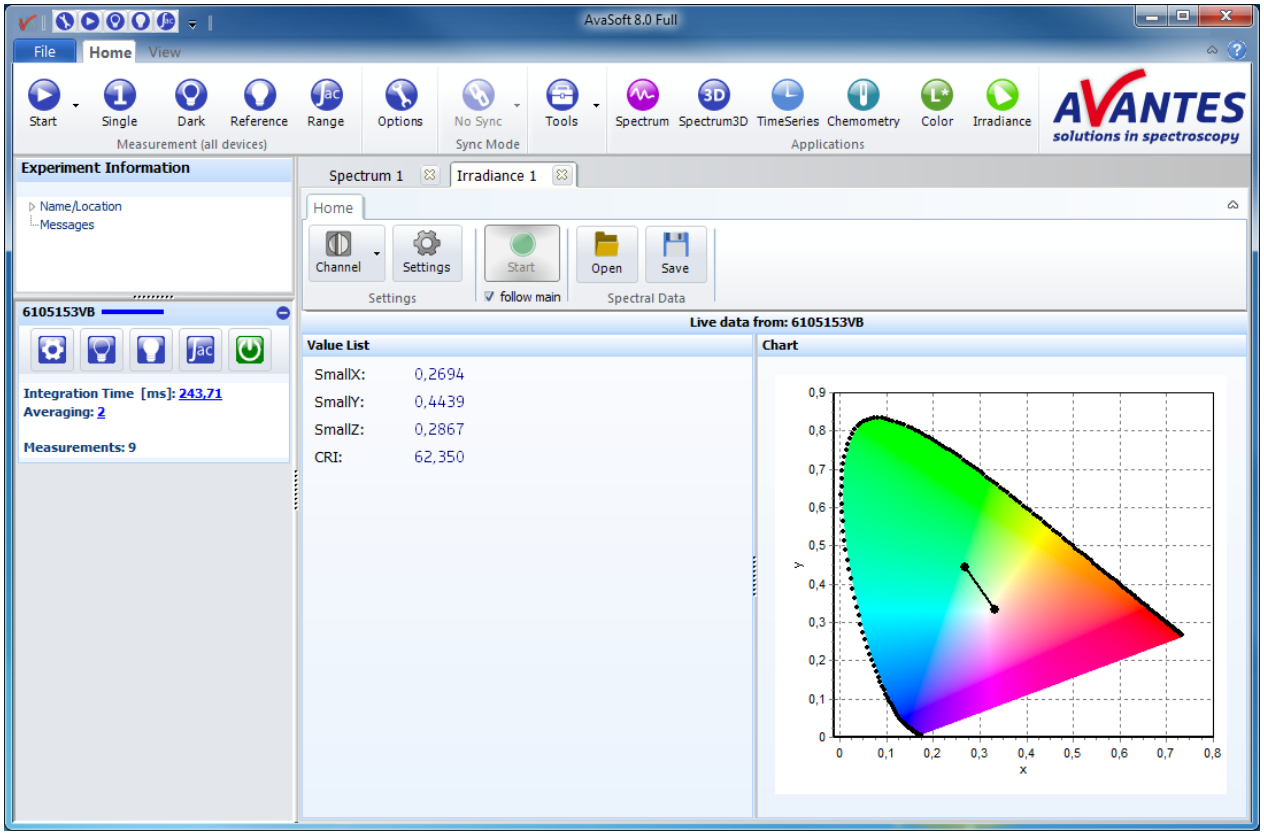
An important assumption is that the source should be an isotropic point source.

Peak Measurement parameters



4.9.5.3 'Home' Ribbon Tab, 'Start/Stop' Button

After all settings are filled in correctly the measurements can be started by clicking the 'Start' button. It might be easier to check the 'follow main' checkbox, in which case starting the spectrometer measurements will also start the irradiance measurements.
The figure below shows a measurement in progress.



The chromaticity diagram is used to visualize the colorimetric measurements. Depending on what has been selected in the irradiance chart settings dialog, it will display the locus for the 2 or 10 degrees standard observer. The measured (x,y) coordinates will be displayed in the diagram and a line will be drawn from the midpoint (x=y=1/3) through the measured (x,y) to the edge of the locus, which represents the dominant wavelength. If you mouse over the black dots on the edge of the locus, the wavelength corresponding to the dot will be displayed in a small popup help window.
The 'Stop' button is clicked to stop the color measurements.

4.9.5.4 'Home' Ribbon Tab, 'Open Spectral Data' Button

4.9.5.5 'Home' Ribbon Tab, 'Save Spectral Data' Button

4.10 Thin Film

4.10.1 Film Thickness Primer

As light is reflected from both sides of a transparent thin film on a reflective surface, an interference spectrum is formed. This spectrum looks generally like a sine wave with a frequency that decreases with the wavelength (a 'chirp'). The thickness of the layer determines the frequency of the sine wave at a given wavelength, where a larger thickness will render a higher frequency (i.e. more waves visible). This means that you can determine the thickness of a layer by either determining the frequency of these sine waves directly from the measured spectrum (through Fast Fourier calculations), or by calculating a theoretical spectrum for lots of different values for thickness, and matching these spectra with the measured one, yielding the best fit as the measured thickness. Both methods are available in the AvaSoft Thin Film application.

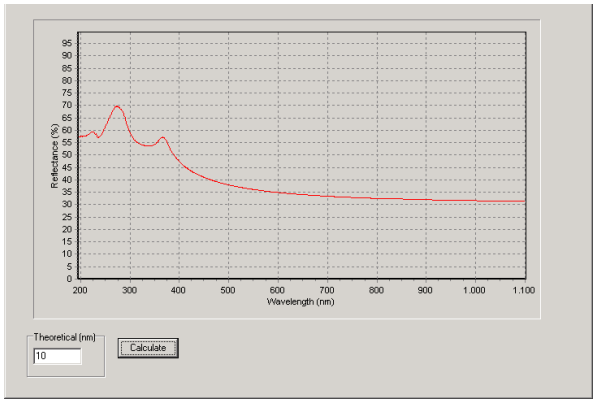
The FFT algorithm can be used if the range to be searched is too large to be calculated in a reasonable amount of time with the "Match Spectrum" algorithm, or if the materials are not well defined. The finish of some materials ("roughness") can influence the reflectance values considerably. The "Match Spectrum" algorithm is the default one. It is most suited for thin layers of well-defined materials, e.g. those used on silicon wafers.

The "Match Spectrum" algorithm has a zooming feature that will speed up readings considerably. A running range is kept from the last 10 values of the Fit Quality value. This value is used as a marker for a stable measurement. If this value drops below a defined level, then the theoretical spectra will not be calculated for the full range between the lower and upper limit. They will only be calculated for a limited range of steps, above and below the current thickness measurement value. A single value above the defined level (meaning the fit is not that good anymore) will undo the zoom, and the full range will be calculated again.

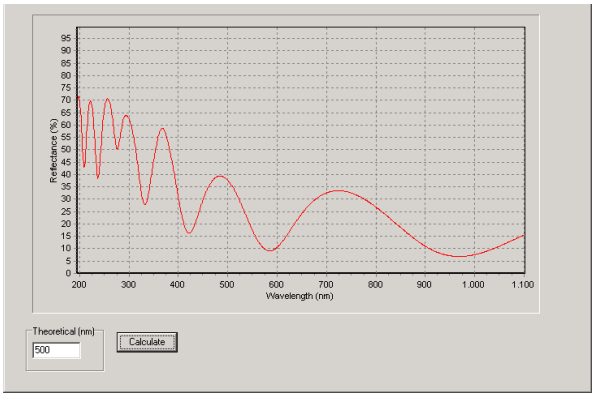
For thin layers, the lower end of the wavelength spectrum will limit the precision with which thin layers can be measured. Very thin layers will yield only part of a single sine. The wavelength range from 200-400 nm can be very important in this case.

For thick layers, the resolution of the spectrometer will be the limiting factor in the measurement, as the sine waves will start to fuse together. The upper end of the wavelength spectrum will yield the best results in this case, as the frequency of the sine waves becomes larger with decreasing wavelength.

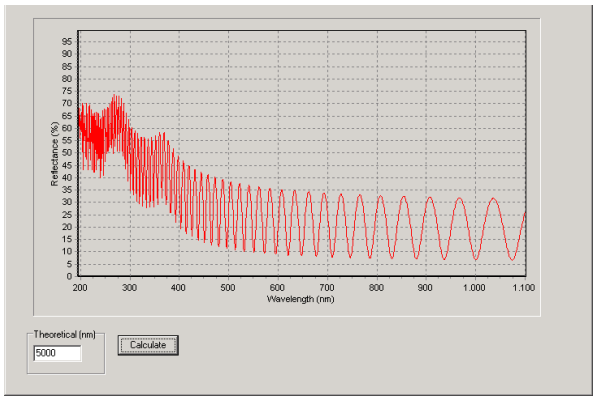
These effects are illustrated in the following figures that show theoretical reflectance spectra for SiO2 layers on Si with a thickness of respectively 10 nm, 500 nm, 5000 nm and 50000 nm.
The wavelength range is 200 – 1100 nm in all four figures.



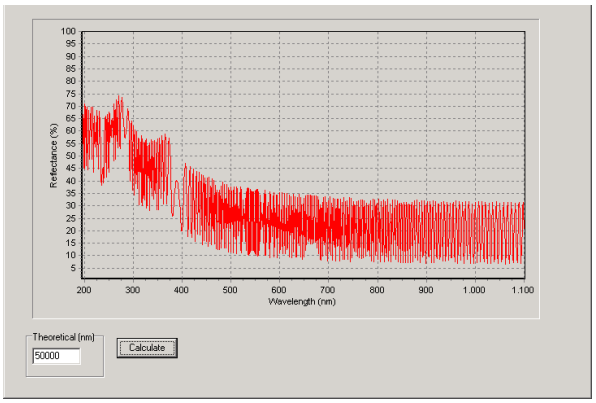
10 nm



500 nm



5000 nm



50000 nm

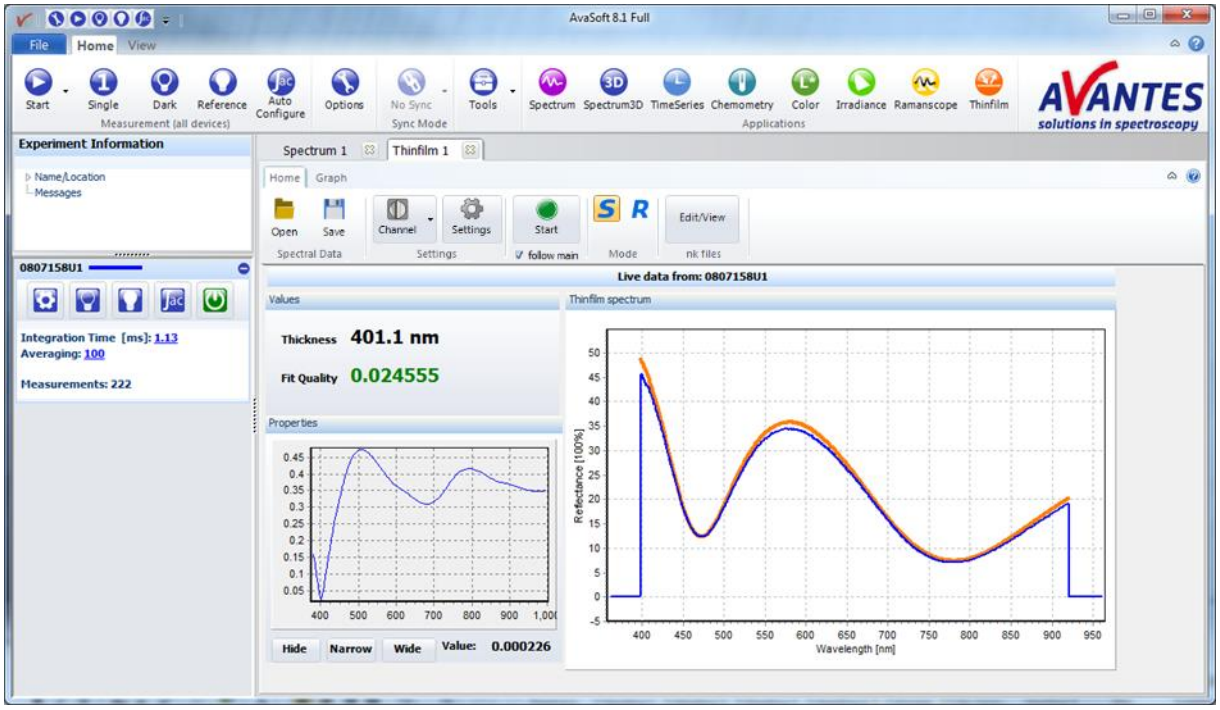
4.10.2 Quick Start: Measuring and Saving a Reflectance Spectrum and a Film Thickness

1. After starting AvaSoft, the Start button needs to be clicked to start measuring.
2. Connect the reflectance probe to the light source and to the spectrometer input port(s) and set up the experiment for taking a reference spectrum. The reference spectrum should be taken from the uncoated substrate material.
3. Select the Thinfilm application in the Applications toolbar.
4. Select Settings and enter correct values for wavelength limits, materials and thickness limits under the Measurement Settings Tab. Select an algorithm under the Calculation options tab. Press ‘Done’ to save.
5. Now turn on the light source. Usually some sort of spectrum may be seen on the screen, but it is possible that too much or too little light reaches the spectrometer at the present data collection settings. This amount of light is controlled by the integration time. Select the AutoConfigure button “∫AC” in the spectrometer window. The integration time can also be changed manually as described in section 4.3.4.1, Measurements Settings.
6. Now turn off the light source and save the Dark data. This is done by pressing the dark bulb icon in the spectrometer window. Always Save Dark after the integration time has been changed.
7. Turn on the light source again. Save the present spectrum as a reference by pressing the lit bulb icon in the spectrometer window (next to the black one). Always use Save Reference

after the integration time has been changed. After saving a reference, replace the reference material by the coated material. Verify that with the coated material, the maximum value of the signal is not overloading the spectrometer. In most cases this will not be the case as the coating will absorb part of the light, but for some coatings the light of the coated material will reflect more than uncoated reference material. If this is the case, a new reference and dark spectrum should be taken at a lower integration time at which the coated material will not overload the spectrometer.

8. Click the reflectance (R) button to switch to reflectance mode. This will also start the Film Thickness measurements, displayed in the Values panel. By clicking the stop button in the top left corner, the data acquisition is stopped and the last acquired spectrum is shown in static mode. The data acquisition can be started again by clicking the same button, which now shows 'Start'.
9. To save the spectrum, select the 'Spectrum 1' application, which allows you to save the spectrum in Scope mode or in Reflectance mode. You can export or print the chart in the 'Graph' ribbon tab.
10. To improve the Signal/Noise ratio, a number of spectra may be averaged. To do this, the Averaging value in the spectrometer window (below the integration time) can be increased.

4.10.3 Thin Film Application Window



The upper left 'Values' panel contains the large type Thickness and Fit Quality fields. These fields are read-only. The Fit Quality is defined as the square root of the average SSR (sum of squared residuals), when comparing a theoretical spectrum with a measured spectrum. The reflectance values are normalized first by dividing them through the calculated reference reflectance.

The middle left 'Properties' panel contains either a display of the settings that can be edited in the 'Settings' dialog, or it shows the Variance Graph. You can switch between these displays by pressing the 'Show/Hide' button.

The upper right panel contains a chart of the Thinfilm spectrum in either Scope mode or Reflectance mode.

The bottom panel (not shown in the figure above) contains the Thinfilm time series chart. Resize the window to show or hide this part of the window.

4.10.3.1 'Home' ribbon tab, 'Open spectral data' Button

Loads spectral data in AvaSoft 8 binary format and recalculates the thickness.

4.10.3.2 'Home' ribbon tab, 'Save spectral data' Button

Saves spectral data in AvaSoft 8 binary format.

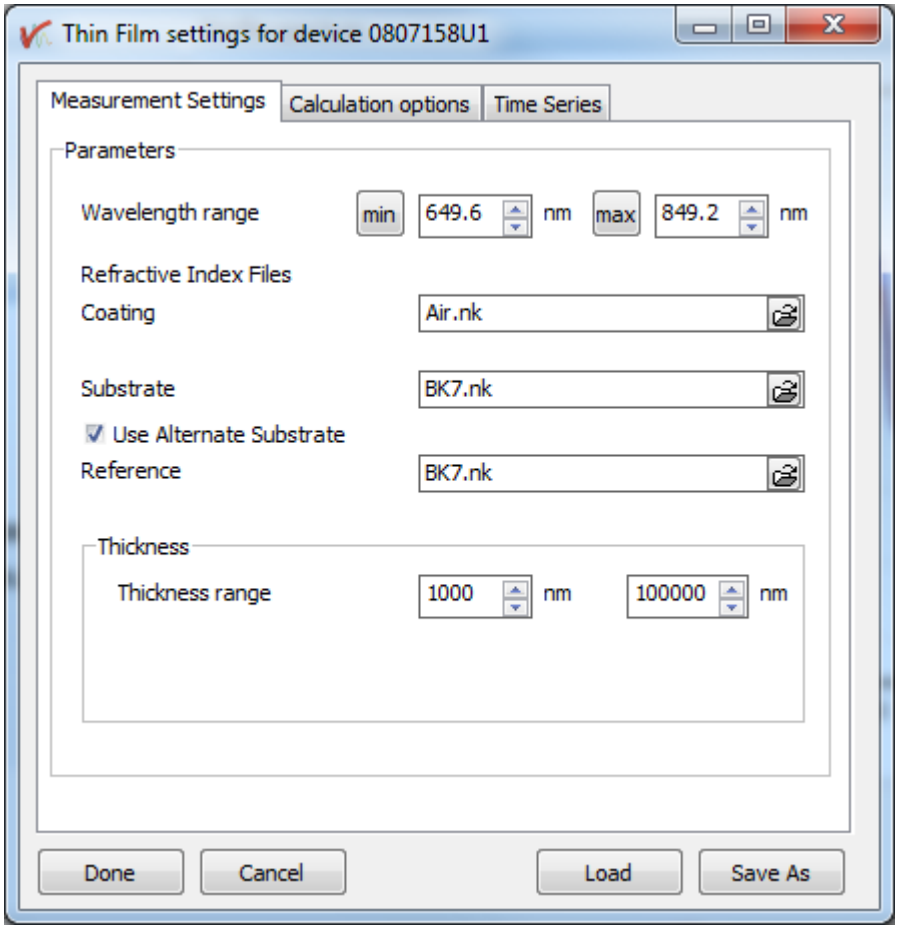
4.10.3.3 'Home' ribbon tab, 'Channel' Button

Allows you to select the spectrometer channel used.

4.10.3.4 'Home' ribbon tab, 'Settings' Button

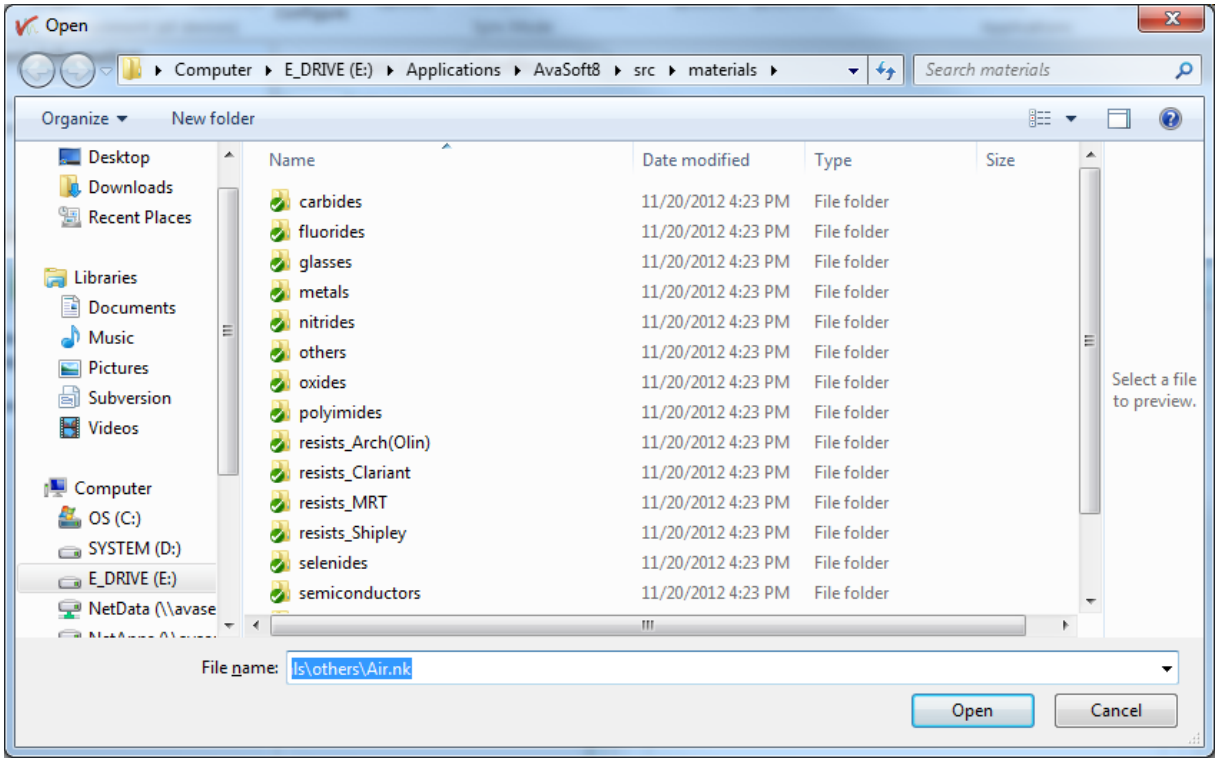
After clicking the 'Settings' button, you can select the parameters that will be used in the thin film application. They are distributed over 3 tab sheets:

- Measurement Settings



The wavelength limits used in the calculations can be edited in the two input fields on the top line. Default values here will reflect the full range of the spectrometer channel. Be sure to view the Reflectance spectrum and limit the range here accordingly. Without a UV light source, you should set the lower limit to about 400 nm, as the Reflectance spectrum will only contain bogus noise information at very low signal values.

The next three edit fields show the filenames for the .nk files used. The default values are for a SiO2 coating layer on a Si substrate.
Normally, you should enter the same filename for Reference and Substrate. To do this, you can also uncheck the 'Use Alternate Substrate' checkbox. The Reference field is available to enable use of a different (uncoated) reference material, in case the substrate material is not available in an uncoated state. You can change the values for the filenames by clicking the button to the right of each field. You will then enter a File Open Dialog, which allows you to select an .nk file for many predefined materials.

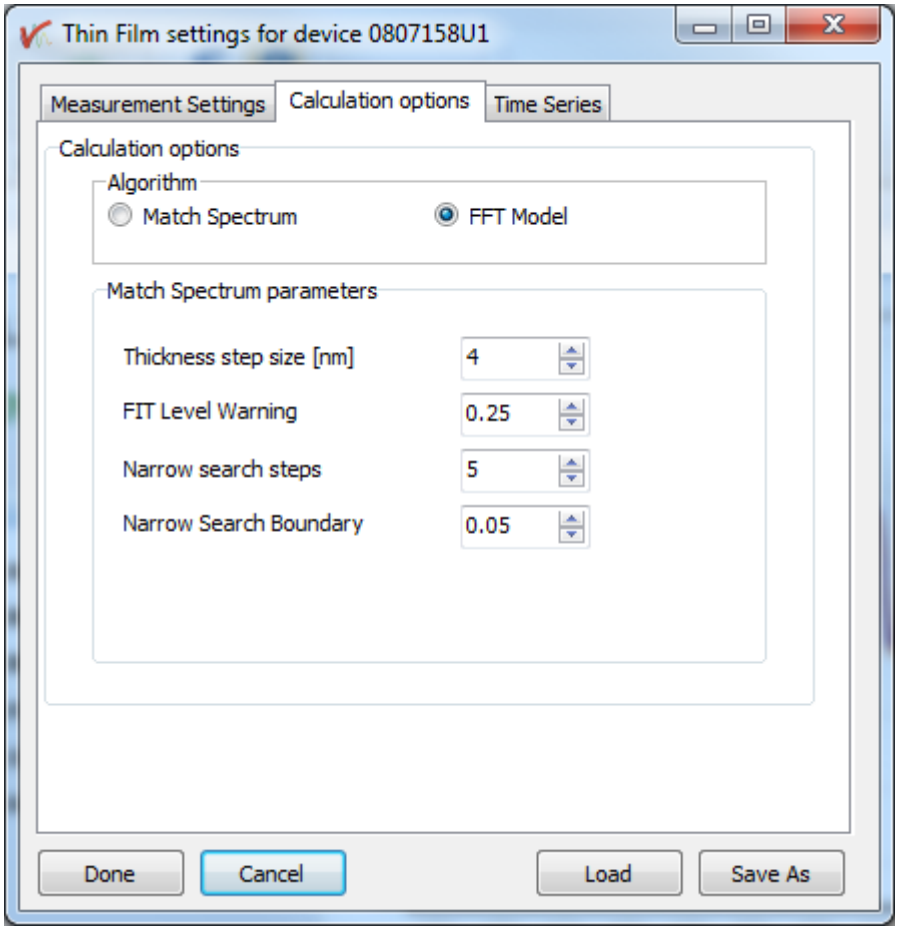


The lower and upper thickness limit values can be edited in the Thickness fields in the lower part of the form. If you are confident about the layer thickness, select a narrow range here. This will significantly speed up your measurement in the default Match Spectrum mode, as it will limit the amount of spectra that are calculated for each reading.

The buttons at the bottom of the Layer Display window allow you to Save and Load the menu settings. The ‘Done’ button will also save the values entered, and the information saved will be reloaded in the next session.

The ‘Load’ and ‘Save As’ buttons allow you to save the same information to a different filename (‘*.tf.ini’) in the user directory, and reload it at a later time.

Calculation Options

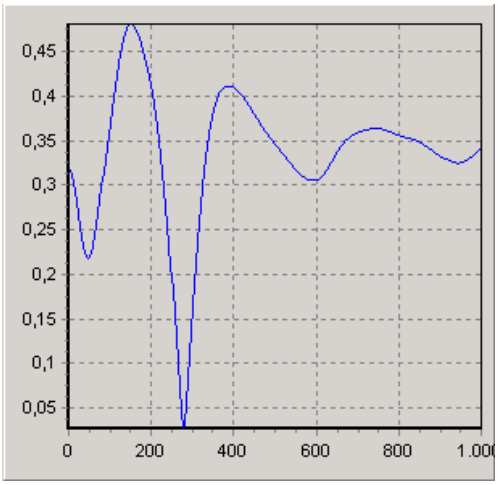


The top of this form allows you to select which algorithm is used to calculate thickness values. The default value is 'Match Spectrum', which is suited best for thin layers of well-defined materials. The 'FFT Model' algorithm is suited best for thick layers, and for materials where roughness of the material influences the reflectance value.

The lower part of the form only applies to the 'Match Spectrum' algorithm.

The 'Thickness Step Size' value determines the interval between the lower and upper thickness limits at which the theoretical reflectance spectrum will be evaluated against the measured reflectance spectrum during the first (global) search. The default step size is 1 nm. By increasing this value, less theoretical spectra will be evaluated during the first step in the algorithm. This will take less time, but it can also decrease the certainty of finding the best solution.

The graph below shows the quality of fit at the Y-axis against the evaluated layer thickness at the X-axis. In this example the thickness limits were set to 0 nm and 1000 nm, as shown at the X-axis. With a 1 nm step size this means that 1001 spectra are evaluated in the first run. From the shape of the curve can be concluded that it is very likely that the best thickness found (= minimum at 277 nm) is the optimum. You can choose to take larger steps here to speed up calculations, but then it would of course also be possible to miss an optimum if this value is set too high.



In the past, a 4 nm step size has been tested on a lot of different materials and it lead to the right optimum in all tests. The graph above is called the response curve and is available in the ThinFilm application to get an impression about the robustness of the solution that was found. A detailed description about this feature can be found below.

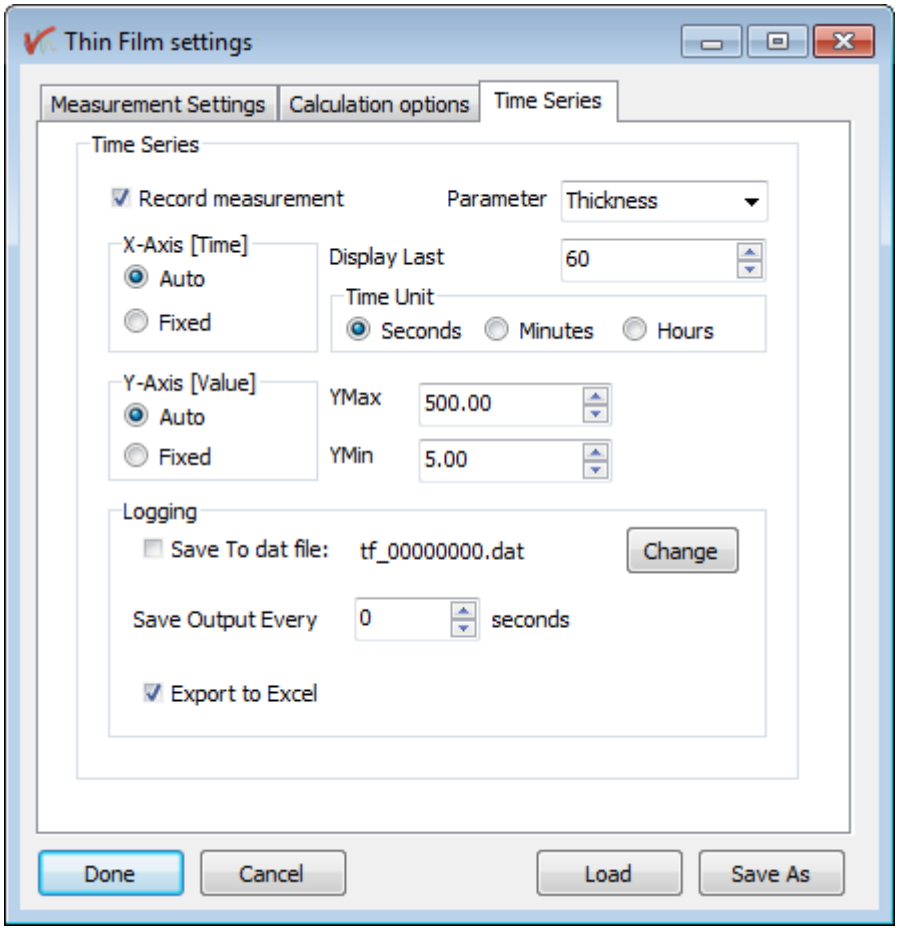
The ‘Fit Warning Level’ can be changed if the default warning level is not correct for your setup. If the ‘Fit Quality’ value exceeds this warning level, the ’Fit Quality’ field in the Values panel will be colored red.

The next two fields, ‘Narrow Search Steps’ and ‘Narrow Search Boundary’, allow you to fine-tune the zooming feature that is part of the ‘Match Spectrum’ algorithm. A running range is kept from the last 10 values of the Fit Quality value. This value is used as a marker for a stable measurement. If this value drops below the ‘Narrow Search Boundary’, then the theoretical spectra will not be calculated for the full range between the lower and upper limit in the Layer Display window. They will only be calculated for a limited range of steps, above and below the current thickness measurement value. The thickness range of steps is the product of the ‘Thickness Step Size’ and the ‘Narrow Search Steps’, both under and over the currently measured thickness value.

A single running range value that is over the limit will undo the zoom effect, and the full range will be calculated again. After at least 10 readings, the algorithm can zoom in again.

If you press the ‘Show’ button, the Properties display will show a graph of the fit quality against layer thickness. This allows you to monitor whether there are more optima present in your range. You can also fine-tune the zooming feature here. The Narrow and Wide buttons force the algorithm to zoom in or out. The ‘Value’ is the running range value, which is the absolute range in the last 10 values of the ‘Fit Quality’ value.

Time Series



This form allows you to set options for a time series measurement.

Check ‘Record measurement’ to chart either thickness or variance against time. The chart will be displayed below the Thinfilm spectrum. You may have to expand the form to view it. You can customize both x and y axis values. You can also log values to disk (by selecting the “Save to dat file” option), and change filename and logging frequency in the bottom part of the form. Export to Excel is also possible, where always both the thickness and fit quality will be exported to the Excel sheet.

4.10.3.5 ‘Home’ Ribbon Tab, ‘Start/Stop’ Button

After all settings are filled in correctly the measurements can be started by clicking the ‘Start’ button. It might be easier to check the ‘follow main’ checkbox, in which case starting the spectrometer measurements will also start the Thinfilm measurements.

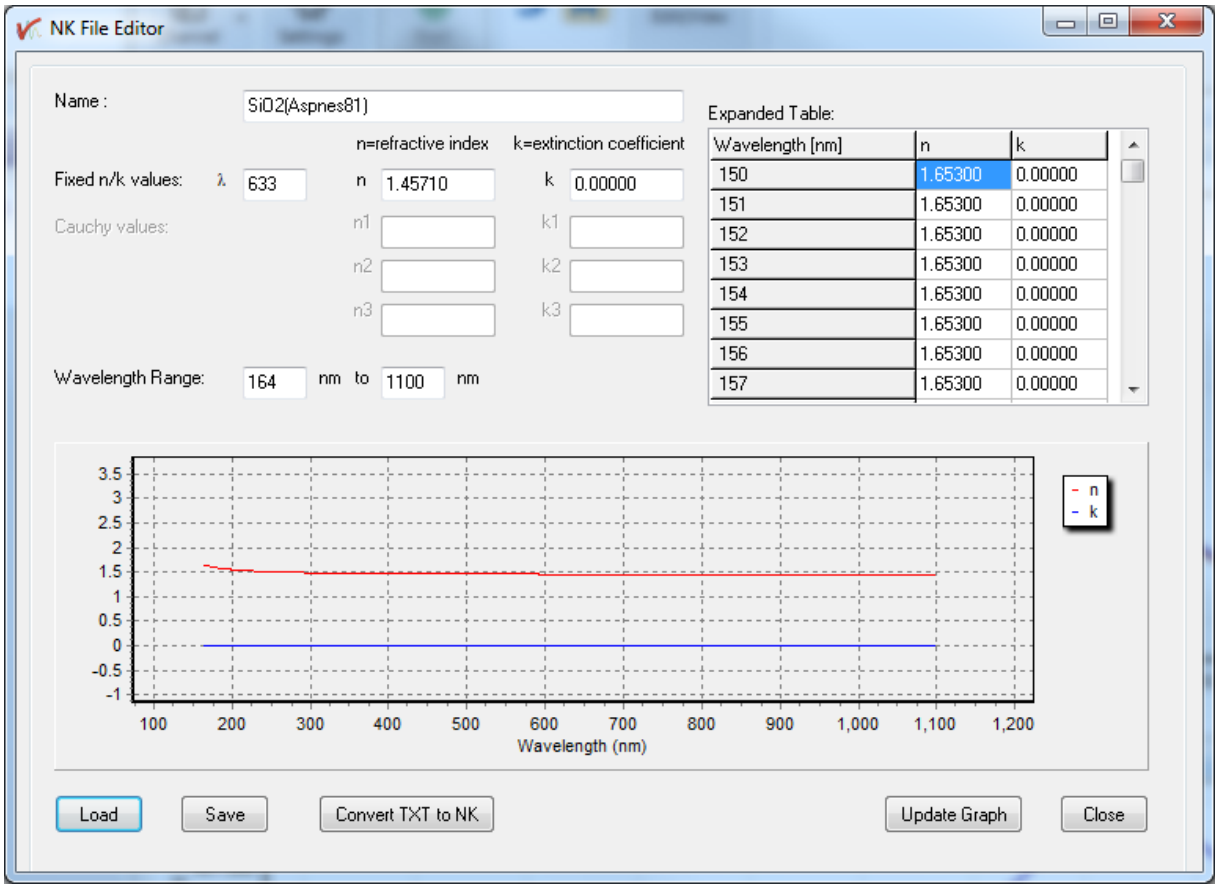
4.10.3.6 'Home' Ribbon Tab, Mode Selection Buttons

S This mode will show a real time raw data signal, with on the Y-axis the read out of the AD-converter and on the X-axis the calculated wavelength.

R In Reflectance Mode, the reflectance at pixel n is calculated using the current sample, reference and dark data sets in the following equation:

$$R_n = 100 * \left(\frac{sample_n - dark_n}{ref_n - dark_n} \right)$$

4.10.3.7 'Home' Ribbon Tab, Edit/View .nk Files



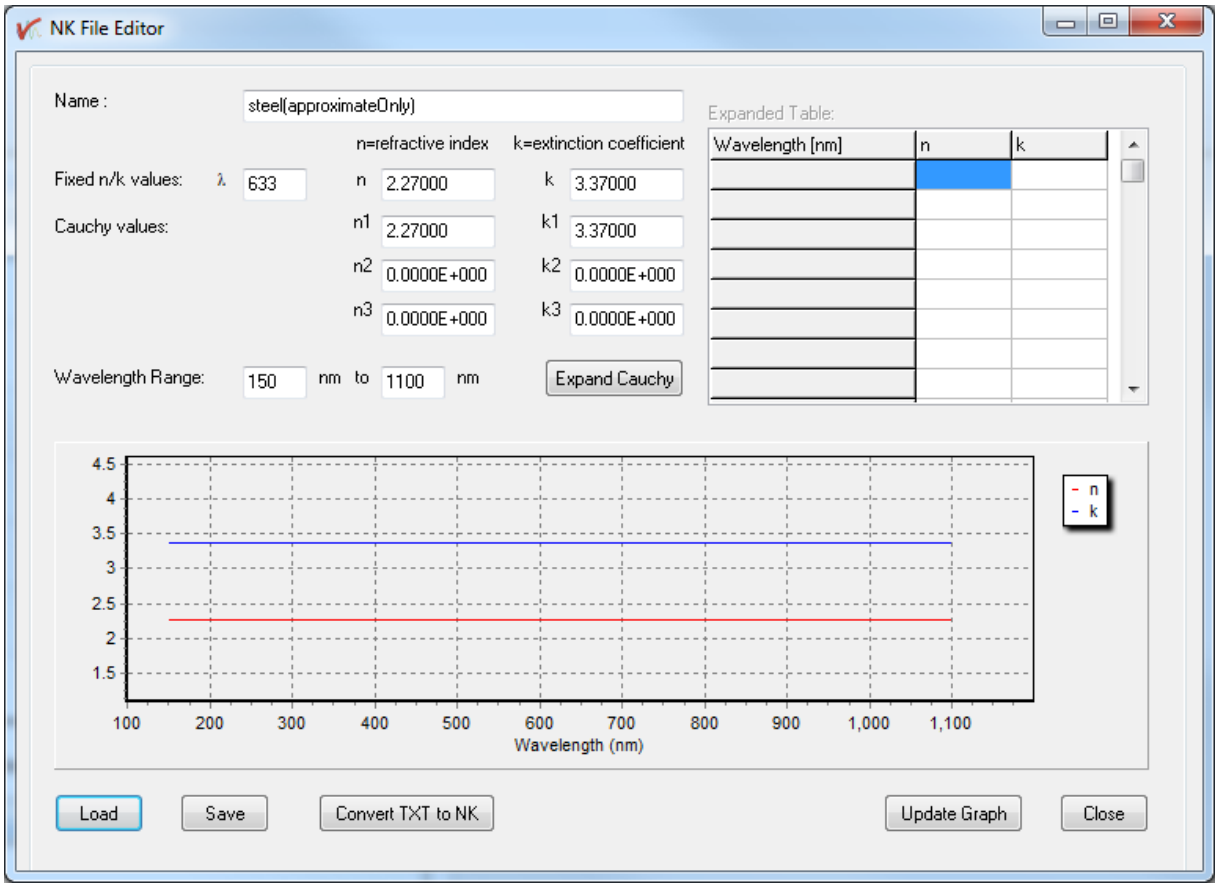
An example of a .nk file with a full list of n and k values being edited

.NK files hold the information about the n-value (real part of complex refractive index) and k-value (extinction coefficient) of a material, as a function of the wavelength. These values can be listed in two different ways.

The first, and most accurate way to list them is as a table (mostly from 150 to 1100 nm) with the n and k value listed for each wavelength, with 1 nm increments for the wavelength.

The second way is with 6 coefficients, the so-called Cauchy coefficients. These allow the n and k value to be calculated for each wavelength. The latter way is less accurate, but is the only one available for many materials.

The ThinFilm application can edit both types of file. You can edit either the Cauchy values, or the n and k values per wavelength. You can evaluate the resultant n and k values in the graph. Press ‘Update Graph’ after a change, to view your changes. The ‘Save’ button allows you to save the .nk file. Click the ‘Close’ button to leave without saving.



An example of a .nk file with Cauchy coefficients being edited

You might want to change a .nk file with Cauchy values to one with a full list of n and k values, in order to fine-tune the values without bothering with the Cauchy formula. The ‘Expand Cauchy’ button allows you to do just that. Load an unexpanded .nk file (with Cauchy values) and save it in an expanded form (without Cauchy values, but with a full list of n and k values).

The format of the .nk tables in the database are rather strict in their layout (wavelength numbers should be incremented with 1 nanometer, starting at 150nm and ending at 1100nm. Also the decimal separator and column separator should be respectively a period (.) and comma (,). Moreover, the first 4 lines in the .nk file are reserved for respectively title, fixed wavelength, wavelength range and Cauchy coefficients.

The button “Convert TXT to NK” has been added to allow an easy import of custom specific materials with known .nk tables. The data in the textfile (.txt extension) should hold 3 columns: wavelength, n-value, k-value. The wavelength incrementation is not restricted, linear interpolation will be used to convert the .txt file to a .nk file. The decimal separator can be a period (.) or comma (,) and the column separator a space, tab, semicolon or other character(s).

After clicking the button, you will be asked to select a .txt that should be converted to the .nk format. After the conversion, the .nk file can be displayed/edited with the “Edit .NK File” menu option and selected in the settings form.

4.10.3.8 'Graph' ribbon tab, 'Export Spectrum Chart' Button

Pull down menu:

- Windows Bitmap (*.bmp)
- Compressed Bitmap (*.jpg)
- Portable Network Graphics (*.png)
- Acrobat Reader (*.pdf)

Exports the Spectrum Chart to a choice of formats.

4.10.3.9 'Graph' ribbon tab, 'ASCII' Button

Exports the Spectrum Chart to an ASCII text file.
It contains measurement input data and results. It also contains a table of the raw data, in the following columns: Wavelength; Calc. Reflectance; Reflectance at Zero Thickness; Reflectance Data

4.10.3.10 'Graph' ribbon tab, 'Copy Spectrum Chart' Button

Copies the Spectrum Chart graph to the clipboard.

4.10.3.11 'Graph' ribbon tab, 'Print Spectrum Chart' Button

Prints the Spectrum Chart.

4.10.3.12 'Graph' ribbon tab, 'Export Time Series Chart' Button

Pull down menu:

- Windows Bitmap (*.bmp)
- Compressed Bitmap (*.jpg)
- Portable Network Graphics (*.png)
- Acrobat Reader (*.pdf)

Exports the Time Series Chart to a choice of formats.

4.10.3.13 'Graph' ribbon tab, 'Copy Time Series Chart' Button

Copies the Time Series Chart graph to the clipboard.

4.10.3.14 'Graph' ribbon tab, 'Print Time Series Chart' Button

Prints the Time Series Chart.

4.11 Raman Application

4.11.1 Raman Primer

In Raman spectroscopy, samples are illuminated with monochromatic laser light. The laser light interacts with the sample, resulting in small energy shifts, which can be measured as wavelength shifts.

The resulting Raman fingerprint spectrum can be used to identify chemicals. This is comparable to Infrared spectroscopy. The advantage of Raman spectroscopy here is the fact that the wavelengths of the fingerprint spectrum are in the sensitivity range of CCD detectors. This is not the case with Infrared spectroscopy.

A Raman spectrum is typically displayed with a calculated wavenumber of the Raman shift (in cm^{-1}) as the parameter on the x-axis, instead of a wavelength (in nm) that is used in the other applications of AvaSoft 8.

4.11.2 Quick Start: Measuring and Saving a Raman Spectrum

1. After starting AvaSoft Raman, the Start button in the upper left corner of the screen needs to be clicked to start measuring.
2. Connect the probe to the laser and to the Spectrometer input port(s).
3. Adjust the Nr of Smoothing Pixel in the Measurement Settings (reachable from the spectrometer window) to optimize smoothing for the Fiber/Slit diameter that is used. In most Raman systems, the slit is 25 micron, and the smoothing parameter should be set to 0. Setting the smoothing parameter to 1 will show a smoother spectrum against the price of a little less resolution (see also section 4.3.4.1)
4. Before switching on the laser, be sure to avoid direct eye contact via the probe tip. Turn on the laser. Usually some sort of spectrum may be seen on the screen. A lot of experiments with a Raman system require a long integration time, e.g. 10000 milliseconds for ethanol measurements. A progress bar (section 4.3.9) can be enabled to visualize the progress of a measurement cycle. The integration time can be changed in the spectrometer window.
5. When a good spectrum is displayed, turn off the laser.
   Optionally the laser can be switched off automatically when saving dark by enabling the option: ‘Settings’, ‘Digital IO’, ‘TTL Shutter on Save Dark’.
6. Now save the Dark data. This is be done by clicking the dark bulb icon in the spectrometer window, or the one in the left top of the screen with the mouse. Always use Save Dark after the integration time has been changed.
7. Turn on the laser again. The measure mode can be changed to ‘Scope minus Dark’ mode by pressing the corresponding button. To have a better look at the amplitude versus wavelength, the Assign Cursor button can be clicked in the Tools menu. A vertical line is then displayed in the graph. If the mouse cursor is placed nearby this line, the shape of the mouse cursor changes from an arrow to a ‘splitter’ shape. If this shape is displayed, the left mouse button can be used to drag (keep left mouse button down) the line with the mouse towards a new position. Moving this line shows the corresponding values of wavelength and amplitude in the status line of the screen. By clicking the stop button, the data acquisition is stopped and the last acquired spectrum is shown in static mode. The data acquisition can be started again by clicking the same button, which now displays ‘Start’.
8. To save the spectrum (in the mode chosen before), choose ‘File’, ‘Save’ from the menu.
9. Other options to save a spectrum can be found under ‘Options’, ‘Save Spectra Periodically’. With this option, spectra can be saved automatically according to instructions entered in "Time delay before first scan", "Time delay between scans" and “Number of scans to save”.
10. To improve the Signal/Noise ratio, a number of spectra may be averaged. To do this, the value in the spectrometer window (below the integration time) can be increased. The new value will take effect when you press the ‘Set’ button.

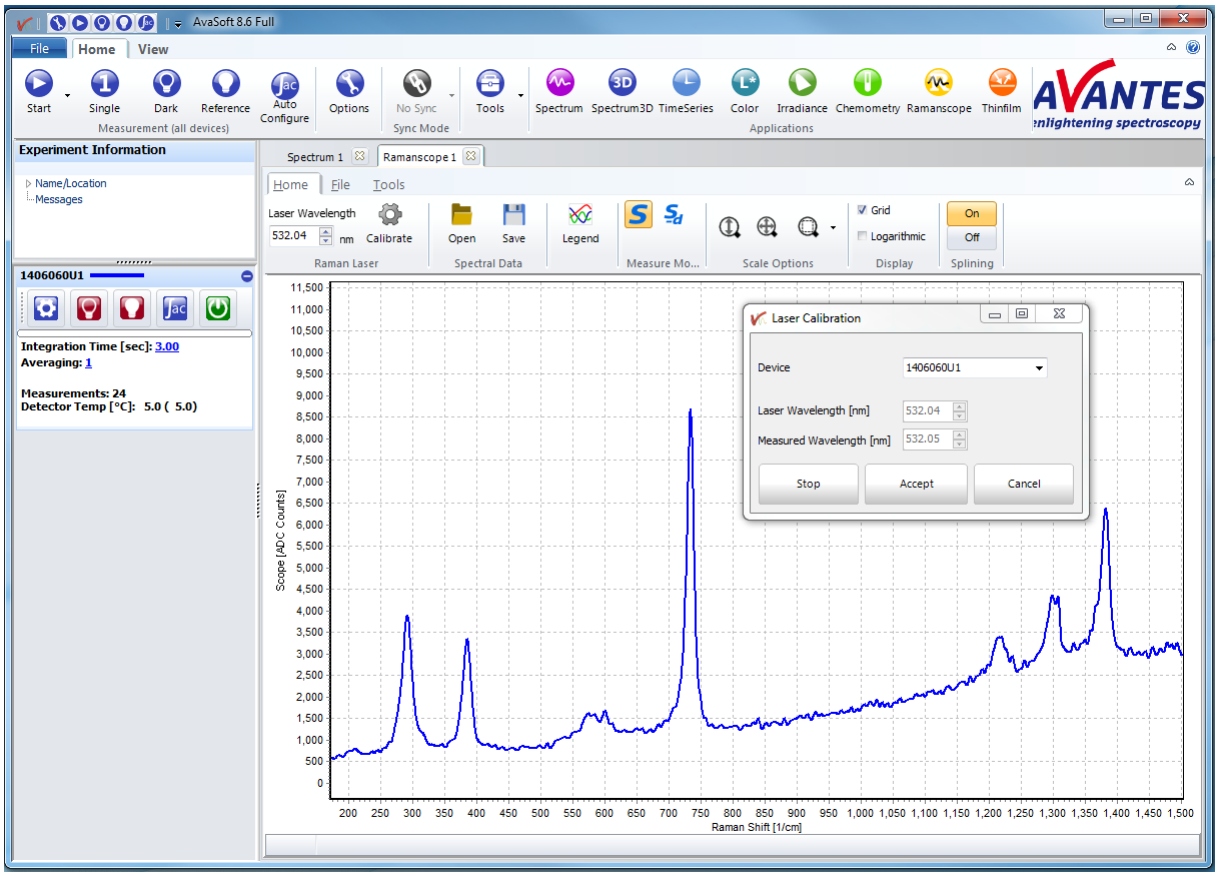
4.11.3 Raman Application Window

4.11.3.1 'Home' Ribbon Tab, 'Laser Wavelength' Edit Box

This edit box contains the laser wavelength. The value can be edited, and is saved in an .XML file between sessions. If the .XML files are deleted, new ones will be saved, with a default wavelength value that is read from the spectrometer EEPROM.

4.11.3.2 'Home' Ribbon Tab, 'Calibrate' Button

Pressing this button will show the Laser Calibration form. Using a Teflon (PTFE) calibration cap, the exact laser wavelength can be calculated from the characteristic PTFE spectrum.



Select the device in the drop down box (if necessary), make sure the measurement is running and press the 'Start' button. If you are satisfied with the measured wavelength, press 'Accept'. This will change the value in the Laser Wavelength box of the main Raman window. It will also save the new value to .XML file.
Press 'Cancel' to leave without saving.

4.11.3.3 'Home' Ribbon Tab, 'Open' Button

Loads spectral data in AvaSoft 8 binary format.

The Raman application uses the following binary files extensions:

- RMN8 Scope Mode
- RMD8 Scope Corrected for Dark Mode

4.11.3.4 'Home' Ribbon Tab, 'Save' Button

Saves spectral data in AvaSoft 8 binary format.

The Raman application uses the following binary files extensions:

- RMN8 Scope Mode
- RMD8 Scope Corrected for Dark Mode

4.11.3.5 'Home' Ribbon Tab, 'Legend' Button

Shows information about the series present in the chart. You can edit visibility of the series, splining of the line, color of the line and width of the line. The default line width value of 2 can be changed with persistence via Option menu item Look and feel. Allowed width range is 1 to 10. If the series was loaded from disk, you can remove it here by pressing the 'Remove' button. You can also add an integral calculation to each of the series. The start and stop Raman shift of the integral calculation can be set, as well as a factor that is applied. Integrals can also be removed in this screen.

4.11.3.6 'Home' Ribbon Tab, 'Scope Mode' Button

This mode will show a real time raw data signal, with on the Y-axis the read out of the AD-converter and on the X-axis the calculated Raman shift wave number.

4.11.3.7 'Home' Ribbon Tab, 'Scope minus Dark Mode' Button

This mode will also show a real time raw data signal, but corrected for the dark signal that is set.

4.11.3.8 'Home' Ribbon Tab, 'Auto Scale Y-axis' Button

By using this option, the graph will be rescaled on-line. A maximum signal will be shown at about 75% of the vertical scale.

4.11.3.9 'Home' Ribbon Tab, 'Graphic Reset' Button

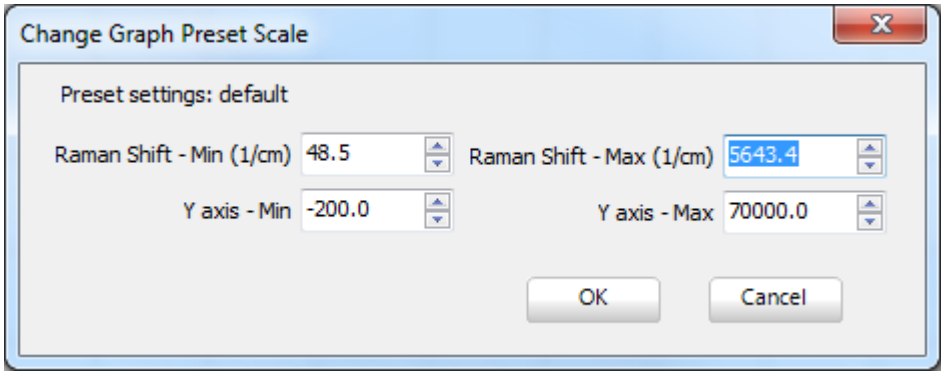
When selecting this option, the graph will be reset to the default X- and Y-axes.

4.11.3.10 'Home' Ribbon Tab, 'Preset Scale' Button

Pull down menu:

- Edit
- Save Current Scale

Pressing this button will set a preset scale. To preset a scale, you can save the current scale as preset scale by selecting the bottom option from the pull down menu.
You can also edit the scale first, with the following form that will appear after selecting 'Edit' from the pull down menu.



4.11.3.11 'Home' Ribbon Tab, 'Grid' Checkbox

With the Grid Enable option activated, a grid will be displayed in the graph.

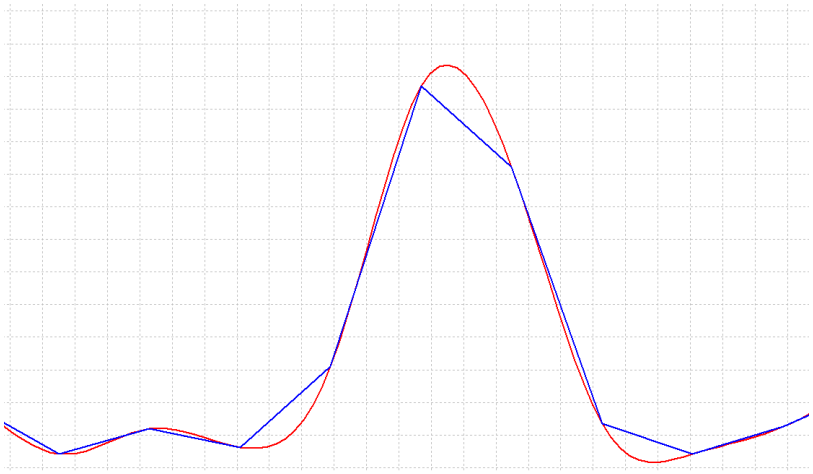
4.11.3.12 'Home' Ribbon Tab, 'Logarithmic' Checkbox

If you select this option, the Y axis will be displayed with a logarithmic scale, rather than a linear one.

4.11.3.13 'Home' Ribbon Tab, 'Splining On' Button

This will switch on a cubic spline interpolation of the spectrum. The spline interpolation can be useful for applications in which the output of line sources (like laser diodes) is displayed, or for other applications which require a high resolution. Note that for the AvaSpec-2048 with 2048 pixels, the effect of spline interpolation is not visible if the data is shown at full scale. The monitor resolution will probably be less than 2048 pixels. The effect of spline interpolation can only be visualized if the number of detector pixels that are displayed is smaller than the number of monitor pixels at the x-axis.

In the figure below, the effect of spline interpolation is illustrated. The blue line shows the AD counts for about 10 pixels, connected by a straight line (linear interpolation). The data for the red line is exactly the same, but this time the cubic spline interpolation algorithm has been applied, resulting in data which is smooth in the first derivative and continuous in the second derivative.



4.11.3.14 'Home' Ribbon Tab, 'Splining Off' Button

Switches off the spline interpolation.

4.11.3.15 'File' Ribbon Tab, 'Open Spectral Data' Button

Loads spectral data in AvaSoft 8 binary format. This option is repeated from the 'Home' menu.

4.11.3.16 'File' Ribbon Tab, 'Open V7 Spectral Data' Button

Loads spectral data in AvaSoft 7 binary format.

4.11.3.17 'File' Ribbon Tab, 'Save Spectral Data' Button

Saves spectral data in AvaSoft 8 binary format. This option is repeated from the 'Home' menu.

4.11.3.18 'File' Ribbon Tab, 'Export Spectral Data' Button

Pull down menu:

- ASCII
- Excel
- JCAMP
- GRAMS

Saves spectral data in one of several popular formats. Note that this only exports the LIVE data. To convert existing files, please use the 'Convert File To' option in the main window. Note that the equidistant version of the ASCII, JCAMP and GRAMS format is not supported in the Raman application.

4.11.3.19 'File' Ribbon Tab, 'Copy Graph' Button

This will store the graph on the clipboard, allowing you to paste it into other applications.

4.11.3.20 'File' Ribbon Tab, 'Save Graph As' Button

Pull down menu:

- Rich Text Format (*.rtf)
- Windows Bitmap (*.bmp)
- Compressed bitmap (*.jpg)
- Portable Network Graphics (*.png)
- Acrobat Reader (*.pdf)

Saves the graph in one of several popular formats. Note that the .rtf format is a Microsoft format that will open in MS Word. The saved file holds a .png graph that you can extract from it if necessary. The .pdf format that we export does not support transparency. If your graph has transparent parts (e.g. when if contains an integral), please select a different format.

4.11.3.21 'File' Ribbon Tab, 'Print Graph' Button

Will open a standard Windows Print dialog.

4.11.3.22 'Tool' Ribbon Tab, 'Magnify Tool On' Button

Switches on the Magnify tool. You can select the magnification in the pull down menu.

4.11.3.23 'Tool' Ribbon Tab, 'Magnify Tool Off' Button

Switches off the Magnify tool.

4.11.3.24 'Tool' Ribbon Tab, 'Assign Cursor' Button

Pull down menu:
- 'None'
- Spectrometer ID

You can assign a cursor to a Chart series here. The cursor consists of a vertical and a horizontal line. If you hover over a line, the mouse cursor will change into a 'splitter' shape, if you then press the left mouse button, you can drag the line to another position. The vertical line will snap to the next pixel position.

The status line will display the cursor position with a value for the Raman shift value and the amplitude.
You can remove the cursor by selecting 'None' in the pull down menu.

4.11.3.25 'Tool' Ribbon Tab, Cursor Raman Shift Wavenumber Edit Box

You can place the vertical cursor line on a specific Raman shift value by entering the value in the edit box and pressing the 'OK' button.

4.11.3.26 'Tool' Ribbon Tab, 'Spectrum Chart Name' Button

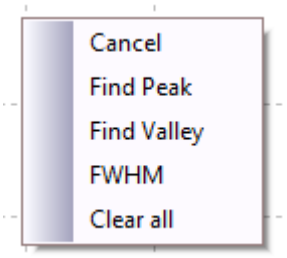
This option allows you to change the name of the application window.

4.11.3.27 Status Bar

The status bar at the bottom of the spectrum application window is used to display wavelength and intensity data for the cursor

4.11.3.28 Peak Submenu

When you click the right button of your mouse in the graphical region, a pop up menu will be shown.



Click 'Cancel' to go back.
Click 'Find Peak' to position a cursor line on the peak nearest to the mouse position. The following procedure is used:

- The Raman shift value is determined from the position the mouse click occurred.
- The data from closest pixel is retrieved
- The direction to search for the peak is determined from the neighbor pixels. If both neighbor pixels have a lower value at the Y-axis than the current pixel, the current pixel is already a peak. If only one of the neighbor pixel values is higher than the current pixel value, the peak

will be searched in the direction of this higher pixel. If both neighbor pixels have a higher value at the Y-axis than the current pixel, the current pixel is in a valley. The peak will in this case be searched in the direction of this neighbor pixel with the highest value.

- The cursor starts moving in the direction, as determined under 3), until it reaches a pixel of which the value is not higher than the last one evaluated. At this pixel the cursor stops.

Click ‘Find Valley’ to position a cursor line on the valley nearest to the mouse position. This uses the same procedure.
Click ‘FWHM’ to calculate an FWHM value of the peak the mouse is over. An area of the chart will be marked in a transparent color with the FWHM width. The FWHM value will be printed to the top right of this area.
Click ‘Clear All’ to clear all Peak, Valley and FWHM markings.

If more than one spectrum is being displayed, a dialog will popup that lets you select which spectrum will be used by the peak finder or the FWHM calculator.

4.11.3.29 Find Peaks or Valleys by CTRL or SHIFT + Right Mouse Button Click

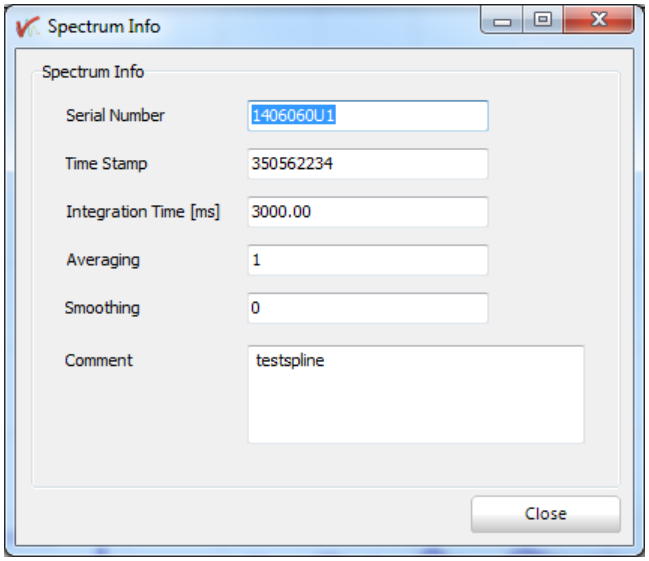
If the cursor is visible, you can use it to find the value of valleys or peaks.
When the right mouse button is clicked in the graphical region, while the CTRL key is down, AvaSoft will follow the procedure described above to run the cursor to the closest peak:

By holding down the SHIFT key instead of the CTRL key, the same procedure will be used to move to the closest valley.

To mark a peak for which the FWHM values need to be calculated, press the ALT key, and click with the right mouse button on this peak.

If more than one spectrum is being displayed, a dialog will popup that lets you select which spectrum will be used by the peak finder or the FWHM calculator.

4.11.3.30 Spectrum Info Window



If you left click on a graph series in the graphical region, a window will appear with some info about the spectrum that is shown in the graph. You can also remove the series by pressing the ‘Remove’ button.

Appendix A: USB Driver Installation

As mentioned in section 1, AvaSoft supports one of two USB drivers under 32 bit Windows Operating Systems:

- The Avantes kernel driver, which has been the standard USB driver on all 32 bit O/S until May 2011.
- The Microsoft WinUSB driver. This driver has been the standard on Windows 64 bit O/S.

Installing the WinUSB driver will be the standard on all recent Windows O/S versions.
At PC's where the Avantes kernel driver was installed before, a dialog is shown in which the user can select to update to the WinUSB driver or to keep the Avantes kernel driver.

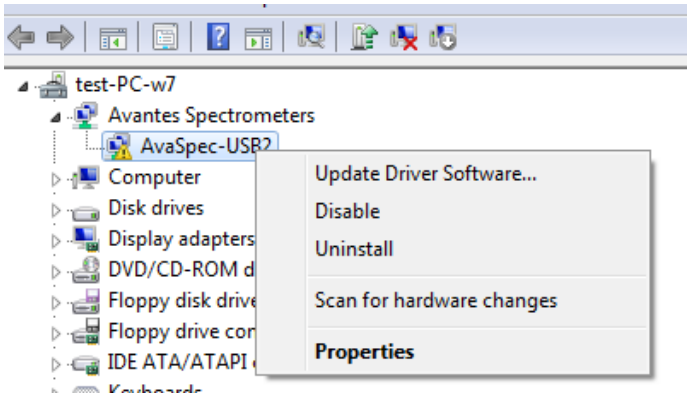
In this Appendix, some compatibility issues will be described that may occur after upgrading to WinUSB:

1. After installing the WinUSB driver and connecting the AvaSpec-USB2 spectrometer, the spectrometer cannot be found.
2. After installing the WinUSB driver, the spectrometers first worked fine, and the Device Manager shows a proper installation of the WinUSB driver. However, after installing some application software the spectrometer cannot be detected anymore. Also AvaSoft cannot detect an AvaSpec-USB2 anymore. The Device Manager still shows a proper WinUSB driver installation.
3. After installing the WinUSB driver, the spectrometer runs fine with AvaSoft, but not with other application software.

A1: Spectrometer cannot be found after update to WinUSB driver

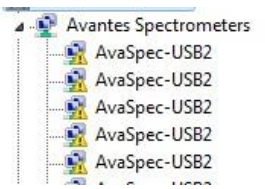
After connecting the spectrometer to a USB port of your PC, Windows will install the device driver. If all goes well, this will be displayed in the lower right corner of your screen with the message 'Device driver software installed successfully'.

We have seen instances, where this message will not appear, and where it is necessary to open the Device Manager, to let Windows find the installed driver files. To open the Device Manager, right click 'Computer' in Windows Start menu, and select 'Properties'. Then click the "Device Manager" option.



The 'Avantes Spectrometers' entry will show a yellow triangle with an exclamation mark. Right-click the AvaSpec-USB2 line and select the "Update Driver Software" option, as shown in the figure at the left. In the next dialog, select "Search automatically for updated driver software". Windows should now find the correct files and install the driver software.

In multichannel spectrometer systems, it may be needed to repeat this step several times (once per channel)



A2: Device Manager shows a proper WinUSB driver installation, but AvaSpec-USB2 cannot be detected anymore

If the WinUSB driver has been installed properly, the Device Manager will display the connected devices without the yellow triangle with exclamation mark. AvaSoft can be executed and everything runs well.

However, after installing some application software, it is possible that the spectrometer cannot be detected anymore. AvaSoft cannot detect the AvaSpec-USB2 spectrometers either. One reason can be that the application software uses an old as5216.dll version 1.7 or earlier, as will be described below under A3.

The problem can also be caused by the installation program that installed the application software. When installing AvaSoft version 7.6.0 or earlier versions, the Avantes kernel driver (AVSUSB2.sys) will be installed, without uninstalling the WinUSB driver. The as5216.dll will try to communicate through the most recently installed driver (avsusb2.sys), while the WinUSB driver is the one that is active in the Device Manager. The problem can be easily solved by reinstalling the most recent application software (AvaSoft 7.6.1 or later). In the driver selection dialog, select the (recommended) WinUSB driver. The same situation may occur when the Avantes kernel driver is installed by other application software (AvaSoft-Thinfilm-USB2, AvaSoft-Raman-USB2, or third party applications).

A3: After installing the WinUSB driver, AvaSoft 7.6.1 (or later) runs fine, but other application software cannot detect the AvaSpec-USB2 spectrometer anymore.

Most likely, the as5216.dll version used by the other application software does not support the WinUSB driver. The WinUSB driver is supported by the as5216.dll since version 1.8.0.0.

Appendix B: Error Messages

AvaSoft can display error messages containing a number. The following table lists these numbers and a description of the error:

Error Code	Description
-1	Function called with invalid parameter
-2	Operation not supported
-3	Opening communication failed or time-out during communication occurred
-4	AvsHandle is unknown in the DLL
-5	Function is called while result of previous function is not received yet
-6	No answer received from device
-7	Reserved
-8	No measurement data is received at the point AVS_GetScopeData is called
-9	Allocated buffer size too small
-10	Measurement preparation failed because pixel range is invalid
-11	Measurement preparation failed because integration time is invalid for selected sensor
-12	Measurement preparation failed because of invalid combination of parameters (e.g. integration time > 600 seconds or averages > 5000)
-13	Reserved
-14	Measurement preparation failed because no measurement buffers are available
-15	Unknown error reason received from spectrometer
-16	Error in communication occurred
-17	No more spectra available in RAM, all read or measurement not started yet
-18	DLL version information cannot be retrieved
-19	Memory allocation error in the DLL
-20	Function called before AVS_Init is called
-21	Function failed because AvaSpec is in wrong state, e.g. AVS_StartMeasurement() while measurement is pending
-22	Reply is not a recognized protocol message
-23	Reserved
-24	Reserved
-25	Spectrometer has encountered an error while reading from its internal non-volatile memory
-26	Spectrometer has encountered an error while writing to its internal non-volatile memory
-27	Error in initializing AvaSoft due to another Avantes (AvaSpec) application running on the same workstation
-28	Invalid spectrometer configuration detected
-100	NrOfPixel in Device data incorrect
-101	Gain Setting Out of Range
-102	Offset Setting Out of Range
-110	Use of Saturation Detection Level 2 is not compatible with the Averaging function
-111	Use of Averaging is not compatible with the StoreToRam function
-112	Use of the Synchronize setting is not compatible with the StoreToRam function

-113	Use of Level Triggering is not compatible with the StoreToRam function
-114	Use of Saturation Detection Level 2 Parameter is not compatible with the StoreToRam function
-115	The StoreToRam function is only supported with firmware version 0.20.0.0 or later
-116	Dynamic Dark Correction not supported
-120	Not supported by sensor type
-121	Not supported by firmware version
-122	Not supported by FPGA version

Appendix C: Using the Ethernet Spectrometer

This section describes some details to avoid common pitfalls that can occur when using the Ethernet interface of the AS7010 spectrometer.

C1: Dynamic (DHCP) vs. Static IP Addresses

The spectrometers are shipped with DHCP enabled. This means that they will be assigned a unique IP address in the correct range if you connect them to a network on which a DHCP server is running. If you connect the spectrometer to your office network for the first time, please ensure that a DHCP server is present on that network.

The spectrometer can also be used with a static IP address configured. You can change the network settings of the spectrometer with the *IP Settings AS7010 utility* that is e.g. distributed with AvaSoft 8. When using the spectrometer with a static IP address please make sure that the used IP address is in the same range as your host PC.

When using the spectrometer within a local network (a network with only one host (PC) and one or more Ethernet spectrometers with static IP addresses), you will have to change the IP settings of your PC from DHCP to static as well. This is also described in the *IP Settings AS7010 manual* in more detail. Of course you can also use DHCP enabled spectrometers within the local network, provided that there is a DHCP server running on your host PC. There are several simple to use and freeware DHCP servers for Windows, such as one available from *www.dhcpserver.de*.

Please consult your network administrator for the availability of any DHCP server on your network or for using static IP addresses on the spectrometers. It is very important that the Ethernet spectrometers are configured with the right network settings, since otherwise major network problems can occur.

C2: Cables

You can use standard Ethernet patch cables to connect the spectrometer to your network. If you use a direct connection to your PC, make sure you have a GigE network connection, if you want to use a standard Ethernet patch cable. If your PC has an older Fast Ethernet connection (100 Mbps), then you will need a cross-connect cable.

C3: Routers

The AvaSpec DLL uses a UDP broadcast to identify the spectrometers on the network. It is sent from each network adapter that is found in the host PC. Most layer 3 switches and routers will not allow this broadcast to pass, which will stop the DLL from working. If there are connection problems, please also test a direct PC connection to make sure your router is not the cause.

C4: Firewall

The Windows Firewall must allow both incoming and outgoing connections to the spectrometer.

If the Windows Firewall is enabled, then a dialog will appear if you first use a program that will access the network:

Make sure you check all three boxes and press the 'Allow access' button, to allow the program access. Switching the firewall off completely will of course also work, but may not be advisable. You may have to restart the program that uses the DLL to have things work correctly.

C5: DLL / Firmware Version Conflicts

With AS7010 firmware version 1.3, the discovery protocol has been changed. If your firmware is older than version 1.3, you will not be able to use the latest versions of the AvaSpec DLL (9.2 and later). Please contact Avantes to upgrade the spectrometer firmware to the latest version with an update utility.

C6: Connecting both Interfaces at the Same Time

If you connect both the USB and Ethernet interfaces, then the USB interface will have priority. If, however, an Ethernet connection has already been made, then plugging in a USB cable will not break the Ethernet connection.

Appendix D: Merge Channels

D1: Introduction

Multichannel spectrometer systems are often setup to achieve a high resolution over a wide range, e.g.

Master: UE 230 to 310 nm
Slave1: UE 303 to 410 nm
Slave2: VE 401 to 490 nm
Slave3: VE 485 to 555 nm

Another example is the UV/VIS/NIR range (e.g. 200-2500nm) which requires at least two different detectors and therefore different channels.

In both examples, there is an overlapping wavelength range between consecutive channels for which the results should be the same, especially when measurements are taken in absorbance, transmittance, reflectance or irradiance mode.

AvaSoft 8 can handle the spectral data in the overlapping range as a single spectrum. It is possible to display, save or export the merged spectrum.
Please note that merging functionality is only available in the file conversions of the main window and in the Spectrum application. It is not available in the other applications.

D2: Settings and requirements

In the AvaSoft options (see section 4.1.15.11) you can define a merge group and add multiple channels to this group. The following requirements should be met:

1. There should not be a “gap” in the wavelength range of the merged spectrum. The start and stop wavelength are used to define the begin and end of the range for a single channel. For example if the stop wavelength of channel 1 is 730 nm and the start wavelength of channel 2 is 740 nm, there would be a 10 nm gap between the channels which is not allowed.
2. A merge group should contain 2 or more spectrometer channels, up to a maximum of 8. A single spectrometer channel in a merge group is not allowed.
3. An overlapping region must contain data of exactly two individual channels.

The merge channel settings dialog allows you to enter a name for each merge group. This name can be used as an identifier when displaying saved graphs, or when converting the graphs to ASCII, Excel, GRAMS or JCAMP.

Due to different sensitivity of gratings, detectors, mirrors, fiber optics and possibly other settings (e.g. integration time), the raw data in scope mode will probably not match in the overlapping wavelength range, and therefore merging data in scope mode does not make much sense. However for some applications, like LIBS, it is more important to identify the location of the spectral peaks than the peak intensity. In such applications, multichannel systems are often used because of the higher peak resolution, and it is convenient to merge these channels into a single spectrum, also in scope mode. It is recommended in this case to save a dark spectrum for all channels and use the “Scope minus Dark Mode” to let the spectrum start at a baseline near zero.

D3: Recalculating the intensity in the overlapping range(s)

In merge mode, recalculating the intensity in the overlapping range can only be done if the data for all channels since the last measurement started is available in the application. Therefore, data processing in merge mode is only done after the data for all channels has been received by the application.

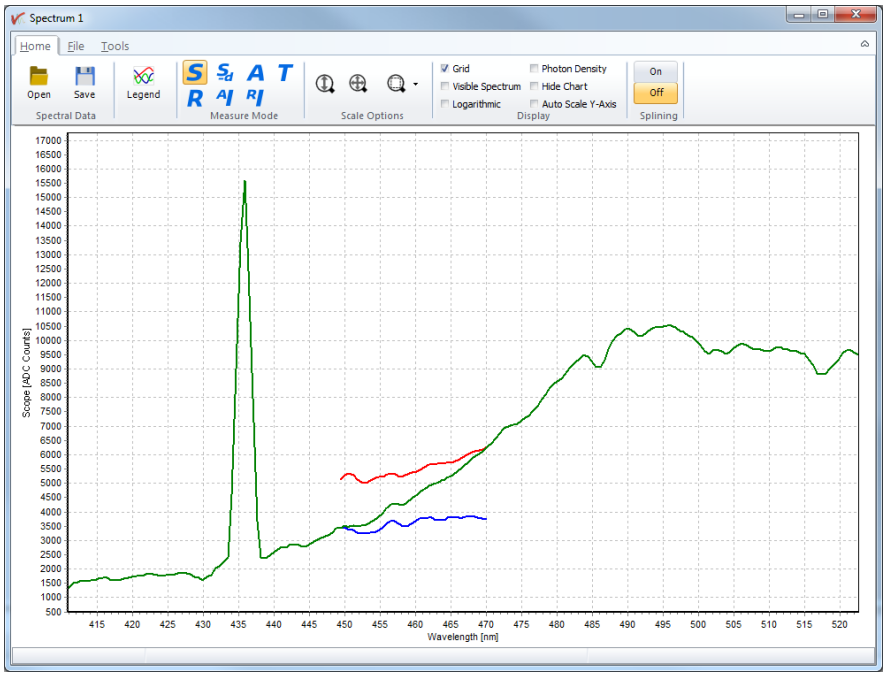
Under perfect conditions, recalculation of the intensity in the overlapping range should not be needed in absorbance, transmittance or irradiance mode, because the intensities measured by both channels in the overlapping range should be the same. However, due to small imperfections like second order effects, stray light, nonlinearity effects and/or temperature drift, minor discontinuities between the intensity of the two channels in the overlapping range may occur. AvaSoft will recalculate the intensity in such a way that a smooth transition between the overlapping channels will take place.

Note that the overlap range is determined by the start and stop wavelength for each spectrometer channel. To minimize recalculation of the intensity, select the start- and stop wavelength such that only a small overlap range remains. The quality of the signal in terms of signal/noise should be used to decide for which spectrometer channel the wavelength range should be reduced. An example is a dual channel UV/VIS/NIR spectrometer system with a 200-1100nm range at channel 1 and 1000-2200nm range at channel 2. The full range for the 200-1100nm channel (UA grating) is probably 200 to 1300nm, but the factory setting for the stop wavelength is only 1100nm, because the CCD is insensitive at wavelengths over 1100nm.

It is not a good idea to use the signal between 1100 and 1300nm when merging this channel with the NIR channel, as this signal is of poor quality. The remaining overlap range between 1000nm (start of NIR channel) and 1100nm can be reduced further. If the quality of channel 1 between 1050 and 1100nm is lower than the quality of the NIR channel, set the stop wavelength for channel 1 to 1050nm. Likewise, if the contribution of the NIR channel around 1000nm should be reduced, increase the start wavelength for channel 2.

When leaving the overlap range between 1000 and 1100nm, the data for both channels in this range will be merged such that the intensity gradually changes from channel 1 to channel 2, using the data from both channels in the overlap range as input.

The figure below illustrates how merging handles a huge discontinuity between two overlapping channels. Since this screenshot was taken in Scope Mode, such a discontinuity is normal. The only purpose for merging these spectra in scope mode is to illustrate how the two channels (blue and red) are merged into a single spectrum (green).



D4: Saving the spectra of all spectrometer channels in the same merge group into one file

In merge mode, the spectra of all spectrometer channels in the same merge group are saved in the same file. Files that are saved in merge mode can be recognized by the addition of an ‘x’ to the file extension: RAW8x, RWD8x, ABS8x, TRM8x, RFL8x, IRR8x and RIR8x. If merge mode is not enabled, the traditional file format and extensions (without ‘x’) are used.

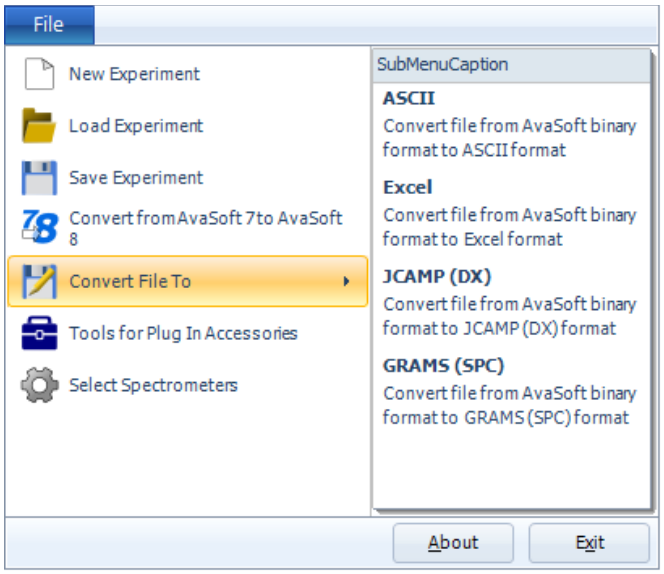
For example, in a 4-channel system in which two merge groups have been defined, saving the spectra will result in three files. One, without ‘x’ in the extension, holding the data for all individual channels and two, with ‘x’ in the extension, holding the data of the channels present in each merge group.

The main reason for developing the merge functionality was the ability to analyze the spectra of a multichannel system as a single spectrum. Therefore, when analyzing the saved spectra (displaying, comparing with other spectra, converting to ASCII, Excel, JCAMP etc..) the file is handled as a single spectrum. Detailed information about the data origin (which channels and settings were used when saving the file) can still be obtained and displayed, but the spectral data will always be represented as a single spectrum (wavelength + intensity).

D5: Displaying merged spectra

In merge mode, all individual channels are hidden by default and only the merged data is visible. The individual channels can be shown by changing the visibility of these channels in the Legend, as described in section 4.4.3.
When loading merged data from a file, only the merged spectrum is shown.

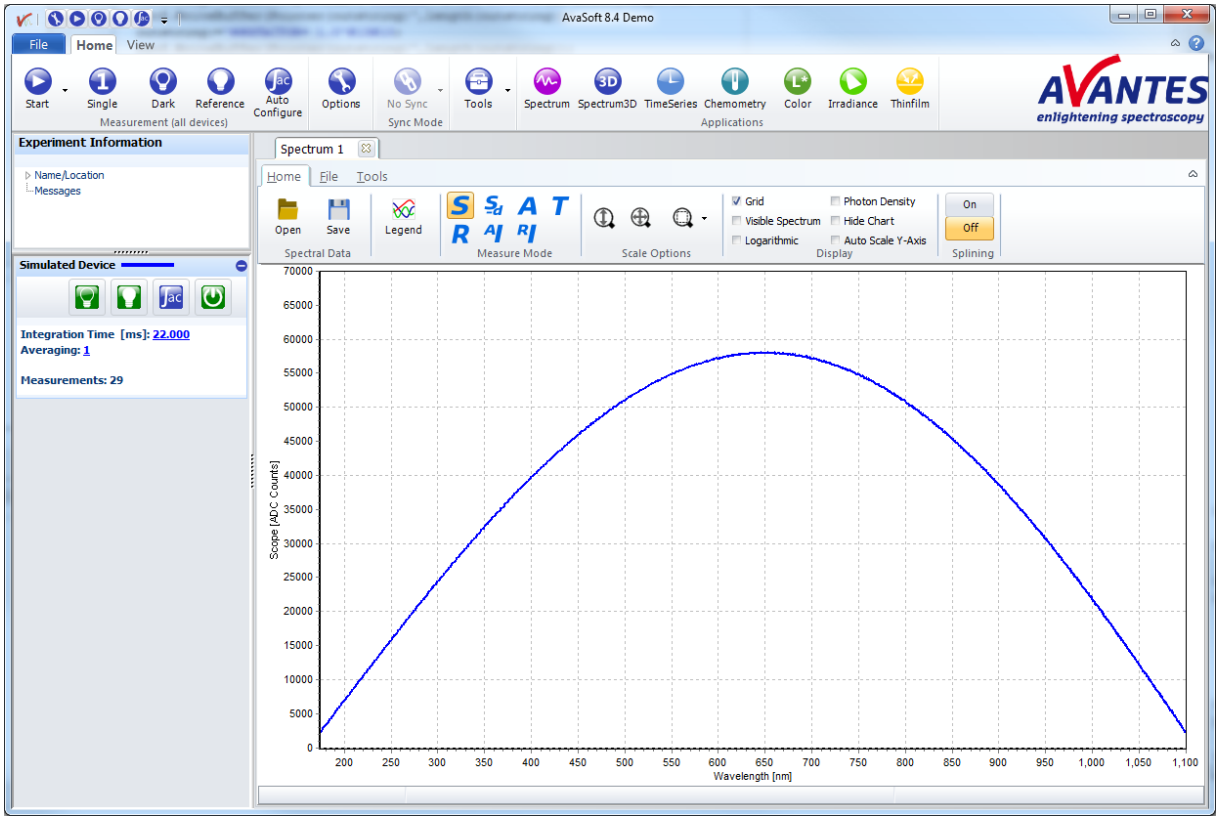
D6: Converting merged spectra to ASCII, Excel, JCAMP and GRAMS



The conversion of merged spectra to ASCII, Excel, JCAMP or GRAMS is the same as for non-merged spectra, see section 4.1.5 for more information.

Appendix E: Demo Mode

To be able to demonstrate and explore the functionality of AvaSoft 8 without the need of a real spectrometer the application can be started in demo mode. If no spectrometer is found during startup of the application the demo mode will be activated. In this mode a ‘Simulated Device’ is present that generates simulated sinusoidal measurement data.



Note that although the simulated data can be used in most of the application it will not always give sensible results.

The demo will be stopped if a real spectrometer is connected.

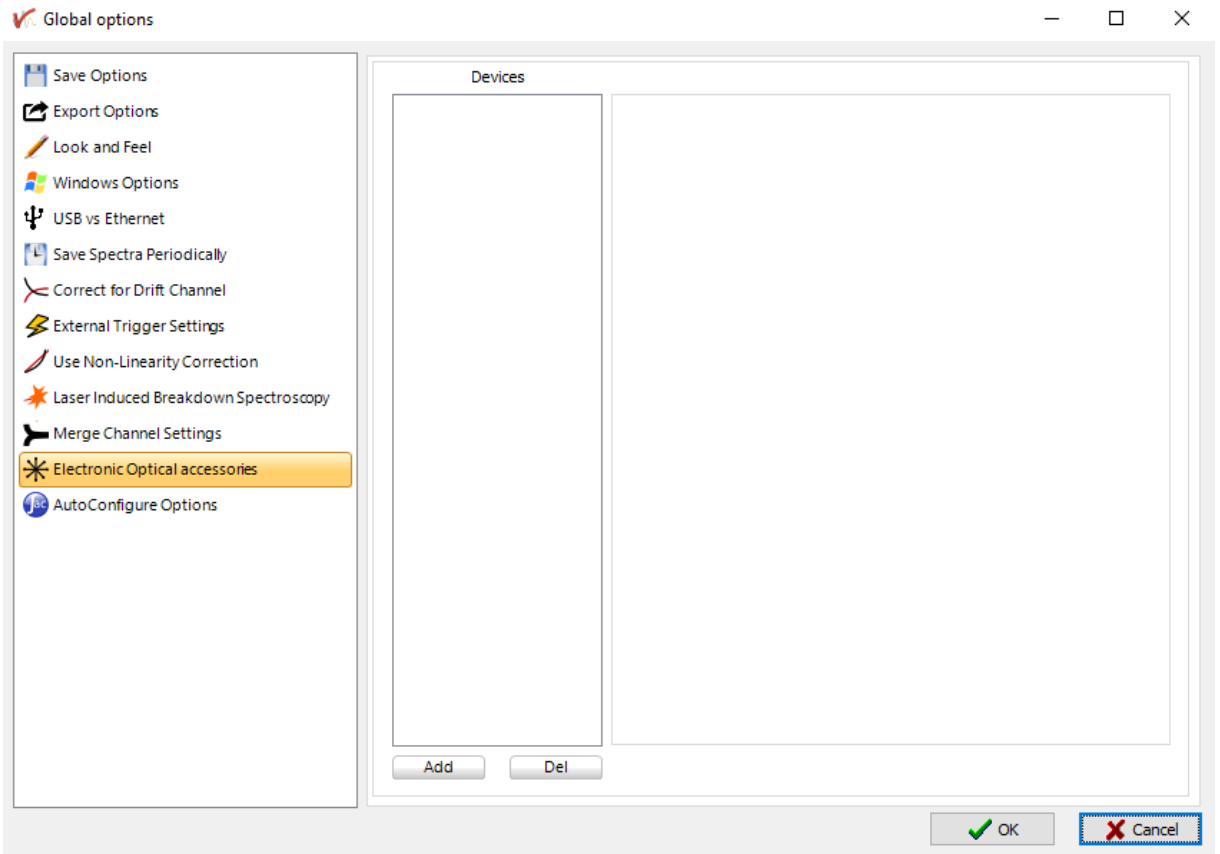
Appendix F: Keyboard shortcuts

Key	Action
F2	Start/Stop a measurement

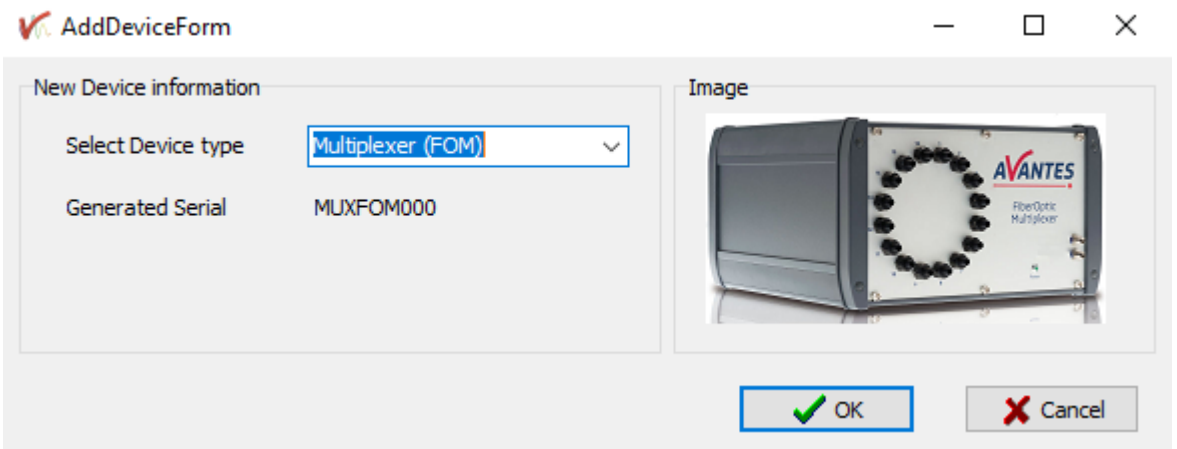
Appendix G: Using the Fiber Optic Multiplexer

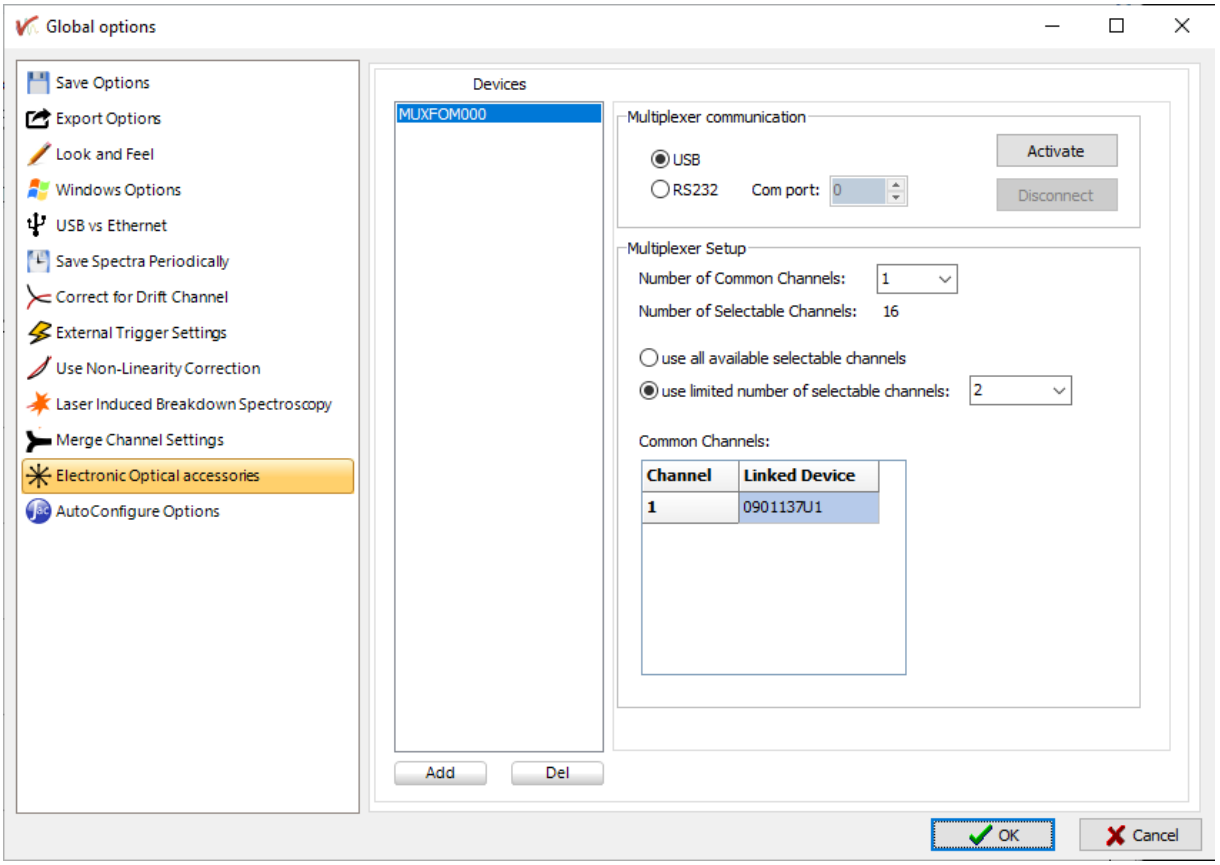
AvaSoft 8 supports the Fiber Optic Multiplexer through virtual channels. You can measure the different positions of the multiplexer as if these were separate spectrometers. You can program a sequence that will change the position of the multiplexer after a pre-set interval.

- Add support of the FOM by selecting ‘Options’, ‘Electronic Optical accessories’.



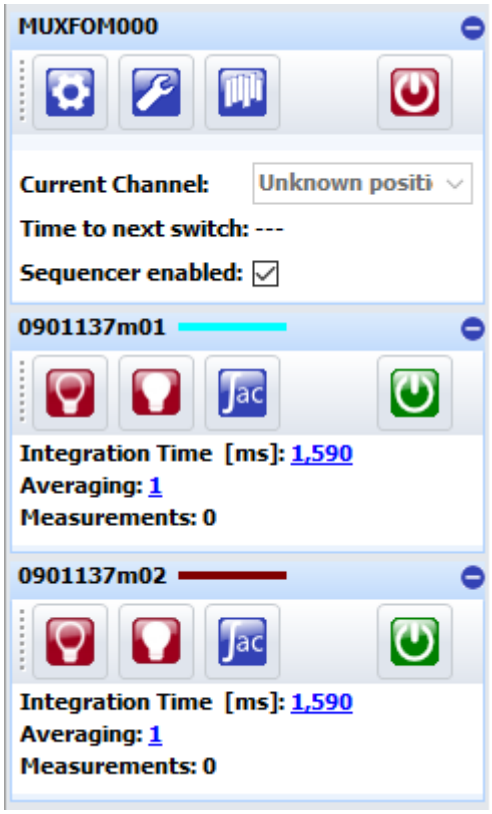
- Click ‘Add’ and select Device type ‘Multiplexer (FOM)’





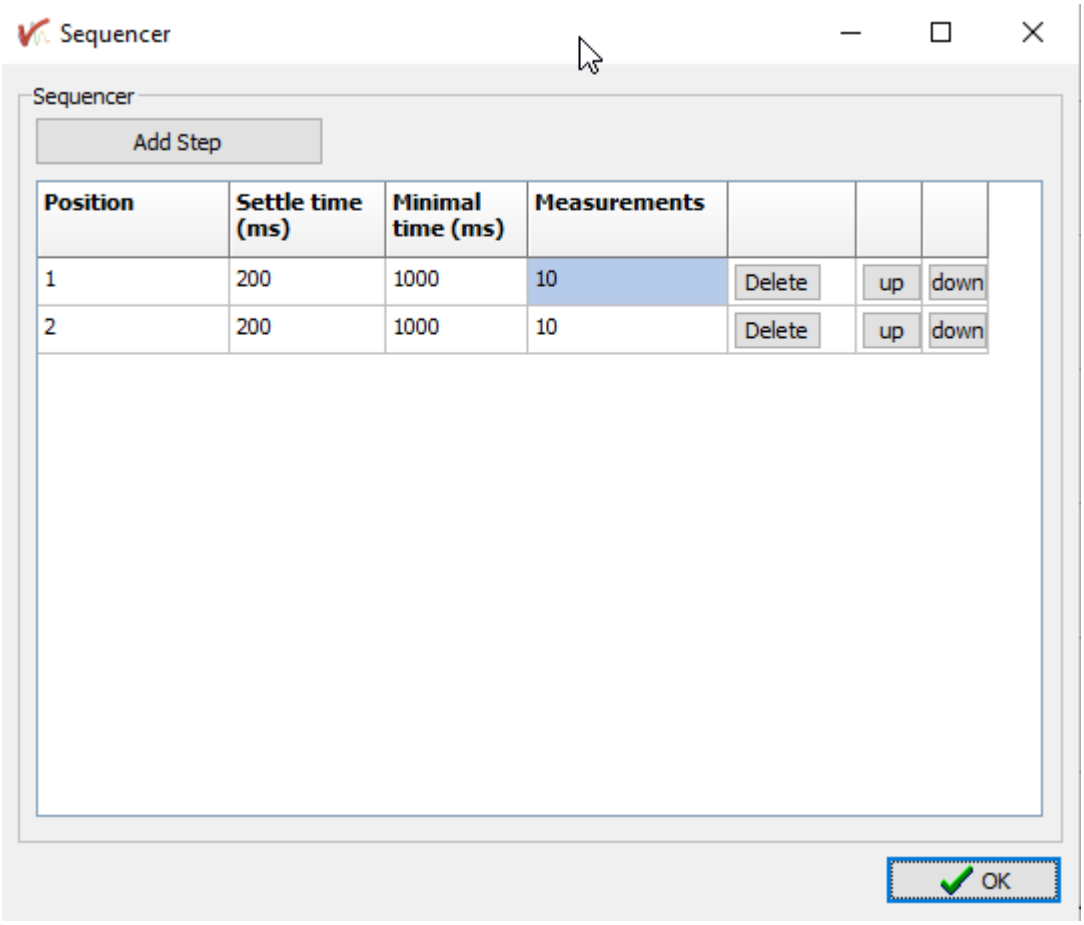
Now select the communication type and press ‘Acivate’
In the ‘Multiplexer Setup’ panel, select the Number of Common Channels. This is the number of physical spectrometers that is attached. Enter the number of selectable channels, and select which spectrometer is attached as Common Channel.

The spectrometer will now show the virtual spectrometers:



You can now program the sequencer by pressing the Sequencer icon:

This will show the sequencer form, that allows you to enter values like the ‘Settle time’, which is the time the multiplexer needs to stabilize after changing position, the ‘Minimal time’ which is a general delay that can be programmed to occur at each position change, and ‘Measurements’, which is the number of measurements to be taken at that position.
You can delete steps, and move steps up or down in the sequence by pressing the appropriate buttons.


Sequencer
Sequencer
Add Step
Position
Settle time (ms)
Minimal time (ms)
Measurements
1
200
1000
10
Delete
up
down
2
200
1000
10
Delete
up
down
OK

Pressing the Settings icon  will put you in the same form that you reached before from the 'Options' form.