Belgian Institute for Space Aeronomy

QDOAS
Software user manual

Thomas DANCKAERT
Caroline FAYT
Michel VAN ROOZENDAEL

Isabelle DE SMEDT
Vincent LETOCART
Alexis MERLAUD
Gaia PINARDI

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aeronomie.be

s[&]t
dependable solutions

QDOAS is free and distributed under the GNU GPL license version 2.0. Please mention the following authors in the acknowledgements when publishing results obtained using QDOAS.

Thomas DANCKAERT thomas.danckaert@aeronomie.be

Caroline FAYT caroline.fayt@aeronomie.be

Michel VAN ROOZENDAEL michelv@aeronomie.be

Tel. +32 (0) 2 373 04 16

Fax +32 (0) 2 374 84 23

Address BIRA-IASB
Avenue Circulaire 3
1180 UCCLE
BELGIUM

Web `http://uv-vis.aeronomie.be/software/QDOAS`

Users can contact us for spectra format adaptations, remarks, suggestions and technical support.

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1 QDOAS Overview

1.1 Introduction

The experience of the Belgian Institute for Space Aeronomy (BIRA-IASB) in the development and improvement of algorithms for the retrieval of trace gas concentrations goes back to the early 1990s, with atmospheric research activities using ground-based UV-Visible spectrometers aiming at the long-term monitoring of minor components involved in the catalytic destruction of the ozone layer or in anthropogenic pollution.

WinDOAS, the first program developed at BIRA-IASB in 1997, knew a success story due to a friendly user interface completed with some powerful DOAS tools. This program, extensively validated through different campaigns, has been used worldwide and for many different DOAS applications (mainly for ground-based and satellite applications).

QDOAS is a cross-platform implementation of WinDOAS: the software is portable to Windows and Unix-based operating systems whereas WinDOAS was designed only for Windows. The user interface and the engine of QDOAS are similar to those of its predecessor. WinDOAS is no longer supported.

QDOAS has been developed in collaboration with S[&]T, a Dutch company well-known for the development of cross-platform products and software tools for the processing of satellite measurements (BEAT, VISAN, . . .). The graphical user interface is built on the Open-Source version of the Qt-4 toolkit, a cross-platform application framework, and Qwt libraries.

QDOAS is free software distributed under the terms of the GNU General Public License; it is open source and the code is available on request by contacting the authors. This document describes the QDOAS user interface and dialog boxes for configuring the software. It completes the online help provided with the package. The algorithms that are used in the software are also summarized. The document assumes that users already have a minimum of experience with Differential Optical Absorption Spectroscopy (DOAS) applications and retrieval.

1.2 Main QDOAS features

General features

- ◇ The main components of the Graphical User Interface (GUI) are organized in multi-page panels with a fixed arrangement and tab-switched access to the different pages;

- ◇ The application is based on a tree structure;
- ◇ Large amount of files can be processed in one shot;
- ◇ Support different spectra file formats (see section 1.4)
- ◇ On line help in HTML format

Plot

- ◇ Visualization of spectra and the results in different tab pages;
- ◇ Possibility to set plot contour and style;
- ◇ Interactive plot mode (zooming, overlay of an existing ASCII file, possibility to fix the scaling of the plot, . . .): activated by right clicking the title of the plot ;
- ◇ Export of plot in different portable image formats (png, jpg)

Analysis

- ◇ DOAS/intensity fitting modes;
- ◇ shift/stretch fully configurable for any spectral item (cross-section or spectrum);
- ◇ possibility to filter spectra and cross-sections before analysis (supported filters include Kaiser, gaussian, boxcar, Savitsky Golay. . .);
- ◇ possibility to define gaps within fitting intervals (e.g. to eliminate bad pixels);
- ◇ possibility to fit an instrumental offset;
- ◇ possibility to define several configurations of spectral windows under a project;
- ◇ possibility to remove spikes.

Calibration And Slit Function Characterization

- ◇ wavelength calibration and instrumental slit function characterization using a Non-Linear Least Squares (NLLS) fitting approach where measured intensities are fitted to a high resolution solar spectrum degraded to the resolution of the instrument. The fitting method (DOAS or intensity fitting) can be different from the method used in the analysis;
- ◇ possibility to correct for atmospheric absorption and Ring effect;
- ◇ supports different analytical line shapes, as described in section 3.3, page 28.

Cross sections handling

- ◇ possibility to calculate differential absorption cross-sections (by orthogonalization or high-pass filtering);
- ◇ possibility to multiply cross-sections with wavelength dependent Air Mass Factors (AMFs);
- ◇ possibility to fix the column density of any selected species;
- ◇ possibility to convolve cross-sections in real time using a user defined slit function or the information on calibration and slit function provided by the wavelength calibration procedure;
- ◇ possibility to handle differences in resolutions between measured and control spectra;

Output The output is fully configurable. Analysis results and various data related to the measurements can be saved to ASCII or HDF-EOS5 files.

Tools Specialized tools are available for the following operations:

Convolution/Filtering (convolution)

- ◇ standard and I_0-corrected convolutions are supported;
- ◇ possibility to create an effective slit function taking into account the (finite) resolution of the source spectrum (using a FT deconvolution method);
- ◇ asymmetric line shapes, wavelength dependent slit functions;

Ring (ring) The ring tool calculates Ring effect cross-sections (Rotational Raman Scattering approach).

Undersampling (usamp) This tool generates undersampling cross-sections.

Batch processing (doas_cl) For batch processing of files, the powerful **command line** tool doas_cl can be used.

1.3 Main differences between QDOAS and WinDOAS

General Differences

- ◇ configuration files are now in XML format, meaning that WinDOAS and QDOAS configuration files are not compatible; it is recommended to start new QDOAS applications from scratch;
- ◇ there is a better separation of the code between the user interface and the engine (completely transparent for users);
- ◇ convolution, ring, undersampling and command line tools are modules completely independent from the QDOAS main user interface. This means that QDOAS comes in five independent executables or modules :
  - qdoas : the user interface similar to the WinDOAS one;
  - convolution : the convolution tool;
  - Ring : the Ring calculation tool;
  - usamp : the undersampling calculation tool;
  - doas_cl : a powerful command line tool that applies on qdoas, convolution, Ring and usamp configuration files.

  convolution, **ring** and **usamp** tools manage their own configuration files and can be called either from the QDOAS user interface or from the system command line.

User Interface

- ◇ The main sub-components of the GUI into resizable panels with a fixed arrangement; tab-switched access for project/analysis windows settings and plotted results;
- ◇ All the spectral windows processed in one shot and tab-switched access between the different fitting windows;

◇ There is no specific processing anymore applied on file format such as MFC (directories were considered as files with multiple records by WinDOAS).

Projects Properties

◇ File format selection is now out of the **Instrumental** page (see page 68) in order to be able to constrain the selection of the fields in the **Display** and **Output** pages.

◇ File formats are now distributed in two groups : ground-based and satellites;

◇ NASA-AMES page doesn't exist anymore.

Analysis Windows Properties

◇ Horizontal scrolling of options;

◇ Shift and stretch in nm units only;

◇ Possibility to constrain the slant column density of a molecule to the value found in a previous window (hidden option in WinDOAS).

1.4 Supported spectra file formats

Satellite Measurements

Spectra measured by the following satellite instruments can be processed by QDOAS :

GOME (ERS-2)

QDOAS supports the original ASCII file format but it is recommended to use the more suitable binary file format created by a modified version of the GDP implemented at BIRA-IASB for the automatic selection of the reference spectrum. Contact the authors for further information about this format.

SCIAMACHY (ENVISAT)

Routines to read the SCIAMACHY PDS file format have been kindly provided by IFE/IUP University of Bremen. SCIAMACHY Level 1C versions up to 7.04 (the SCIAL1C utility converts files from L1 to L1C)

GOME2 (MetOp)

QDOAS uses the Basic Envisat Atmospheric Toolbox (BEAT) library to read spectra from GOME2. The package can be downloaded from the S[&]T web site. Before using QDOAS on GOME2 spectra, BEAT should be installed and the `CODA_DEFINITION` environment variable should be defined.

QDOAS supports GOME2 Level 1B, PPF 5.0 product format version 12.0 and below.

OMI (AURA)

OMI spectra are read using the HDF-EOS2 library, which is based on HDF4.

Ground-based Measurements

The most popular file formats supported by QDOAS for ground-based measurements are :

SAOZ Système d'Analyse par Observation Zénitale developed by the aeronomy lab of the CNRS (JP Pommereau, F Goutail,...), France, and largely used in the NDACC network for stratospheric total ozone and NO_2 monitoring. Both PCD/NMOS 512 and EFM 1024 (SAM) formats are supported.

MFC STD This ASCII format is produced by the well-known DOASIS program designed by the atmospheric research group at IUP Heidelberg, Germany and widely used in the DOAS community. It can be obtained from the following URL:

`https://doasis.iup.uni-heidelberg.de/bugtracker/projects/doasis/`

This format can also be produced by other program or converted from other format, e.g. the Spectra Suite Ocean Optics software. QDOAS requires the size of the detector and the format of the date (for example, MM.DD.YYYY). The equivalent MFC binary file format is not supported by QDOAS.

MKZY PAK developed at the Chalmers University of Technology, Goteborg, Sweden (MANNE Kihlman and ZHANG Yan) and used in the NOVAC network.

OCEAN OPTICS very simple ASCII file format developed by the spectrometers manufacturer.

The ASCII File Format Other formats are specific to the different institutes that developed them. If a format is not supported by QDOAS, it should be possible to convert the files to ASCII. When the ASCII format is selected, spectra can be provided in the file one record per line **(line format)** or one spectral value per line **(column format)**. According to the checked flags in the **Read from file** group box, the following information are expected strictly in the given order :

- ◇ Solar Zenith Angle
- ◇ Azimuth Viewing Angle
- ◇ Elevation Viewing Angle
- ◇ Date in the DD/MM/YYYY (day/month/ year) format
- ◇ Fractional time

In the column format, angles have to be given on the same line and a wavelength calibration can be provided with spectra. Some examples of ASCII files supported by QDOAS are given in appendix **A**.

1.5 System requirements and installation

System Requirements The GUI is built on the Open-Source version of the Qt-4 toolkit. As a result, QDOAS is portable to Windows, Unix/Linux and Mac, and the user interface is effectively the same on all platforms. The software is free and distributed under the GNU GPL version 2.0 (see `http://www.gnu.org/licenses/gpl-2.0.html` for further details).

To obtain the software, to get support or to be notified of new releases, please register on the following page :

`http://uv-vis.aeronomie.be/software/QDOAS/QDOAS_Register.php`

Install QDOAS on Windows

Windows users can download the executables and all needed dynamic libraries from a FTP server (address provided after registration).

GOME2

For GOME2 applications, the `CODA_DEFINITION` environment variable must be defined. This variable should point to the location on the filesystem where is the .codadef file that describes the file format of the GOME2 input data. In windows, it can be set via

Control Panel → System → Advanced → Environment variables

Install QDOAS on Linux

Users who wish to use QDOAS on linux will have to compile the program from the source code, which is provided after registration. Very likely, a number of libraries must be installed as well. This section gives an overview of the installation steps.

Users without administrator privileges will typically have to install QDOAS and some of the required libraries in their home directory. In the following instructions, we will assume that the user wants to install qdoas and any libraries that might need to be installed in her home directory, `/home/username`. Executable files will be installed in `/home/username/bin`, libaries and headers in `/home/username/lib` and `/home/username/include`. When you want to install the software in a different directory, you will need to replace `/home/username` by the directory of choice in the following instructions.

In order that the operating system can find the QDOAS executable files, the `/bin` subdirectory must be added to the `$PATH` system variable. To do this, the user will add the following entry in to her shell profile (typically the file `/home/username/.profile`), or execute this command directly from the shell[1]:

```
export PATH=/home/username/bin:$PATH
```

C++ compiler

g++ version 4 or higher is recommended. See the compiler notes on the Qt website for further details.

Qt (`http://qt.digia.com`)

The easiest solution is to install the Qt packages available for your Linux flavour, including the headers (development packages). We recommend Qt version 4.6 or higher.

Alternatively, you can download the latest source package from the Qt website. Download the "Qt/X11 Open Source Edition" and follow the installation instructions for that source package.

Qwt (`http://sourceforge.net/projects/qwt`)

Either install the Qwt development package available for your linux distribution, or install the Qwt library using the source code.

To install Qwt manually, download the latest source package from the Qwt project website and unpack it in a temporary directory. The current QDOAS version requires Qwt version 6.0.2.

[1] When you execute this command from the shell, the changes are lost at the end of your session, and you will have repeat the command every time you start a new session. Adding the command to your shell profile will cause it to be executed automatically at the start of every session.

Open a shell and change to the Qwt root directory: edit the qwtconfig.pri and change the variables according to your installation. A sysadmin will set the `QWT_PREFIX_INSTALL` to `/usr/local`, while a regular user will set it to `/home/username`.

Once the changes are made accordingly to your installation, run the command **qmake qwt.pro** followed by **make** and finally **make install**. This will build the Qwt libraries and install the development package (headers, documentation and runtime libraries).

BEAT (`http://www.stcorp.eu/beat`)

QDOAS uses the BEAT library developed by the Dutch private company S[&]T to read GOME2 data. BEAT is provided as an open source library and has to be linked with QDOAS during compilation. After the installation of BEAT, the environment variable `CODA_DEFINITION` must be set as well.

BEAT can be installed using the usual "configure/make/make install" procedure. From the directory where you have downloaded the BEAT library files, type

```
$ ./configure --prefix=/home/username
```

This configures the install script to use the directory structure we described earlier. To complete the installation, type `make`, which will compile the library files, and finally `make install`, which will copy the compiled files, headers and other resources to the right subdirectories in `/home/username`.

To use QDOAS with GOME2 files, you should define the environment variable `CODA_DEFINITION`. This variable should contain the location of the .codadef files required by BEAT. For example:

```
In c-shell:
   setenv CODA_DEFINITION "/home/username/share/beat/definitions"
In bash:
   export CODA_DEFINITION="/home/username/share/beat/definitions"
```

Again, it is practical to add these commands to your shell profile.

HDF-EOS2

QDOAS uses the HDF-EOS2 library to read OMI spectra. The HDF-EOS2 library itself relies on the HDF4 library. If these libraries are not yet available on your system, you can install them using your linux distribution's package management system, or install them from the source code.

If you want to install the libraries from source, HDF4 must be installed first. The HDF4 source code package is available from `http://www.hdfgroup.org/ftp/HDF/HDF_Current/src`. You can install it using the usual "configure/make/make install" procedure. To avoid a conflict with the HDF5 library, we have found it practical to install the HDF4 header files in a separate subdirectory. To do this, use the `configure` with the following arguments:

```
$ ./configure --prefix=/home/username \
    --includedir=/home/username/include/hdf4
```

Now, use `make` and `make install` to complete the installation of HDF4.

Once you have installed the HDF4 library, download the source for HDF-EOS2 from `ftp://edhs1.gsfc.nasa.gov/edhs/hdfeos/latest_release/`. The library comes with an installation script, but we recommend installing it with the same "configure/make/make install" procedure, which is also available. If you installed HDF4 according to the previous instructions, the following command should allow you to install HDF-EOS2:

```
$ ./configure --prefix=/home/username CC=/home/username/bin/h4cc \
    --enable-install-include
```

When `configure` has finished its job, run `make` and `make install`.

HDF-EOS5

QDOAS can write output data in the HDF-EOS5 format, for which it needs the HDF-EOS5 and HDF5 libraries. Again, if these libraries are not installed on your system yet, you can either install the appropriate packages for your linux distribution, or compile the libraries from source yourself.

To install the libraries from source, you should first install the HDF5 library. Source code packages are available from `http://www.hdfgroup.org/ftp/HDF5/current/src`. Again, the installation follows the standard "configure/make/make install" procedure. You only need to set `--prefix`, to the path where you want to install the library:

```
$ ./configure --prefix=/home/username
```

After installing HDF5, you can obtain the HDF-EOS5 source code[2] at `ftp://edhs1.gsfc.nasa.gov/edhs/hdfeos5/latest_release`. This package can then be installed using configure and make. Again, you should set `--prefix=/home/username` to install the library at the correct location.

QDOAS

The QDOAS build configuration uses the Qt utility **qmake**. The configuration file is **Src/all.pro**, and it assumes that Qwt is installed in the default location – edit the file **Src/config.pri** to change this. Typically, the unix section of **config.pri** contains the following values:

```
INSTALL_PREFIX = /home/username

INCLUDEPATH += $$INSTALL_PREFIX/include
INCLUDEPATH += $$INSTALL_PREFIX/include/hdf4
INCLUDEPATH += /usr/include/qwt
QMAKE_RPATHDIR += $$INSTALL_PREFIX/lib
QMAKE_LIBDIR += $$INSTALL_PREFIX/lib
```

This configuration assumes that the BEAT, HDF4, HDF-EOS2, HDF5 and HDF-EOS5 libraries were installed at the location `/home/username`, that Qwt header files are installed at /usr/include/qwt, and that the user wishes to install the QDOAS executable files in `/home/username/bin`. When some of the include files and/or libraries are installed in other locations, you should add the include files' and library files' directories to the variables `INCLUDEPATH` and `QMAKE_RPATHDIR/QMAKE_LIBDIR` respectively. If you followed the instructions so far, you should only need to change `/home/username` to your actual username in order to install Qdoas.

To enable online help from Qdoas, you should adapt the following line:

```
QDOAS_HELP= '\\"/home/username/share/qdoas/Help\\"'
```

[2]The current version 1.14 of the HDF-EOS5 source code contains a bug. Until a fixed version of the HDF-EOS5 library is available, we recommend also applying the patch "strcopy-overlap.patch" contained in `https://launchpad.net/ubuntu/+archive/primary/+files/hdf-eos5_5.1.14%2Bdfsg.1.orig.tar.gz` to the downloaded HDF-EOS5 source code.

Change **/home/username/share/qdoas/Help** to the location where you want to put the qdoas help files.

When you have adapted `config.pri`, go to the Src directory of the QDOAS source distribution. Run the command **qmake all.pro** followed by **make**. This will create the executable files, `qdoas`, `doas_cl`, `convolution`, `ring` and `usamp`. The command `make install` copies the executable files to the directory `$$INSTALL_PREFIX/bin`. To copy the help files to the correct location, type (from the `Src` directory):

```
$ mkdir -p /home/username/share/qdoas
$ cp -r qdoas/Help /home/username/share/qdoas/Help
```

QDOAS uses the Qt resource system so that the executable only depends on system Qt and Qwt libraries. The executable can therefore be safely moved to another directory. To rebuild QDOAS after an update of the package, run the following commands from the `Src` directory:

```
$ make distclean
$ qmake all.pro
$ make
```

Install QDOAS on MAC

As BIRA-IASB doesn't have experience with MAC systems, we present the following guidelines which have been kindly provided by two different users. Warm thanks to Will and Anoop.

QDOAS build details on Mac OS X 10.6

1. Make sure you have Xcode installed. This comes on the DVDs included with the Mac, or the Apple developer website.
2. Qt and Qwt can be built separately, but allowing MacPorts (`http://www.macports.org/install.php`) to do it for you is much easier - it will automatically pull in the required dependencies.
```
sudo port selfupdate
sudo port install qt4-mac
sudo port install qwt-60
```
3. Install BEAT as per S&T instructions
4. Get QDOAS source (svn address provided after registration)
```
cd trunk/Src
```
5. Edit config.pri to reflect the paths on your system, if using MacPorts; they will be something like :
```
QWT_INC_PATH = /opt/local/include/qwt
QWT_LIB_PATH = /opt/local/lib
QWT_LIB = qwt
INSTALL_PREFIX = /usr/local/Qdoas
CODA_LIB_PATH = /usr/local/lib
CODA_INC_PATH = /usr/local/include
```
6.
```
/opt/local/bin/qmake -spec macx-g++42 all.pro
make
```
7. If it fails on make, so we then go into the individual QDOAS program folders, e.g.:
```
cd qdoas

g++-4.2 -headerpad_max_install_names -Wl,-rpath
Wl,/opt/local/lib -Wl,-rpath -Wl,/usr/local/lib -arch x86_64
-Xarch_x86_64 -mmacosx-version-min=10.6 -o
+../../qdoas/release/qdoas.app/Contents/MacOS/qdoas
*.o  L/opt/local/lib -lqwt -L/usr/local/lib -lcoda -lm
-lQtXml -lQtGui -lQtCore

sudo make install
```

Another experience with MAC

1. Check whether you are working on 32 bit of 64 bit architecture. Change this accordingly in src/all.pro, e.g. :

   ```
   CONFIG += ordered -arch x86_64
   ```

2. Darwin does not allow for -Wl and -rpath, you need to change this in all your .pro files in the src folder. E.g. in the gui.pro file, change the unix dependency to

   ```
   unix {
   INCLUDEPATH  += /usr/local/qwt/include ../engine
   LIBS         += -L/usr/local/qwt/lib -lqwt -lm
   QMAKE_LFLAGS += -rpath=/usr/local/qwt/lib
   }
   ```

3. Link of the binaries to the library needs to be done in the config.pri file, so I changed the unix dependency to:

   ```
   unix {
   QWT_INC_PATH   = /usr/local/qwt/include
   QWT_LIB_PATH   = /usr/local/qwt/lib
   QWT_LIB        = qwt
   DYLD_LIBRARY_PATH=/usr/local/qwt/lib
   INSTALL_PREFIX=
   /Users/userName/Documents/installed_programs/qdoas/app
   CODA_LIB_PATH = /usr/local/lib
   CODA_INC_PATH = /usr/local/include
   # for trace-write debugging ...
   DEFINES += DEBUG
   DEFINES += LVL4
   CONFIG += x86_64
   }
   ```

4. Finally, once you compile it, hopefully without any problems, the app will still not work from the finder. It will however work from the terminal. If you want to make sure that the app runs in the finder by double clicking, you need to change the framework in its resources (right click: package contents).

   ```
   // copy library into bundle:

   mkdir DupsApplication.app/Contents/Frameworks

   cp /usr/local/qwt-6.0.1/lib/libqwt.6.dylib \
     DupsApplication.app/Contents/Frameworks/

   // change library:

   install_name_tool \
     -id @executable_path/../Frameworks/libqwt.6.dylib \
     DupsApplication.app/Contents/Frameworks/libqwt.6.lib

   // change executable:

   install_name_tool \
     -change libqwt.6.dylib \
     @executable_path/../Frameworks/libqwt.6.dylib \
     DupsApplication.app/Contents/MacOS/DupsApplication

   ---------- run these commands----------

   sudo mkdir qdoas.app/Contents/Frameworks

   sudo cp /usr/local/qwt-6.0.1/lib/libqwt.6.dylib \
     qdoas.app/Contents/Frameworks/

   sudo install_name_tool \
     -id @executable_path/../Frameworks/libqwt.6.dylib \
     qdoas.app/Contents/Frameworks/libqwt.6.dylib

   sudo install_name_tool \
     -change libqwt.6.dylib \
     @executable_path/../Frameworks/libqwt.6.dylib \
   ```

```
  qdoas.app/Contents/MacOS/qdoas

sudo mkdir convolution.app/Contents/Frameworks

sudo cp /usr/local/qwt-6.0.1/lib/libqwt.6.dylib \
  convolution.app/Contents/Frameworks/

sudo install_name_tool \
  -id @executable_path/../Frameworks/libqwt.6.dylib \
  convolution.app/Contents/Frameworks/libqwt.6.dylib

sudo install_name_tool \
  -change libqwt.6.dylib \
  @executable_path/../Frameworks/libqwt.6.dylib \
  convolution.app/Contents/MacOS/convolution

sudo mkdir ring.app/Contents/Frameworks

sudo cp /usr/local/qwt-6.0.1/lib/libqwt.6.dylib \
  ring.app/Contents/Frameworks/

sudo install_name_tool \
  -id @executable_path/../Frameworks/libqwt.6.dylib \
  ring.app/Contents/Frameworks/libqwt.6.dylib

sudo install_name_tool \
  -change libqwt.6.dylib \
  @executable_path/../Frameworks/libqwt.6.dylib \
  ring.app/Contents/MacOS/ring

sudo mkdir doas_cl.app/Contents/Frameworks

sudo cp /usr/local/qwt-6.0.1/lib/libqwt.6.dylib \
  doas_cl.app/Contents/Frameworks/

sudo install_name_tool \
  -id @executable_path/../Frameworks/libqwt.6.dylib \
  doas_cl.app/Contents/Frameworks/libqwt.6.dylib

sudo install_name_tool \
  -change libqwt.6.dylib \
  @executable_path/../Frameworks/libqwt.6.dylib \
  doas_cl.app/Contents/MacOS/doas_cl

sudo mkdir usamp.app/Contents/Frameworks

sudo cp /usr/local/qwt-6.0.1/lib/libqwt.6.dylib \
  usamp.app/Contents/Frameworks/

sudo install_name_tool \
  -id @executable_path/../Frameworks/libqwt.6.dylib \
  usamp.app/Contents/Frameworks/libqwt.6.dylib

sudo install_name_tool \
  -change libqwt.6.dylib \
  @executable_path/../Frameworks/libqwt.6.dylib \
  usamp.app/Contents/MacOS/usamp
```

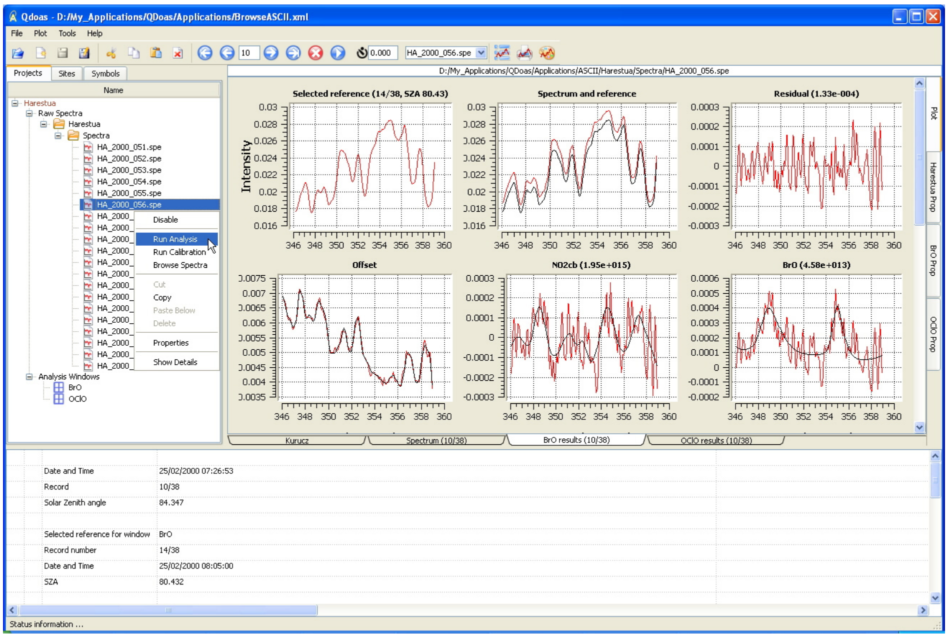
Online Help Online help is available as HTML pages. The content is similar to chapters 3, 5 and 6 of this document. HTML files have to be copied on your disk (usually a subfolder Help of the directory where executables are installed on Windows systems; a dedicated subfolder of your system share directory on Linux systems). The HTML pages are reachable from the Help button of the configuration dialog boxes. If the page can not be found, the root path of the index.html file is requested then the **Help** button has to be clicked again.

2 General Description of the User Interface

2.1 The user interface components

QDOAS is based on the notion of *projects*. A project is as a set of files sharing the same configuration of analysis, i.e. the definition of spectral windows and the list of files to be analysed with this configuration.

QDOAS allows defining several projects in a session, giving users the possibility to handle several analysis configurations.



QDOAS user interface and dialog boxes are very similar to WinDOAS but now, the main components are distributed into three resizable panels with a fixed arrangement :

- ◇ the elements of the application organized in tree structures presented in three tab pages (**Projects**, **Sites** and **Symbols**) in the upper-left one;
- ◇ dialog boxes for the configuration of the elements of the application and the plot of spectra and results in the upper-right one; all the spectral windows are processed in one shot; right and bottom tab-switched access possible between all these pages;

◇ the available information on the current spectrum and analysis results are displayed in the third one;

The Menu Bar

File Usual option to create a new application, open an existing one or save the current settings. QDOAS configuration files are in XML format. WinDOAS configuration files (*.wds) are not compatible with QDOAS.

Plot New option to organize the plots on the page (see below), to print the plot page or to save it in a png file;

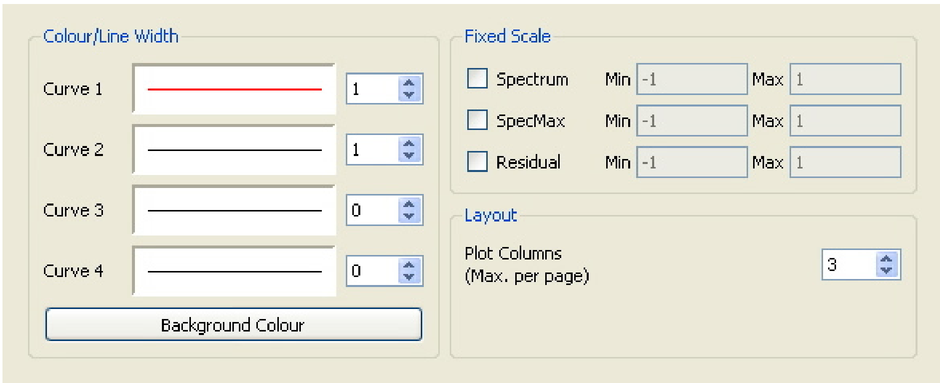
Tools The Convolution, Ring and undersampling tools, already present in WinDOAS, are now modules completely independent from the QDOAS application but they can still be called from the user interface;

Help Access to on-line help

The Toolbar

The toolbar gives access to the same **File** and **Plot** options of the menu bar. It contains also buttons to move easily in the current file or to use another file in the case a multiple files selection has been performed.

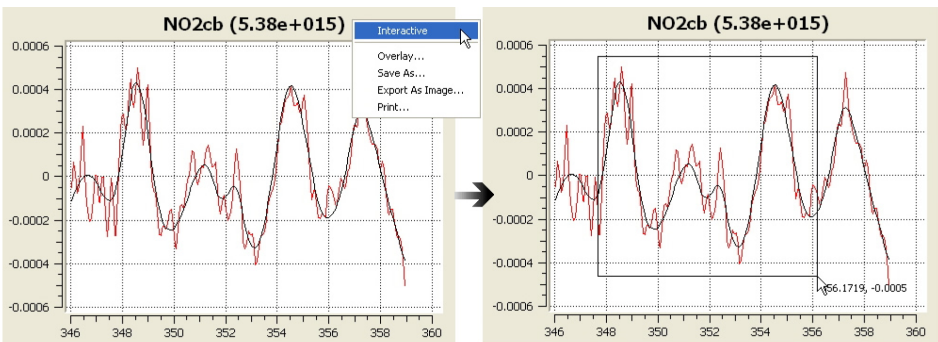
Plot Properties



This dialog box allows selecting a different color and a different line thickness for curves 1 and 2 (respectively the spectrum and the reference or the observed optical depth and the calculated optical depth). The number of plot columns impacts the size of the plots.

Handling plots

It is not possible to display a specific plot in another window as it was in WinDOAS but zoom can be made by right-clicking the **Interactive** option from **the title of a plot**.



The **Save As** option saves the plotted curves in a ASCII file (useful for example to create a reference spectrum). **Export As** image exports the selected plot in a png file while **Print** sends it to printer. **Overlay** will load a spectrum from a given file and superpose it over the already plotted curves but this option is not yet implemented.

2.2 The projects tree

The organisation of projects, analysis windows, spectra files and directories in a tree structure completed with the definition of right-click shortcut menus at each level of the tree makes the access, manipulation and configuration of all these objects very easy.

Raw Spectra

Spectra to analyze have to be inserted under this projects tree node. Individual files and complete directories structures are accepted. The "New Folder" option allows organizing spectra files and directories within a user-defined catalog (folder that is not physically present on the disk). The following actions can be performed from any node:

Browse Spectra browses spectra in the selected file(s);

Run Analysis analyses spectra using the configuration of the project and analysis windows; this step includes the correction of the wavelength calibration of the reference spectrum if it has been requested in the configuration of the analysis windows;

Run Calibration uses the options defined in the **Calibration page** of **Projects properties** (see page 65) to apply it on spectra.

To move from one record to the other or from one file to the other (in case of multiple files selection), use the adequate buttons in the toolbar:

Other options :

Disable/Enable Disables the selected file or directory from the list of files to browse/analyze. Enable option re-enables previously disabled files.

Refresh Refreshes the list of files in the selected directory;

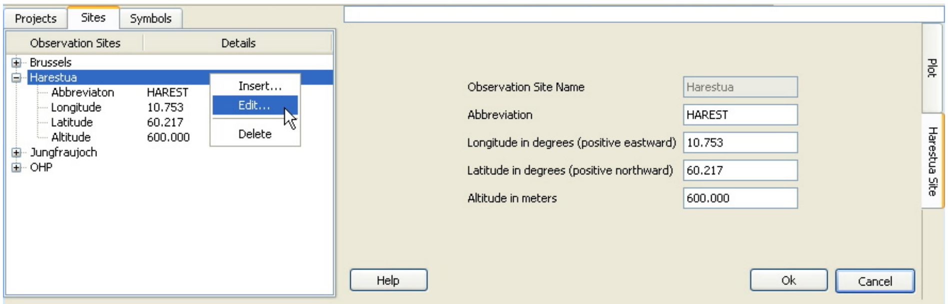
Show/Hide Details Shows/hides file information (last modification date and time, size). The file size information is useful to indicate if the selected file is empty or not.

Analysis windows

A project can include several spectral analysis windows. A specific analysis window can be disabled in order not to process it without removing it from the list. The **View Cross Sections** option is useful to check that the requested cross-sections files exist.

2.3 The observation sites

In the **Observation Sites** page, a list of observation sites can be specified by their location coordinates:



QDOAS applies the following conventions :

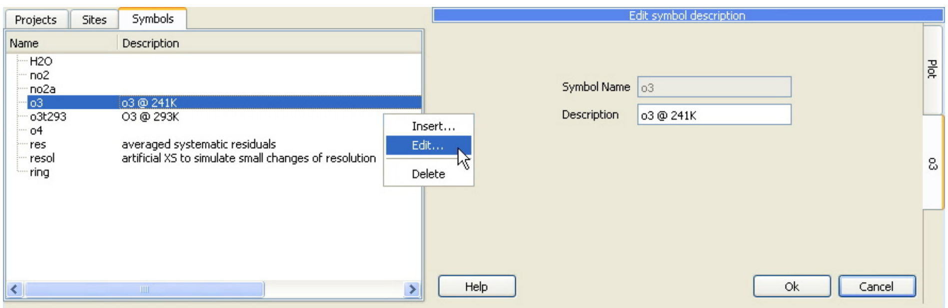
◇ longitudes are positive eastwards; negative westwards;
◇ latitudes are positive northwards; negative southwards.

For ground-based measurements, information on the observation site can help to [re-]calculate the solar zenith angle as far as the measurement date and time are correct (see the **Instrumental page** of **Projects properties**, page 68). For satellite measurements, this page can be used to define a list of overpasses (see the **Selection** page of Projects properties, page 61). In both cases, the **Abbreviation** is used as prefix of the name of the output files when the automatic creation of the output file name is requested.

The **Altitude** information is just for the user.

2.4 The symbols

Before configuring the analysis, the user must define the list of all relevant symbols that will be used. These symbols are needed to build cross-sections files filters, to link AMF and cross-section files and for internal manipulations (**Molecules** and **Shift and Stretch** pages of **Analysis Windows properties**).



Cross-sections symbols can be completed with a short description. The deletion of a symbol is possible only if this symbol is not used in the configuration of a project or an analysis window.

3 Description of Algorithms

This chapter summarizes the main features of QDOAS and describes the structure of the program and the algorithms.

3.1 Differential Optical Absorption Spectroscopy

DOAS is a widely used inversion method for the retrieval of atmospheric trace gas abundances from multi-wavelength light measurements. It uses the structured absorption of many trace gases in the UV, visible and near-infrared spectral ranges. The DOAS method was originally developed for ground-based measurements (Platt [17]; Platt and Stutz [18]) and has been successfully adapted to nadir measurements from UV-Vis spaceborne spectrometers (Gottwald et al. [9]). It relies on the application of the Beer-Lambert law to the whole atmosphere in a limited range of wavelengths.

The Beer-Lambert law states that the radiant intensity traversing a homogeneous medium decreases exponentially with the product of the extinction coefficient and the path length. Applying this law to the atmosphere, we obtain

$$I(\lambda) = I_0(\lambda) \exp\left(-\sum_{j=1}^{n} S^j(\lambda) c_j \right), \qquad (3.1)$$

where

- I_0 is the spectrum at the top of the atmosphere, without extinction;
- I is the measured spectrum after extinction in the atmosphere;
- S^j is the absorption cross section of the species j, with wavelength dependent structures [cm2/molec.];
- c_j is the column density of the species j [molec./cm2].

The logarithm of the ratio of the spectrum I_0 (also called the control spectrum) and the measured spectrum I is denoted optical density (or optical thickness) τ

$$\tau \equiv \ln\left(\frac{I_0(\lambda)}{I(\lambda)}\right) = \sum_{j=1}^{n} S^j(\lambda) c_j. \qquad (3.2)$$

The key idea of the DOAS method is to separate broad and narrow band spectral structures of the absorption spectra in order to isolate the narrow trace gas absorption features. In order to do this, some approximations are made:

1. In the case where the photon path is not defined (scattered light measurements), the mean path followed by the photons through the atmosphere up to the instrument is considered;
2. The absorption cross sections are supposed to be independent of temperature and pressure, which allows us to introduce the concept of Slant Column Densities (SCDs);
3. Broadband variations, such as loss and gain from scattering and reflections by clouds and/or at the earth surface, are approximated by a common low order polynomial.

Molecular absorption cross sections are fitted to the logarithm of the ratio of the measured spectrum and the reference spectrum (i.e. an extraterrestrial irradiance spectrum for satellite measurements, or a spectrum measured around the local noon when the light path is minimum for ground-based measurements). The resulting fit coefficients are the integrated number of molecules per unit area along the atmospheric light path for each trace gas, the differential SCD. The slant column depends on the observation geometry, the position of the sun and also on parameters such as the presence of clouds, aerosol load and surface reflectance.

3.2 DOAS retrieval

DOAS fitting

In the DOAS analysis, high frequency spectral structures of the various absorbing species are used to resolve the corresponding contributions to the measured optical density. This is achieved using a least squares fitting procedure for the differential slant column densities of the various species. Large band contributions to the atmospheric attenuation (Rayleigh and Mie scattering) are accounted for by including a low order polynomial $P(\lambda) = \sum b_k \lambda^k$ in the fit. Other effects, such as the Ring effect or instrument undersampling can be treated as pseudo-absorbers.

According to eq. (3.2), the DOAS retrieval is a linear problem. This linearity is unfortunately broken down by the need to account for additional effects, namely:

1. small wavelength shifts $\Delta(\lambda)$ between I and I_0 spectra must be corrected using appropriate shift and stretch parameters;
2. possible instrumental and/or atmospheric stray light or residual dark current signal require the introduction of an offset parameter.

Including these necessary non-linear corrections and the polynomial component $P(\lambda)$, we obtain the modified equation

$$\ln\left(\frac{I(\lambda + \Delta(\lambda)) - \text{offset}(\lambda)}{I_0(\lambda)}\right) + \sum_{j=1}^{n} S^j(\lambda) c_j + P(\lambda) = 0\,. \tag{3.3}$$

Marquardt-Levenberg Algorithm

The SCDs c_j can be retrieved by performing a least squares fit of the measurement data to equation (3.3). Due to the shift, stretch and offset parameters, this is a non-linear least squares problem, which can typically be solved using a Marquardt-Levenberg (M-L) algorithm (see Marquardt [15]; Bevington [2]). Starting from given initial values, this algorithm searches the parameter space using a combination of Gauss-Newton and gradient descent steps. The M-L algorithm is an efficient minimization algorithm for a wide range of non-linear functions, but it may converge to a local minimum if the initial values are too far from the global minimum. In QDOAS, this problem can occur during the wavelength calibration, when the initial calibration is not accurate enough (see Calibration problems in section C.2 of the appendix).

In QDOAS, the M-L algorithm is used to find the set of parameters that minimizes the weighted[1] sum of squares

$$
\begin{aligned}
F(\vec{\alpha}) =& \frac{1}{2}\sum_{i=1}^{M}\left(\frac{f^i(\vec{\alpha})}{\sigma^i}\right)^2 \\
=& \frac{1}{2}\sum_{i=1}^{M}\left(\frac{\ln(I^i(\vec{a})) + \sum_{j=1}^{n} S^{ij}c_j + \sum_{k=0}^{d} b_k(\lambda_i)^k - \ln(I_0^i)}{\sigma^i}\right)^2 ,
\end{aligned}
\qquad (3.4)
$$

where

$\vec{\alpha} = (\vec{a}, \vec{b}, \vec{c})$ is the vector containing all fitted parameters;

$\vec{a}$ is the set of parameters describing the shift, stretch and offset of the measured spectrum;

$b_k,\ k = 1, \ldots, d$ are the fitted polynomial coefficients;

$c_j,\ j = 1, \ldots, n$ are the fitted SCDs;

$\lambda_i,\ i = 1, \ldots, M$ is the wavelength grid of the reference spectrum I_0, calibrated with respect to a high resolution solar spectrum (see section 3.3).

$I^i(\vec{a})$ is the measured spectrum, including shift, stretch and offset corrections, interpolated at wavelength λ_i;

S^{ij} is the absorption cross section of absorber species j, as measured in a laboratory, interpolated at wavelength λ_i;

I_0^i is the reference spectrum at wavelength λ_i and

σ^i is the standard error on the measurement at wavelength λ_i.

In each iteration, the fitting algorithm will choose new values for the parameters using the Marquardt-Levenberg algorithm, and recompute the sum of squares F. The algorithm assumes that it has converged to a solution when the difference between two succeeding values of F is smaller than a fixed small number ϵ. The convergence criterion ϵ can be chosen by the user (see Convergence Criterion in section 5.1).

For a given value of the non-linear parameters $\vec{a}$, the determination of the parameters c_j and the polynomial coefficients b_k is a linear least squares problem. Explicitly, we can rewrite equation (3.4) as

$$
F = \frac{1}{2}\sum_{i=1}^{M}\left(\frac{\ln(I^i(\vec{a})/I_0^i) + (A\cdot\vec{x})^i}{\sigma^i}\right)^2 , \qquad (3.5)
$$

[1] Weighting the residuals by the instrumental errors σ^i is optional in QDOAS. When no measurement uncertainties are used (or no error estimates are available), all uncertainties in equation (3.4) are set to $\sigma^i = 1$, giving all measurement points equal weight in the fit. See analysis properties in section 5.1

where the matrix A contains the polynomial basis $(\lambda_i)^k, k = 0, \ldots, d$ and the absorption cross sections $S^{ij}, j = 1, \ldots, n$ and $\vec{x}$ represents the combined linear parameters $\vec{b}$ and $\vec{c}$:

$$A^{il} = \begin{pmatrix} (\lambda_i)^d & S^{ij} \end{pmatrix} , \qquad (3.6)$$

$$\vec{x} = \begin{pmatrix} \vec{b} \\ \vec{c} \end{pmatrix} . \qquad (3.7)$$

This fact is exploited in QDOAS to limit the parameter space of the M-L algorithm to the non-linear parameters: once a new set of values $\vec{a}'$ for the non-linear parameters is chosen, the linear parameters b_k and c_j are updated using a linear least squares algorithm, minimizing the sum of squares (3.4) for the given values of the non-linear parameters.

In QDOAS, the linear least squares problem is solved using the Singular Value Decomposition (SVD) of the matrix A defined in equation (3.6).

QDOAS can include further parameters in the fits (3.4), which we omitted from the previous description for the purpose of clarity. Such parameters include the width of the instrument's slit function and wavelength shifts in the reference absorption cross sections $S^j(\lambda)$. Mathematically, they play the same role as the shift, stretch and offset parameters $\vec{a}$. Section 5.3 describes the available fitting options in QDOAS and their configuration.

Intensity fitting

QDOAS also supports the so-called intensity fitting (or direct fitting) method where measured intensities are directly fitted instead of their logarithms. The equation used in the least squares fitting procudure is then

$$\frac{I(\lambda + \Delta(\lambda)) - \text{offset}(\lambda)}{I_0(\lambda)} - P \exp(-\sum_{j=1}^{n} S^j c_j) = 0 , \qquad (3.8)$$

This method involves a decomposition of equation (3.8) in its linear and non-linear parts: column densities are fitted non-linearly, but the polynomial, which is taken out of the exponential function using a Taylor expansion, and offset are linear parameters.

Intensity fitting is sometimes preferred to optical density fitting, for example when a poor signal leads to numerical problems when taking the logarithms of the intensity ratio.

Errors On Slant Column Densities

Uncertainties on the retrieved slant columns c_j depend on:

- ◇ the sensitivity of the sum of squares F (3.4) with respect to variations of the fitted parameters around the minimum and
- ◇ the noise on the measurements.

Formally, the covariance matrix of the fitted parameters of a least squares estimate may be estimated by the inverse of the Hessian of the sum of squares F, evaluated at the fitted values of the parameters

$$\Sigma_{\vec{\alpha}} = H^{-1} , \qquad (3.9)$$

where H is given by

$$H_{kl} = \frac{\partial^2 F}{\partial \alpha_k \partial \alpha_l} . \qquad (3.10)$$

The actual approach used to calculate H in QDOAS is different in optical density fitting mode and in intensity fitting mode. In optical density fitting mode, the slant column density is fitted linearly according to equation (3.5) and we use the following expression for the covariance matrix $\Sigma_{\vec{x}}$ of the weighted linear least squares parameter estimate:

$$\Sigma_{\vec{x}} = \left(A^T W^2 A\right)^{-1} , \tag{3.11}$$

where the matrix A contains the linear components of the fit, as described in equation (3.6) and the $(M \times M)$ diagonal matrix W contains the measurement errors

$$W_{ij} = \frac{1}{\sigma^i} \quad \text{if } i = j \, . \tag{3.12}$$

Equation (3.11) implies that uncertainties on estimated values of the non-linear parameters are not taken into account in the reported errors on the slant columns.

When the individual measurement errors σ^i are not available (or the user has chosen not to weight the fit by the instrumental errors), the weight matrix W is just the identity matrix. In this case, the mean squared error on the measurements σ^2 may be estimated by the reduced χ^2, e.g. the sum of squares F divided by the number of degrees of freedom in the fit

$$\chi^2 = \frac{F}{M - N} , \tag{3.13}$$

where M is the number of wavelengths included in the fit, and N is the total number of fitted parameters. Equation (3.11) then becomes

$$\Sigma_{\vec{x}} = \chi^2 \left(A^T A\right)^{-1} . \tag{3.14}$$

In intensity fitting mode, the slant column densities are determined using non-linear least squares fitting, and the Hessian is approximated by the square of the Jacobian of the fitting functions f^i

$$H_{kl} \simeq \sum_{j=1}^{M} \frac{\partial f^j}{\partial \alpha_k} \frac{\partial f^j}{\partial \alpha_l} \frac{1}{(\sigma^j)^2} . \tag{3.15}$$

This implies that, in intensity fitting mode, uncertainties on the linear parameters are not taken in to account in the reported slant column errors. As in the linear case, the instrumental errors are approximated using the reduced χ^2 of the fit when the σ^i are not available. Equation (3.9) then becomes

$$\Sigma_{\vec{\alpha}} = \chi^2 H^{-1} . \tag{3.16}$$

Limitations

The estimates for the uncertainties of the fitted parameters rely on the statistical model used for the DOAS retrieval. The model assumes that the errors on the measurements at each frequency are independent and normally distributed. When measurement errors are correlated or contain systematic components, or in case of fitting errors such as a wrong fit for shift and stretch parameters, or relevant absorbers that are not included in the fit, the uncertainties calculated by QDOAS will underestimate the true error on the slant column density. Remaining residual structures after the fit, or a value of $\chi^2 \gg 1$ when measurement errors σ^i are taken into account, are an indication of such a bad fit. A discussion can be found in Stutz and Platt [23].

We also note that the errors in QDOAS do not take into account the uncertainties on the cross sections. A way to achieve this is given in Theys et al. [24].

3.3 Wavelength calibration

The quality of the retrieval fit strongly depends on a perfect alignment between the spectrum to analyze, the reference spectrum and the cross sections. The wavelength-pixels relation (see Platt and Stutz [18]) of the reference spectrum, previously determined in laboratory using a lamp spectrum can be corrected using a procedure based on the alignment of the Fraunhofer structures of the reference spectrum I_0 with those of an accurately calibrated high-resolution solar reference atlas, degraded at the resolution of the instrument, i.e. convolved with the instrumental slit function. The reference atlas used for this purpose is usually the Chance and Kurucz [7] spectrum.

During the calibration process, the instrumental slit function can also be characterized by repeatedly convolving the highly resolved solar atlas with the slit function and adjusting the parameters until the best match with the reference spectrum is found. QDOAS allows fitting the parameters of different line shapes, as well as their wavelength dependence. This is useful when the slit function provided with the instrument is not described precisely enough in the wavelength interval used for the retrieval. In the same way, to account for the moderate resolution of satellite or ground-based instruments (about a few tenths of a nanometer), the absorption cross sections of the trace gases have to be convolved with the instrumental slit function (and interpolated on the final I_0 wavelength grid). A good knowledge of the instrumental slit function and its potential wavelength variation is important to avoid systematic errors in the retrieved slant columns due to spectral shape mismatch between the reference and atmospheric spectra [25].

Fit of shift and stretch

Shift and stretch (see Shift on page 31) can be taken into account in the wavelength calibration scheme. To this end, the spectral interval is divided into a number of equally spaced sub-intervals. The fitting algorithm used for the DOAS retrieval is then applied in each sub-interval to fit the measured intensities to those of the high-resolution solar spectrum, according to the equation

$$I_0(\lambda) = I_S(\lambda - \Delta_i) \exp(-\sum_{j=1}^{m} S^j c_j)\,, \tag{3.17}$$

where I_S is the solar spectrum convolved at the resolution of the instrument, Δ_i is a fitted constant shift in sub-interval i, and the c_j are optional absorber coefficients accounting for possible light absorption in the reference spectrum I_0. A value of the shift Δ_i is calculated in each sub-interval

i and a polynomial is fitted through the individual points in order to reconstruct an accurate wavelength calibration $\Delta(\lambda)$ for the complete analysis interval.

Several tests may be needed to determine the best configuration. One has to find the right compromise between using enough sub-intervals to represent the wavelength variation of the shift, and having enough spectral information in each sub-window. The interval calibration should cover all analysis spectral windows.

The algorithm can take into account molecular absorption and offset correction. In order to help the algorithm to converge to the exact solution, it is important to start with a preliminary wavelength grid close enough to the real one and to limit the number of fitting parameters (for example by fixing the value of some parameters, typically the concentration of the fitted molecules after a first estimation).

Ref2/Ref1 Alignment

If two reference spectra are given (see section 5.1 and figure 5.5), the wavelength calibration described in the previous section is applied to the first one. The shift between both reference spectra is then determined using a least squares fit. This shift is then applied to the reference absorption cross sections in order to align them on the second reference spectrum. The measured spectra are then analyzed with respect to the second reference spectrum.

Characterization Of The Line Shape

If the slit function varies strongly in the fitting window and is symmetric enough to be approached by an analytical function like a Gaussian, it can be fitted together with the shift during the calibration procedure. A high resolution solar spectrum is needed. The wavelength variation of the line shape can be accounted for in order to convolve high-resolution cross sections before the analysis. The equation (3.17) used in the calibration is then modified as follows:

$$I_0(\lambda) = (L_{a_i} * I_S)(\lambda - \Delta_i) \exp\left(-\sum_{j=1}^{m} c_j S^j\right) , \tag{3.18}$$

where $L_{a_i}(\lambda)$ is the line shape with Full Width at Half Maximum (FWHM) parametrized by a_i. QDOAS can fit the parameters for a number of different analytical line shapes, which we describe in more detail in the Analytical line shapes section on page 40.

3.4 Fit parameters

Absorption cross sections

In principle, DOAS measurements are applicable to all gases with suitable narrow absorption bands in the UV, visible or near IR regions. However, the generally low concentrations of these compounds in the atmosphere and the limited signal-to-noise ratio of the spectrometers restrict the number of trace gases that can be detected. Figure 3.1 shows the absorption cross sections of a number of trace gases that are regularly measured using the DOAS technique.

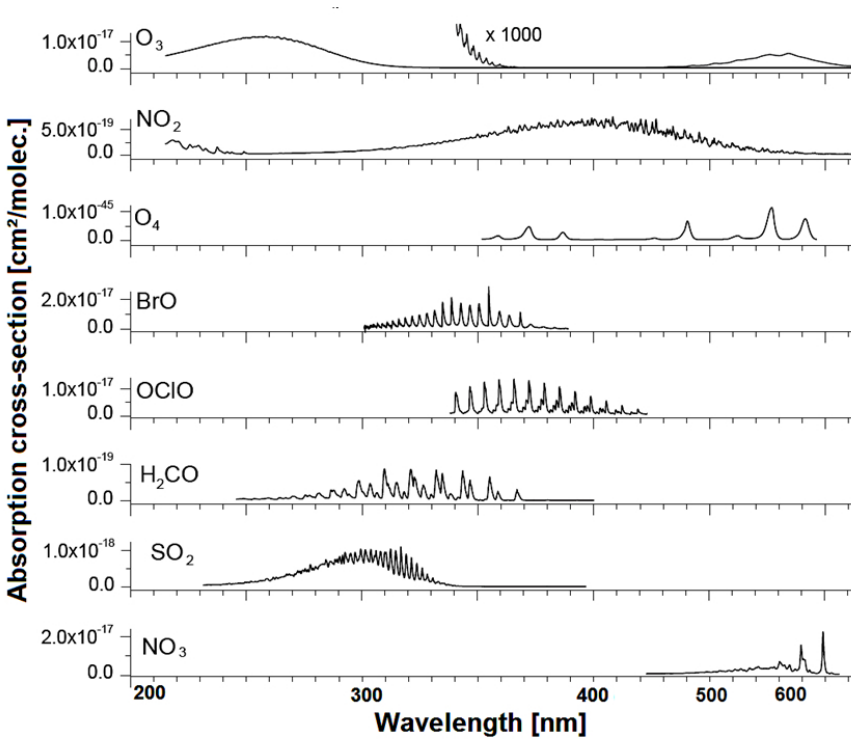


Figure 3.1.: Absorption cross sections of various absorbers retrieved with the DOAS method (figure taken from Platt and Stutz [18]).

Many spectral regions contain a large number of interfering absorbers. In principle, because of their unique spectral structure, a separation of the absorption is possible. However, correlations between absorber cross sections sometimes lead to systematic biases in the retrieved slant columns. In general, the correlation between cross sections decreases if the wavelength interval is extended, but doing so is at odds with the assumption that a single effective light path for the entire wavelength interval is defined, leading to systematic misfit effects that may also introduce biases in the retrieved slant columns. To optimize DOAS retrieval settings, a trade-off has to be found between these effects. A basic limitation of the classical DOAS technique is the assumption that the atmosphere is optically thin in the wavelength region of interest. At shorter wavelengths, the usable spectral range of DOAS is limited by rapidly increasing Rayleigh scattering and O_3 absorption. In addition, 'line-absorbers' such as H_2O, O_2, CO, CO_2 and CH_4 usually cannot be retrieved precisely by standard DOAS algorithms because their strong absorption also depends on pressure and temperature.

The selection of the spectral analysis window determines which absorbers have to be included in the fitting procedure. The pressure dependence of absorption cross sections can be neglected in UV-Visible region. However, the temperature dependence of cross sections can be significant (for example that of O_3 and NO_2). This can be corrected in a first approximation by introducing correction factors during the AMF calculation [3] or, assuming a linear dependence on temperature, by fitting two absorption cross sections at different temperatures as described in Van Roozendael et al. [25].

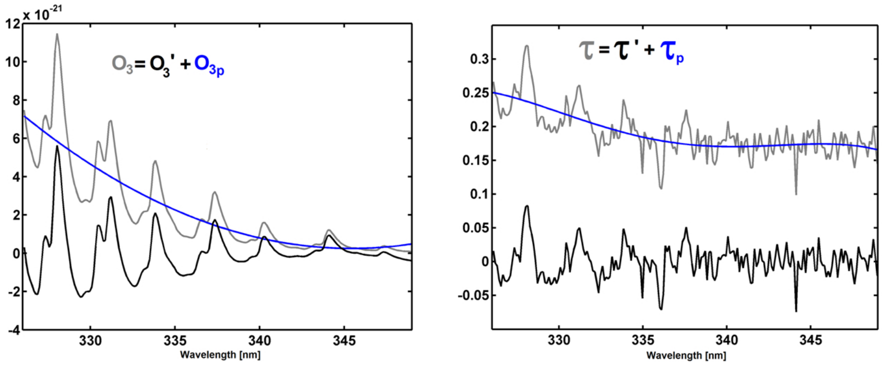


Figure 3.2.: Cross section O_3 and optical thickness τ are separated into a narrow (O_3' and τ') and a broad band part (O_{3p} and τ_p) by an adequate filtering procedure.

Shift

Before analysis, absorption cross sections are interpolated on the final grid of the reference spectrum which may be determined by the program itself (automatic reference selection mode). Moreover, shift and stretch parameters can be fitted during the processing of a spectrum in order to obtain the best match of the absorption structures.

Interpolation/Convolution

Cross sections can be pre-convolved and interpolated[2] on an appropriate wavelength grid prior to the analysis. However, the direct use of high-resolution cross sections which can be convolved in real-time with a predefined slit function or with the slit function determined by the wavelength calibration procedure, is more convenient.

Differential cross sections

The aim of calculating differential absorption cross sections is to separate narrow spectral features from unstructured absorption not useful in the DOAS method. Figure 3.2 gives an illustration.

Differential cross sections can be calculated by orthonormalization with respect to an orthogonal set formed with the low order component vectors (usually a base of order 2 or 3) of the polynomial. The vectors are orthogonalized using the Gram-Schmidt algorithm. This method gives also the possibility to separate the spectral structures of temperature dependent cross sections by mutually orthogonalizing them. Differential cross sections can alternatively be obtained by high-pass filtering: a filter is applied iteratively on the cross section and the resulting cross section is subtracted from the original one. High-pass filtering is presently only supported in optical density fitting mode (DOAS mode). Note that it is not necessary to calculate differential cross sections when the baseline is around 0 such as for H_2O, O_4 or H_2CO.

Low-pass filtering

Low-pass filters can be applied to both spectra and absorption cross sections. A large choice of filters is proposed (see 'Filtering Page', section 5.1).

[2]By default, QDOAS uses cubic spline interpolation.

Wavelength-dependent AMF Absorption cross sections can be replaced by geometrically corrected cross sections that take into account the wavelength dependency of the AMF. The correction is based on the equation

$$\ln(I_0) - \ln(I) = S(\lambda)\mathrm{AMF}(\lambda, \mathrm{SZA}), \tag{3.19}$$

where $\mathrm{AMF}(\lambda, \mathrm{SZA})$ is the AMF calculated for a given wavelength λ and a given Solar Zenith Angle (SZA).

Polynomial In the DOAS technique, absorption cross sections of the considered molecules are highly structured, while scattering by molecules and particles (Rayleigh and Mie scattering), as well as reflection at the surface, have broadband dependencies that can be approximated by a low order polynomial. In QDOAS, polynomials up to degree 5 can be fitted. The low order components of the polynomial can be used to calculate differential cross sections when this is preferred to high-pass filtering.

Shift and Stretch Shift and stretch parameters allow to correct possible misalignment between the various wavelength-dependent quantities involved in the data evaluation (i.e. measured and reference spectra as well as absorption cross sections). Shift and stretch parameters may be fitted or simply applied to any wavelength-dependent quantity, according to the equation

$$\Delta\lambda = a + b(\lambda - \lambda_0) + c(\lambda - \lambda_0)^2, \tag{3.20}$$

where λ is the wavelength according to the original calibration and λ_0 is the center wavelength of the current spectral range. The parameters a,b and c describe the offset and the first and second order stretch applied to λ.

Offset Correction An ideal spectrometer in an ideal atmosphere would measure the part of the sunlight that has been elastically scattered by air molecules and particles. In a real experiment, however, a number of possible additional sources may contribute to the measured intensity, adding an "offset" to the ideal Rayleigh/Mie contribution. In addition to the Ring effect, which is, to a first approximation, a natural source of offset, one must also account for instrumental sources of offset, such as stray light in the spectrometer and dark current of the detector. The offset component in equation (3.3) accounts for these effects. QDOAS models the offset using a polynomial

$$\mathrm{offset}(\lambda) = (a + b(\lambda - \lambda_0) + c(\lambda - \lambda_0)^2)\bar{I}, \tag{3.21}$$

where λ_0 is the center wavelength of the spectral analysis window, $\bar{I}$ is the average intensity and a, b and c are fitted parameters.

Due to the normalization by $\bar{I}$, the offset values can be easily interpreted relatively to the absolute intensity of the spectrum (percent offset). In DOAS, the offset is usually fitted as a non-linear parameter. Sometimes, this could lead to numerical errors in the evaluation of the logarithm, typically in the near UV region where the level of the signal is very low. In this case, we can fit the offset as a linear parameter. Expanding the left-hand side of equation (3.3) to first order, we obtain

$$\ln(I(\lambda + \Delta(\lambda))) = \ln(I_0(\lambda)) - \tau(\lambda) + \frac{\mathrm{offset}(\lambda)}{I(\lambda + \Delta\lambda)}. \tag{3.22}$$

Ring Effect Because of Rotational Raman Scattering (RRS), a small fraction of the incident photons undergo a wavelength change of a few nanometres, i.e. a part of the scattering is inelastic. This causes an intensity loss at their incident wavelength and a gain at the neighbouring wavelengths to which they are redistributed. RRS causes the so-called "filling-in" of Fraunhofer lines, which have a slightly different shape in the earthshine radiance than in the direct solar light. This effect was first discovered by Grainger and Ring [10] and is referred to as the Ring effect. The atmospheric absorption lines are also broadened by RRS events occurring after absorption (molecular Ring effect). Although RRS accounts for only a few percent of the measured intensity, it significantly affects DOAS measurements of scattered radiation since typical trace gas absorptions are of the order of a percent or less. If not properly corrected, the Ring effect produces strongly structured residuals in the differential optical density, due to the fact that Fraunhofer lines do not cancel perfectly between I and I_0. Especially in the UV spectral range, the remaining spectral structures can by far exceed the structures of weak atmospheric absorbers.

Usually the Ring effect is taken into account by including an additional 'absorber' in the DOAS fit. Ring cross sections $S_{\mathrm{Ring}}(\lambda)$ can be measured [22] or calculated [8]. The Ring effect can be approximated using the following development for an optically thin atmosphere [27; 25]:

One can consider that in any scattered light observation, the light detected by the satellite instrument (I_{meas}) is the sum of elastic and inelastic scattering processes:

$$I_{\mathrm{meas}} = I_{\mathrm{elastic}} + I_{\mathrm{RRS}} = I_0 e^{-\tau} + I_{\mathrm{RRS}}\,. \tag{3.23}$$

To analyze a measured spectrum, the logarithm of I_{meas} is taken. Since I_{RRS} is very small compared to I_{elastic}, the logarithm can be approximated by the first two terms of the Taylor expansion:

$$\ln(I_{\mathrm{meas}}) = \ln(I_{\mathrm{elastic}}) + \frac{I_{\mathrm{RRS}}}{I_{\mathrm{elastic}}} = \ln I_0 - \tau + \frac{I_{\mathrm{RRS}}}{I_{\mathrm{elastic}}}\,. \tag{3.24}$$

The last term $I_{\mathrm{RRS}}/I_{\mathrm{elastic}}$ is the Ring term which can be approximated by the product of a Ring coefficient α_{Ring} and a Ring cross section S_{Ring}. α_{Ring} can be fitted together with other absorbers in the DOAS procedure.

A good approximation of the Ring cross section can be obtained from calculation of a source term I_0^{Raman} for Raman scattering derived by simple convolution of the solar spectrum with Raman cross sections, i.e with calculated N_2 and O_2 RRS cross sections. The term $I_{\mathrm{RRS}}/I_{\mathrm{elastic}}$ in equation (3.24) is then substituted by $\alpha_{\mathrm{Ring}} S_{\mathrm{Ring}}$ (where $S_{\mathrm{Ring}} = I_0^{\mathrm{Raman}}/I_0$), assuming that the molecular Ring effect can be neglected [8]. The QDOAS Ring tool calculates a normalized Ring cross section according to this approach [27].

Undersampling Correction The undersampling is a well-known problem of GOME [6]. It arises from the poor sampling ratio of the GOME instrument, which results in a loss of spectral information when interpolating earthshine spectra during the DOAS fitting process. Undersampling is only a major problem when the sampling ratio is close to 1. In the case of GOME, this ratio is estimated at 0.16/0.112=1.43 at 340 nm.

The undersampling artifacts can be corrected using an ad-hoc cross section obtained by simulating the effect based on a high-resolution solar reference [6]. This cross section is fitted as a linear parameter, in both intensity fitting and in optical density fitting modes. The procedure to calculate the correction differs slightly between the two fitting modes:

In intensity fitting mode, oversampled and undersampled spectra are calculated as follows:

$$U(\lambda+\Delta) = \mathrm{over}(\lambda+\Delta) - \mathrm{under}^{(\Delta)}(\lambda)\,, \tag{3.25}$$

where $\mathrm{over}(\lambda+\Delta)$ is a high-resolution solar spectrum convolved on its original grid and interpolated on the final grid $\lambda+\Delta$ and $\mathrm{under}^{(\Delta)}(\lambda)$ is a high-resolution solar spectrum convolved on grid λ and subsequently interpolated on the final grid $\lambda+\Delta$.

Residuals are improved by adding a "second phase" of undersampling

$$U_2(\lambda) = \mathrm{over}(\lambda) - \mathrm{under}^{(\Delta)}(\lambda)\,. \tag{3.26}$$

In optical density fitting, we fit the logarithm of the ratio of the measured intensities. We therefore use the corresponding equations

$$U(\lambda+\Delta) = \ln\left(\frac{\mathrm{over}(\lambda+\Delta)}{\mathrm{under}^{(\Delta)}(\lambda)}\right), \tag{3.27}$$

$$U_2(\lambda) = \ln\left(\frac{\mathrm{over}(\lambda)}{\mathrm{under}^{(\Delta)}(\lambda)}\right). \tag{3.28}$$

Undersampling cross sections can be pre-calculated using the QDOAS undersampling tool or they can be calculated in real time, just after the wavelength calibration procedure using the corrected wavelength grid and the characterized slit function.

AMF

To obtain the Vertical Column Density (VCD) from the fitted SCD, we have to divide the SCD by the AMF

$$\mathrm{VCD} = \frac{\mathrm{SCD}}{\mathrm{AMF}}\,. \tag{3.29}$$

AMF's are not calculated by QDOAS but may be imported from ASCII files (for details, refer to appendix A). QDOAS supports solar zenith angle-dependent AMF, wavelength-dependent AMF and climatological AMF.

Graphical Display Of Spectral Fit Results

According to the selected fitting method, different formulas are used to display the measured data and the calculated fit results. Tables 3.1 and 3.2 explain which quantities are displayed on the fit results page for optical density fitting mode and intensity fitting mode. The following quantities

	Calculated	Measured
Residual		R_{od}
Cross sections	$S^j \cdot c_j$	$S^j \cdot c_j + R_{\text{od}}$
Polynomial	P	$P + R_{\text{od}}$
Offset	O	$O + R_{\text{od}}$

Table 3.1.: Formulas used by QDOAS to display the results of a fit in optical density fitting mode. S^j is the reference cross section for species j and c_j the corresponding SCD. $P(\lambda)$ is the polynomial obtained from the fit. See equations (3.30)-(3.34) for the definitions of the quantities R_{od} and O.

	Calculated	Measured
Normalized Residual		R_{norm}
OD Residual		R_{i}
Cross sections	$S^j \cdot c_j$	$S^j \cdot c_j + R_{\text{i}}$
Polynomial	P	P_{meas}
Offset	O	$O + R_{\text{i}}$

Table 3.2.: Formulas used by QDOAS to display the results of a fit in intensity fitting mode. S^j is the reference cross section for species j and c_j the corresponding SCD. $P(\lambda)$ is the polynomial obtained from the fit. See equations (3.30)-(3.34) for the definitions of the quantities $R_{\text{norm}}, R_{\text{i}}$ and O.

are used:

$$R_{\text{od}} = \ln\left(\frac{I_0 \cdot e^{-\sum S^j c_j - P}}{I - \text{offset}}\right), \tag{3.30}$$

$$R_{\text{norm}} = \frac{P \cdot I_0 \cdot e^{-\sum S^j c_j}}{I - \text{offset}} - 1, \tag{3.31}$$

$$R_{\text{i}} = \ln\left(\frac{P \cdot I_0 \cdot e^{-\sum S^j c_j}}{I - \text{offset}}\right), \tag{3.32}$$

$$P_{\text{meas}} = \frac{I - \text{offset}}{I_0 \cdot e^{-\sum S^j c_j}}, \tag{3.33}$$

$$O = \ln(1 - \text{offset}/I), \tag{3.34}$$

where I is the measured spectrum, I_0 is the reference spectrum, P the fitted polynomial, S^j the absorption cross section for absorber species j and c_j the corresponding fitted concentration.

3.5 Block-diagram structure of the program

The following figures give an overview of the structure of the program. Figure 3.3 describes the general organization of the processor. Figures 3.4 and 3.5 show the structure of the wavelength calibration and slant column fitting modules, while the coupled non-linear least squares fitting algorithm is sketched in Figure 3.6.

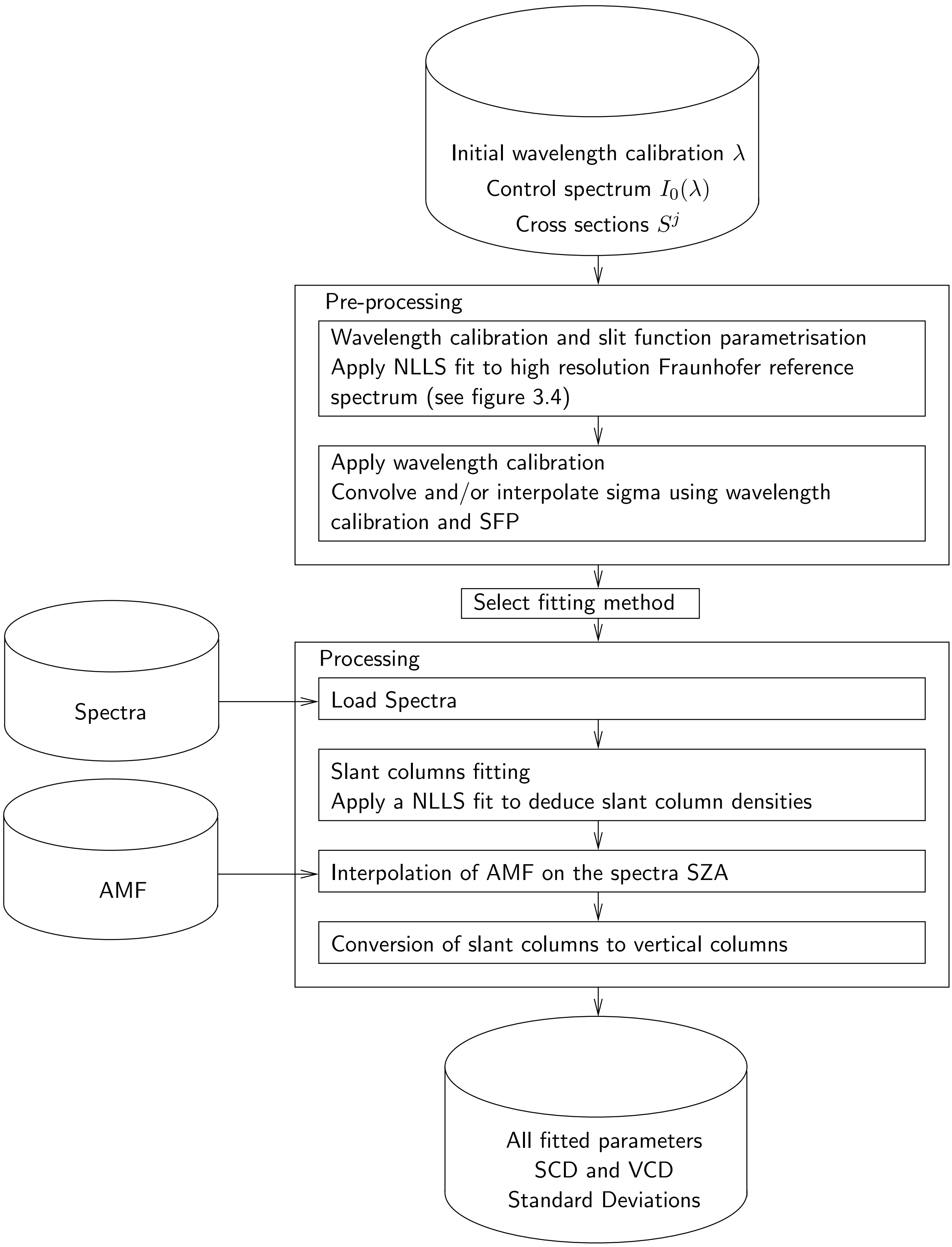


Figure 3.3.: Overall structure of the spectral analysis program.

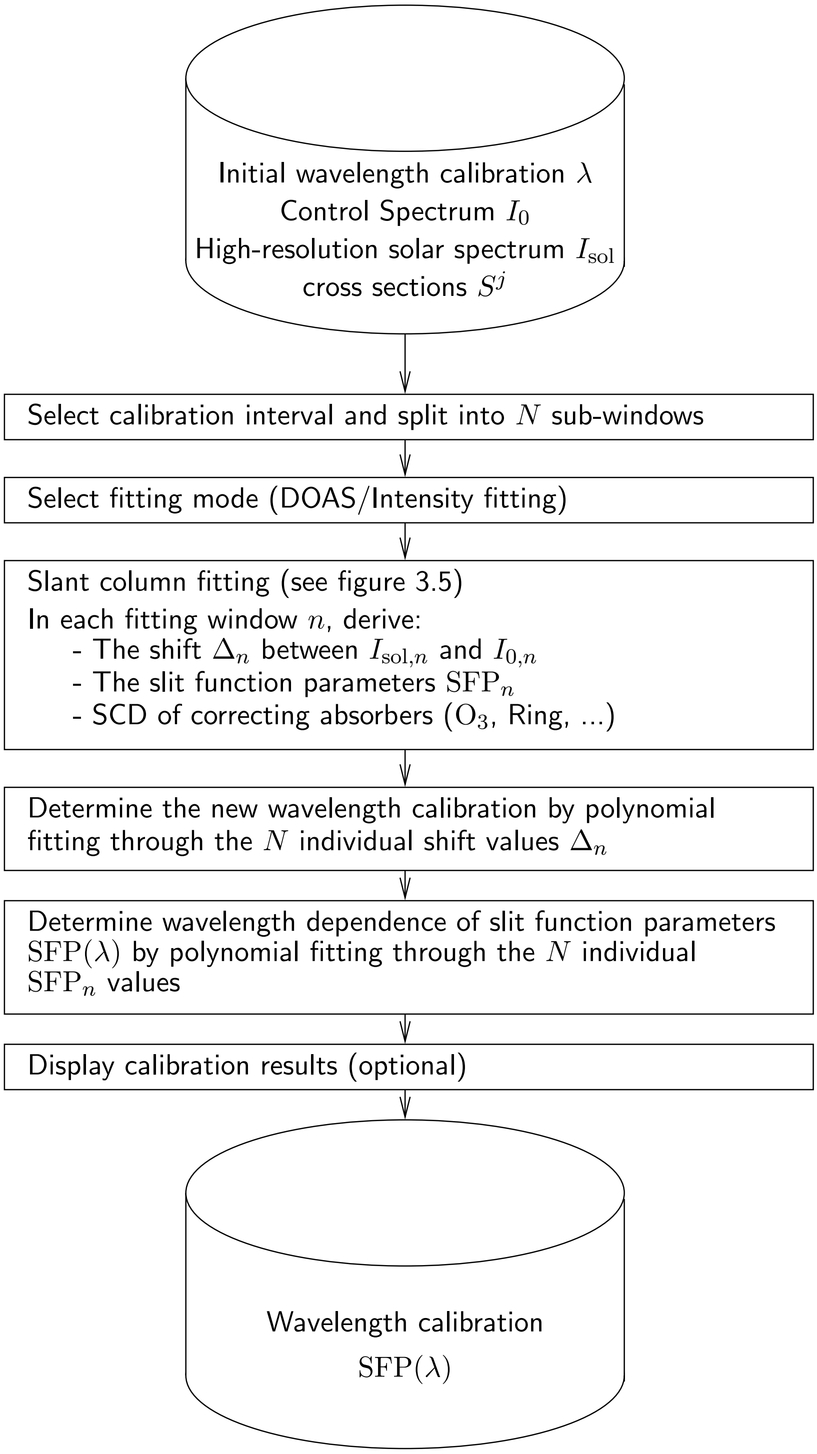


Figure 3.4.: Structure of the wavelength calibration module.

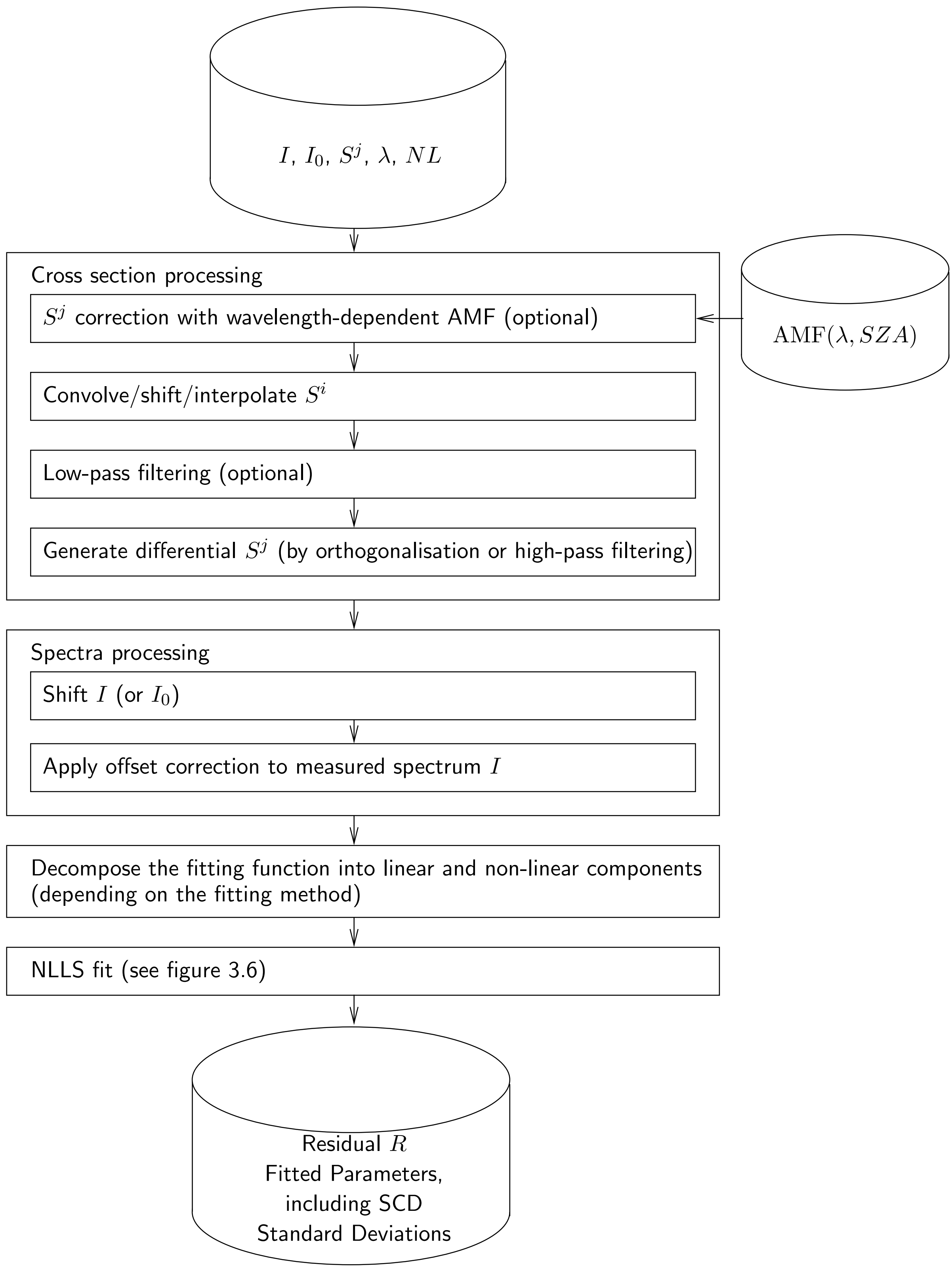


Figure 3.5.: Structure of the slant column fitting module. Cross section processing only takes place during the pre-processing phase, unless cross sections must be dynamically modified during the fit (e.g. when fitting a cross section shift).

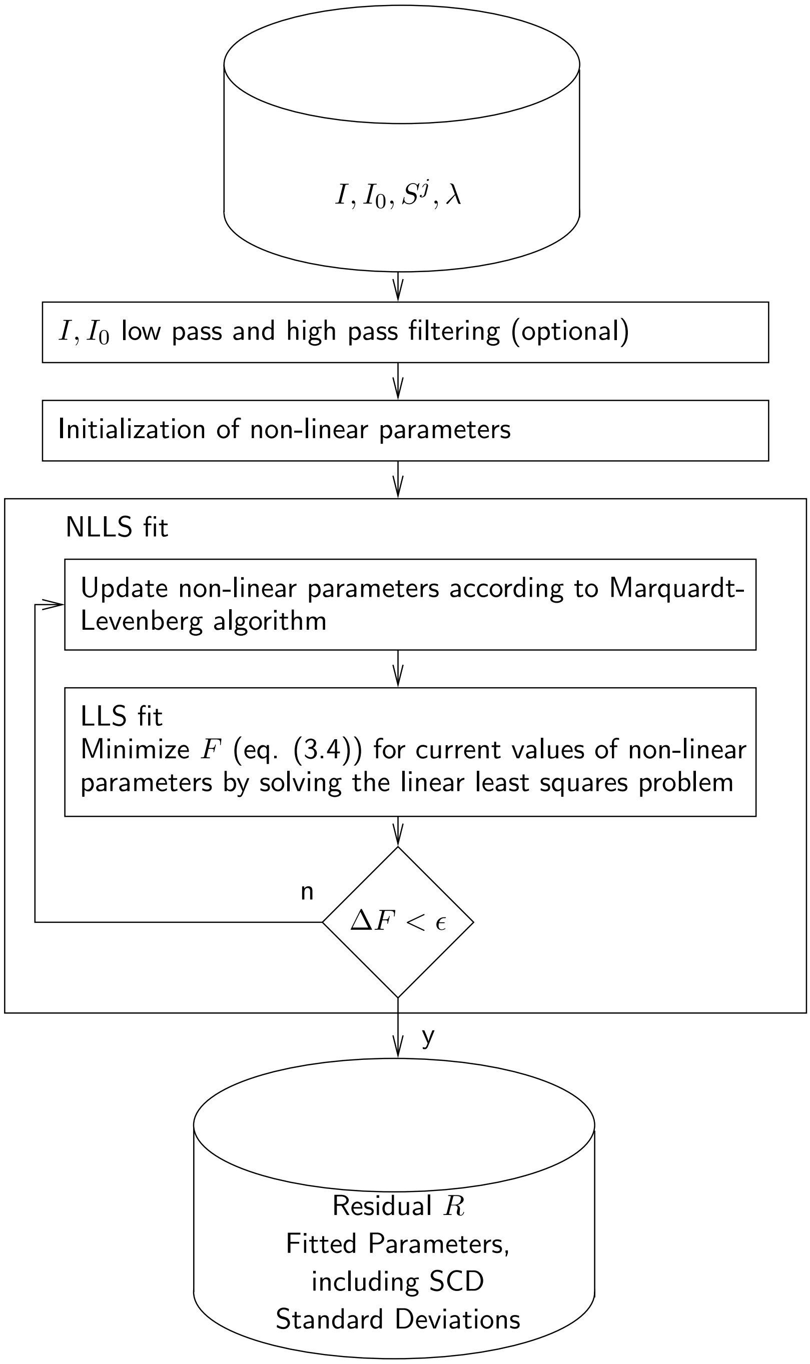


Figure 3.6.: Structure of the non-linear least squares fitting algorithm used in the slant column fitting module and in the wavelength calibration module.

3.6 Convolution

Definition

The convolution of a spectrum I by an instrumental slit function F is given by the integral

$$(F * I)(\lambda) = \int I(\lambda')F(\lambda - \lambda')\mathrm{d}\lambda\,. \tag{3.35}$$

In QDOAS, this integral is calculated using the trapezoidal rule. The integration interval is defined by the width of the slit function.

The three tools (Convolution, Ring and Usamp) provided in the QDOAS package, support convolution with one of the following functions:

- the Gaussian line shape,
- the $2n$-Lorentzian line shape,
- the Voigt profile,
- the error function,
- an asymmetrical line shape,
- a boxcar (using Fourier Transform)
- Norton-Beer strong (using Fourier Transform)
- arbitrary line shapes provided in ASCII files.

Analytical line shapes

QDOAS can calculate the Gaussian, Lorentzian, Voigt, assymetrical and error function line shapes for different values of their parameters. When one of these analytical line shapes is used, QDOAS can fit its parameters during the wavelength calibration procedure (see section 3.3, page 29).

In order to make the convolution algorithm faster, analytical slit functions are pre-calculated on a suitable wavelength grid (determined in order to

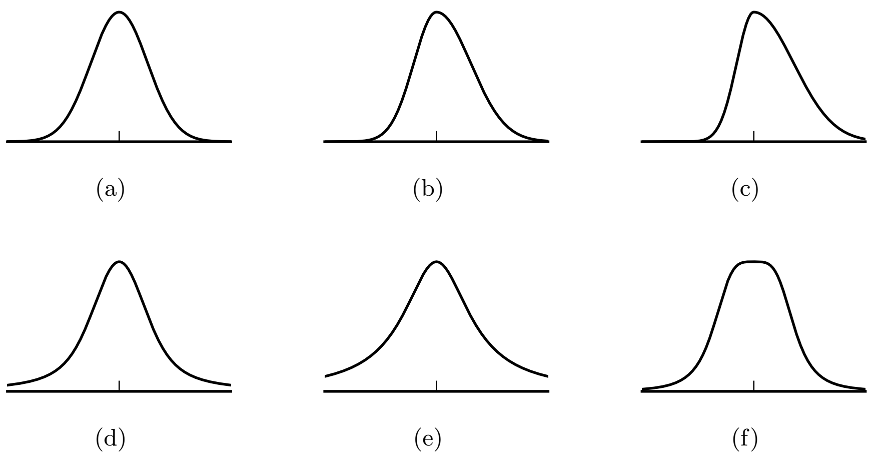


Figure 3.7.: QDOAS can use different line shapes to describe the instrumental slit function. The plots above illustrate the Gaussian (a), asymmetrical (b, c), Voigt (d) and Lorentzian (e, f) profile shapes. The asymmetry factor in (b) is 0.2, that of line shape (c) is 0.4. The Lorentzian (e) is the standard Lorentzian ($n = 1$) and the Lorentzian in (f) has $n = 2$.

have 18 pixels at FWHM) and then interpolated on the grid of the spectrum. For Gaussian and error function line shapes, a Fast Fourier Transform (FFT) algorithm is used whenever possible to speed up the calculation (e.g. within the wavelength calibration procedure).

Gaussian

The standard expression used to approximate instrumental slit functions is the Gaussian function (see figure 3.7(a)). The Gaussian is the exact line shape in the diffraction limit, i.e. in the case of an infinitely thin entrance slit. The normalized Gaussian is given by

$$G_\sigma(x) = \frac{1}{a\sqrt{\pi}} \exp\left(-\frac{x^2}{a^2}\right) , \tag{3.36}$$

where a depends on the Gaussian width at half-maximum σ as follows:

$$\sigma = 2\sqrt{\ln 2}a\,. \tag{3.37}$$

Error function

For a large entrance slit, the slit function can be approximated by the convolution of a boxcar and a Gaussian function. The resulting slit function is given by

$$E_a(x) = \frac{1}{4\Delta}\left(\operatorname{erf}\left(\frac{x+\Delta}{a}\right) - \operatorname{erf}\left(\frac{x-\Delta}{a}\right)\right) , \tag{3.38}$$

where Δ is half the pixel size and $\operatorname{erf}(x)$ is the error function, defined by

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-t^2)\mathrm{d}t\,. \tag{3.39}$$

2n-Lorentzian This line shape is a generalization of the well-known Lorentzian function ($n = 1$, see figure 3.7(e)). It is useful to approximate slit functions with a shape significantly different from the Gaussian one. Low order $2n$-Lorentz can mimic line shapes with large wings (typically the standard Lorentzian profile), or line shapes having a flat top (for higher values of n, see figure 3.7(f)). The generic expression for this function is

$$L_{2n}(x) = \frac{\sigma^{2n}}{x^{2n} + \sigma^{2n}}, \tag{3.40}$$

where σ is the half-width at half maximum.

Voigt profile The Voigt profile function (see figure 3.7(d)) is the convolution of a Gaussian and a Lorentzian function. This function is used in a wide range of contexts, and the optimization of its computation has received much attention. The Voigt profile is usually expressed as

$$K_(x, y) = \frac{y}{\pi} \int_{-\infty}^{\infty} \frac{\exp(-t^2)}{(x-t)^2 + y^2} \mathrm{d}t\,, \tag{3.41}$$

where x is the distance from the line center in units of Gaussian half-widths and y is the ratio of the Gaussian to the Lorentzian half-width. Numerous ways have been proposed to compute the Voigt function. A rather efficient algorithm is described by Kuntz [13].

Asymmetrical line shape To handle asymmetrical line shapes, QDOAS can fit an asymmetry factor in addition to the FWHM. The line shape used is a modified version of the Gaussian line shape (3.36)

$$G'(x) = \frac{1}{a\sqrt{\pi}} \exp\left(-\frac{x^2}{a^2(1 + \mathrm{sign}(x)b)^2}\right), \tag{3.42}$$

where, in addition to the FWHM σ, the asymmetry factor b is now fitted as well. For a value of $b = 0$, it reduces to the ordinary Gaussian line shape. Figure 3.7(b) illustrates the line shape with an asymmetry factor of $b = 0.2$ and 3.7(c) gives an illustration for $b = 0.4$.

User-defined line shape An alternative to fit asymmetrical slit functions is to provide a line shape in an ASCII file and fit a different stretch factor (applying on the wavelength grid of the line shape) for each side of the line shape. In this specific case, the output of the two parameters (SFP1 and SFP2) has to be merged in a three columns file (the first column is the final wavelength calibration) before being used as “Stretch on wavelength” file in the **Convolution tool**.

Lookup tables of slit functions are also accepted. This means that a line shape is provided for different wavelengths. For a specific wavelength, a line shape is first calculated by linear 2D-interpolation in the lookup table and the fitted stretch factors are then applied to the line shape wavelength grid before convolution.

Wavelength dependency QDOAS supports convolution with wavelength-dependent slit functions:

- ◇ Slit function files provided by the user may contain multiple columns describing the shape of the slit function at various wavelengths. The first line of the file should list the wavelengths for which the slit function is provided. QDOAS will then generate a lookup table from the provided slit functions, and calculate the slit function at intermediate wavelength values using linear interpolation.
- ◇ For analytical line shapes, the user can provide a two-column ASCII file containing the wavelengths and corresponding values of the parameters for each requested parameter (for example, the Gaussian width and the boxcar width for the error function). Files with the correct parameter calibration can be saved from the SFP plots obtained after the wavelength calibration procedure.

For more details on how to compute such a convolution using QDOAS, see section 6.1, page 91.

Correction for the Solar I_0-effect

The I_0-effect is due to the difference between cross sections measured in the laboratory with a smooth light source and the atmospheric absorption measured by an instrument of lower resolution with a structured solar light source [1]. As described in equation (3.2), the DOAS technique attempts to isolate the atmospheric absorptions by calculating the ratio of a reference spectrum I_0 and a measured spectrum I. However, because the two spectra in this ratio have been filtered by the instrument function before the calculation of the ratio, complete removal of the Fraunhofer structure is not possible:

If the I_0-effect is not accounted for, the cross sections S used in the DOAS retrieval are laboratory cross sections S_0 convolved with the instrumental slit function F:

$$S(\lambda) = (F * S_0)(\lambda) = \int S_0(\lambda')F(\lambda - \lambda')\mathrm{d}\lambda' . \tag{3.43}$$

The intensities measured by the spectrometer can be defined as

$$I_0^{\text{meas}}(\lambda) = (F * I_0)(\lambda) , \tag{3.44}$$

$$I^{\text{meas}}(\lambda) = (F * I)(\lambda) = (F * I_0 \exp(-S_0 \cdot c))(\lambda) . \tag{3.45}$$

Taking into account the instrumental function F, equation (3.2) becomes:

$$\tau = \ln \frac{I_0^{\text{meas}}(\lambda)}{I^{\text{meas}}(\lambda)} = \ln \frac{(F * I_0)(\lambda)}{(F * I_0 \exp(-S_0 \cdot c))(\lambda)} \tag{3.46}$$

$$\simeq \ln \frac{1}{(F * \exp(-S_0 \cdot c))(\lambda)} \tag{3.47}$$

$$\simeq (F * S_0)(\lambda) \cdot c . \tag{3.48}$$

Thus, the fitting of convolved cross sections to the optical depth measured by a low resolving instrument relies on two approximations:

- ◇ variations in I_0 at a scale below the resolution of the instrument function F can be ignored, i.e. $(F * I_0) \simeq I_0$,
- ◇ the absorber is optically thin ($\tau \ll 1$), so a first order approximation of the exponential and the logarithm in (3.47) is accurate.

For most of the atmospheric absorbers the I_0-effect is negligible but in some cases, the approximations used in equations (3.47) and (3.48) break down. This is particularly the case for strong atmospheric absorbers like O_3.

This effect may be dealt with to a good approximation by correcting the laboratory cross sections with the solar Fraunhofer spectrum: for a particular absorber, a highly resolved solar spectrum $I_0(\lambda)$ and an absorption spectrum $I(\lambda)$ calculated with a known slant column c are both convolved with the instrument slit function

$$I_0^*(\lambda) = (F * I_0)(\lambda)\,, \tag{3.49}$$

$$I^*(\lambda) = (F * I_0 \exp(-S_0 \cdot c))(\lambda)\,. \tag{3.50}$$

The I_0-corrected cross section is then

$$S^*(\lambda, c) = -\ln\left(\frac{I^*(\lambda)}{I_0(\lambda)}\right)\,. \tag{3.51}$$

The I_0-corrected cross section derived in this manner perfectly matches the absorptions in the measured atmospheric spectrum provided that the SCD used for the calculation is equal to the true atmospheric SCD. However, this is not a critical point and the I_0 corrected cross sections can be used for a large range of atmospheric slant column densities [27].

Deconvolution The QDOAS convolution tool implements a de-convolution option. In this case, the convolution is performed using an effective slit function obtained after Fourier transform manipulation of specified convolution and de-convolution functions. The effective slit function is calculated as follows:

$$S_{\text{eff}} = \mathfrak{I}^{-1}\left[\frac{\mathfrak{I}(S_1)}{\mathfrak{I}(S_2)}\right]\,, \tag{3.52}$$

$\mathfrak{I}$ represents the Fourier transform, and S_1 and S_2 are respectively the convolution and de-convolution slit functions. Great care is taken in the algorithm to avoid noise-corruption effects when taking the ratio of the Fourier transforms.

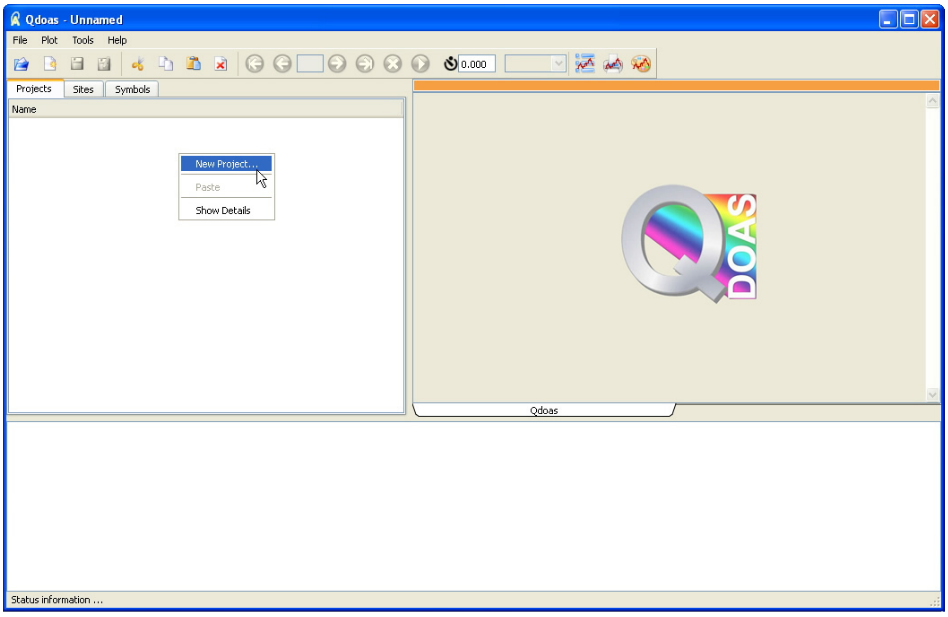
4 Quick start

This chapter guides you step by step towards the complete configuration of a project using a predefined configuration provided with the package (setup for NO_2 retrieval from ground-based MAXDOAS measurements). The retrieval settings are those recommended during the CINDI intercomparison campaign (see Roscoe et al. [21]).

4.1 Creating a project to browse spectra

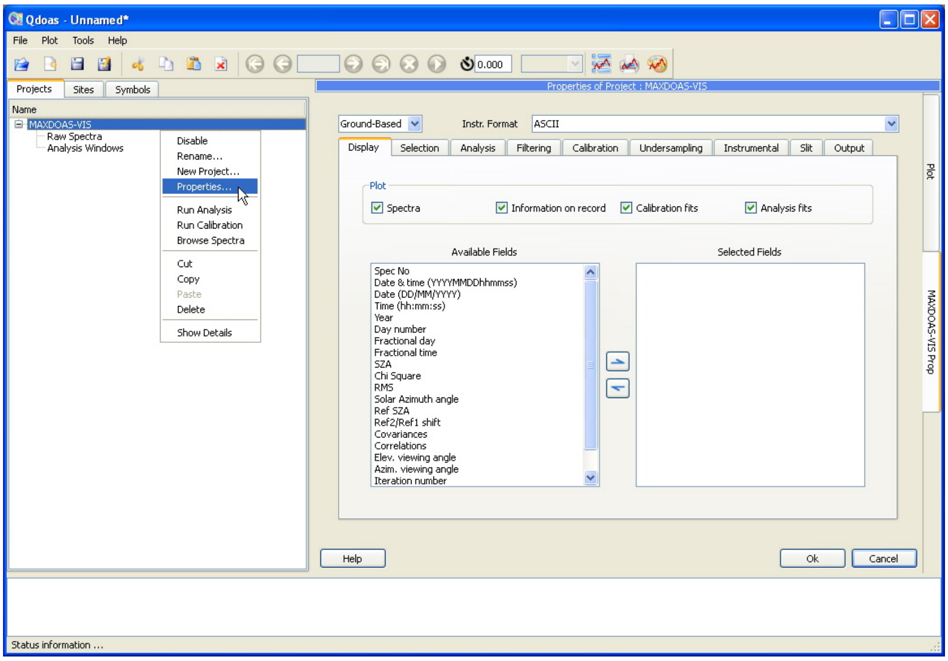
Creating a New Project

When QDOAS starts on an empty application, the user interface looks like :

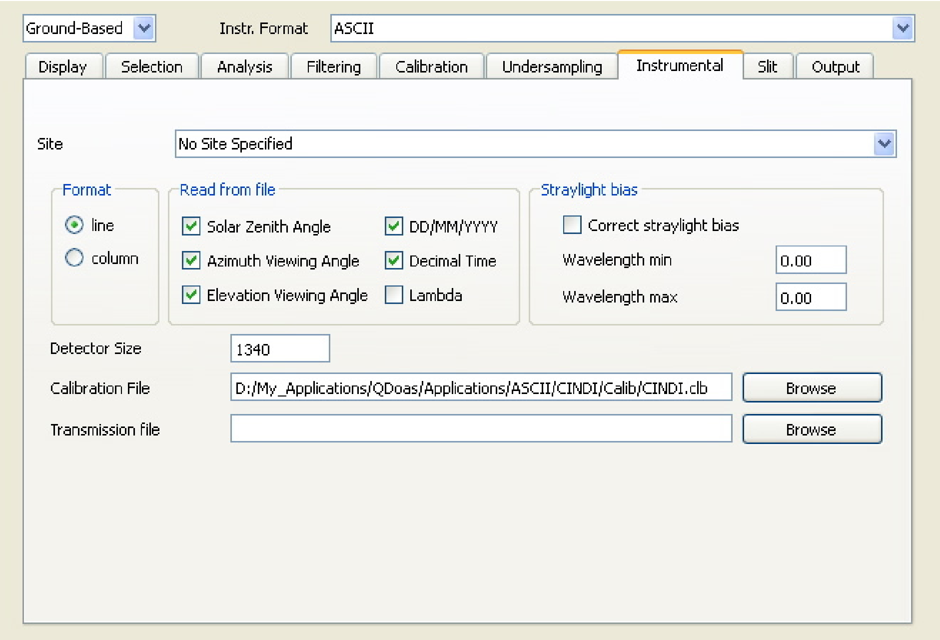


From the upper-left panel, right-click the **New Project** option, and give it a name, for example MAXDOAS-VIS as the purpose of the application here is to retrieve NO_2 from MAXDOAS measurements in the visible region.

Project properties



From the MAXDOAS-VIS tree node, right-click **Properties** to open the **Properties** dialog box on the upper-right panel. Switch to the **"Instrumental"** page to complete information on the format of the files to read. The default file format (**Ground-based, ASCII**) is correct for the example :

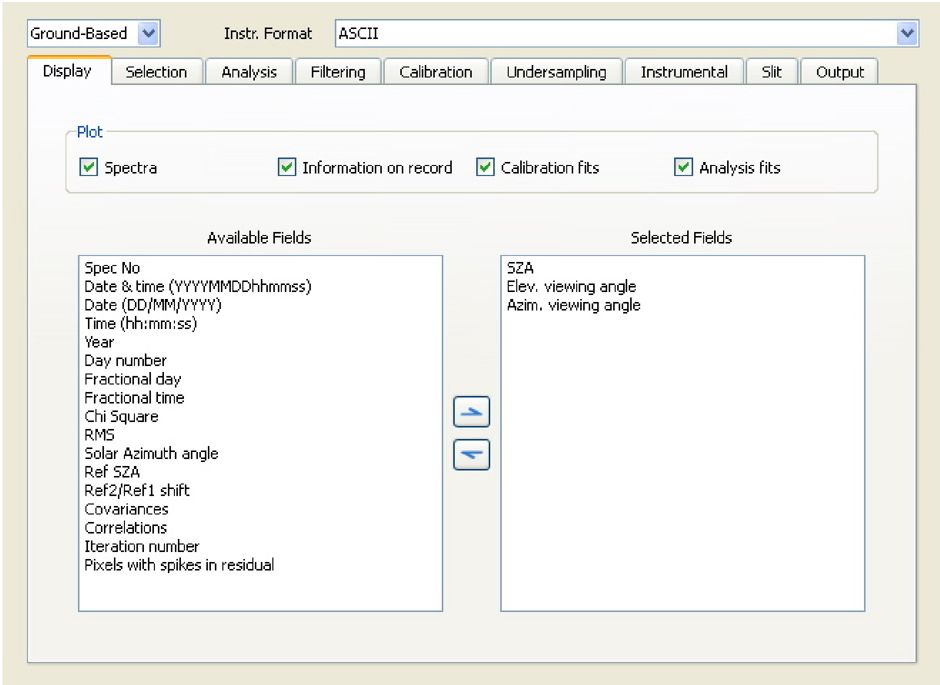


The detector size has to be specified. The files in the example contain one record per line and the following information are given in the expected order :

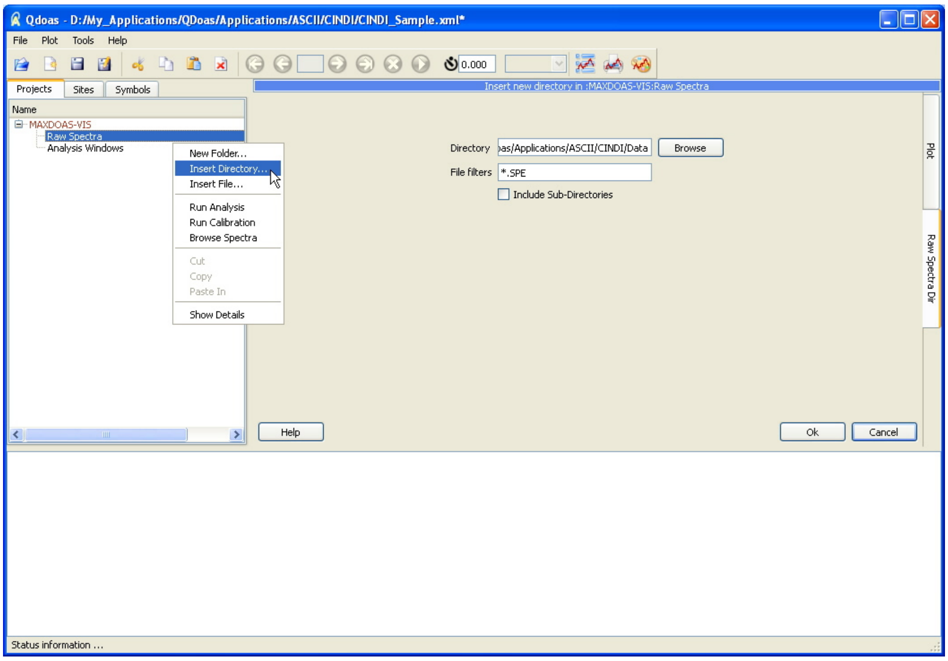
- ◇ Solar Zenith Angle
- ◇ Azimuth Viewing Angle
- ◇ Elevation Viewing Angle
- ◇ Date in the DD/MM/YYYY (day/month/year) format
- ◇ Fractional time

The wavelength calibration is provided in a separate file.

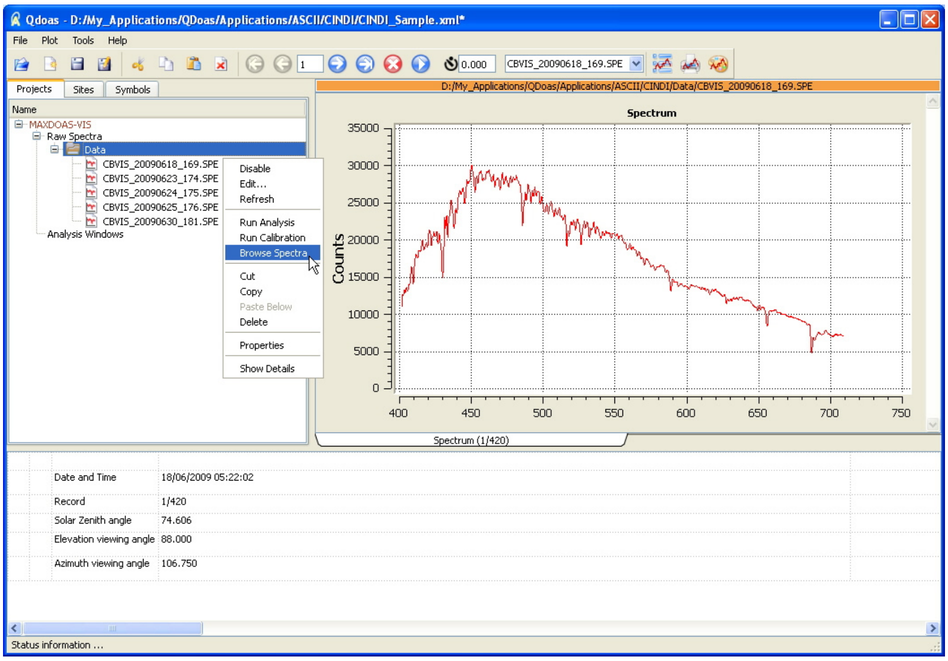
Switch back to the **"Display"** page to select information you want to see when browsing spectra and click ok to save **Projects properties** :



Inserting Files To insert files under the new project, right-click **Insert File** or **Insert Directory** from the **Raw Spectra** node. We prefer to select the directory :



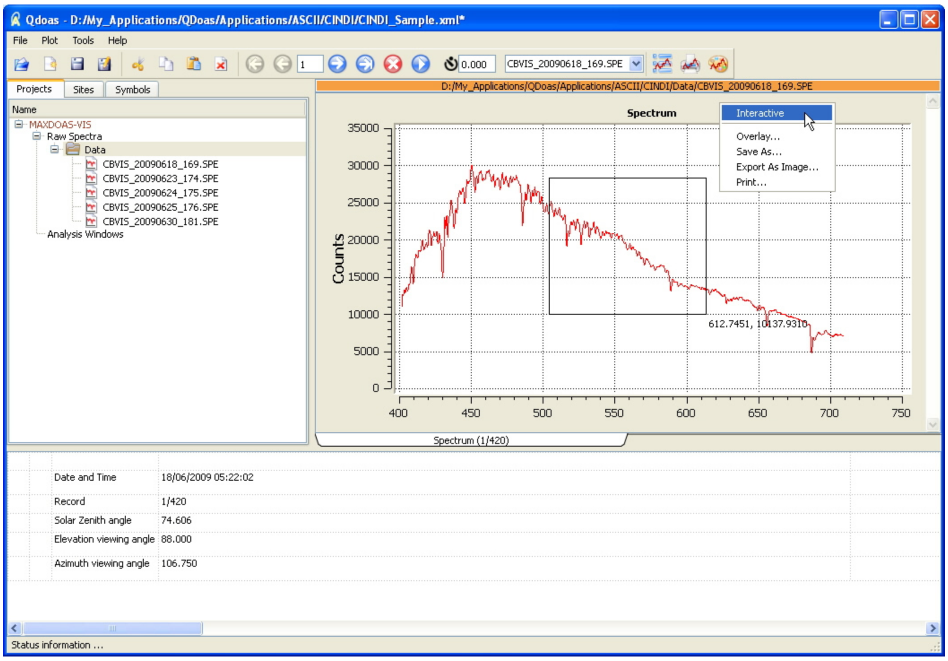
Browsing Files Right-click the **Browse Spectra** option from the **Data directory** name to browse spectra :



Buttons of the toolbar allow moving from one record to the other but also to switch to another file of the directory (possible if the **Browse spectra** option has been clicked from the root directory and not from a file).

Handling Graphs

Zoom is possible by right-clicking the **Interactive** option from the **plot title** :



Other options such as export the plot in ASCII (**Save As**) or PNG (**Save As Image**) are also available. Reference spectra used in the retrieval can be saved in ASCII by this way.

Saving Your Work

Be sure to save your work regularly using **File** → **Save** or **File** → **SaveAs**. The format of configuration files is XML. Always use the **Stop** button (cross in a red circle) in the toolbar before coming back to the project configuration.

4.2 Example : Configuration of a project for NO_2 retrieval

Configuring A Project For Spectra Analysis

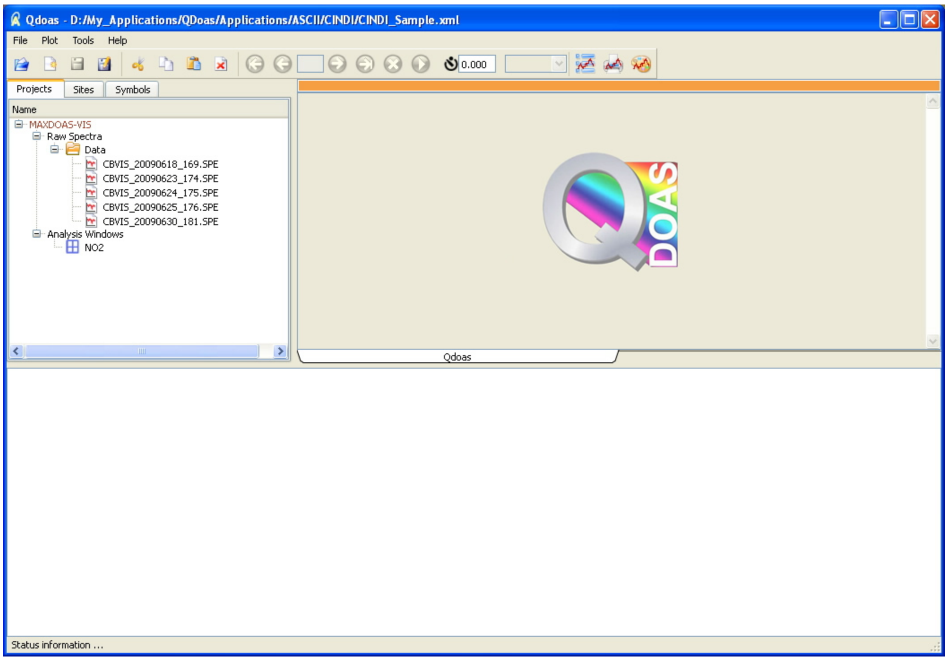
The configuration of a project requires the following steps :

- define all symbols related to the cross-sections files that will be used in the analysis;
- call back the **Projects properties** dialog box to parameterise the wavelength calibration procedure and to setup analysis options independent of the spectral window (fitting method, unit for shifts);
- create an **'Analysis Window'** item in the **Projects** tree for each spectral window to process, and parameterise it.

These steps are described through the example file **CINDI_Sample.xml** provided with the package.

Description of CINDI_Sample.xml

The file **CINDI_Sample.xml** contains the configuration of a project for NO_2 retrieval. Before using the file, you may change the paths according to your installation. The fastest way to do it is to edit the file and replace all **D:/My_Applications/QDoas/Applications/ASCII/CINDI** according to your installation. Then, use **Files** → **Open** command from the QDOAS menu bar or the equivalent button in the toolbar to load the application.



Settings For NO_2 Retrieval

Calibration interval : depends on the wavelength range covered by the detector. It should include all spectral windows. In our application, we have selected 405-580 nm. A preliminary calibration has been previously measured in laboratory and already improved with the wavelength calibration procedure of QDOAS (see section 3.3)

Spectral window : 425-490 nm;

Main Cross-sections :

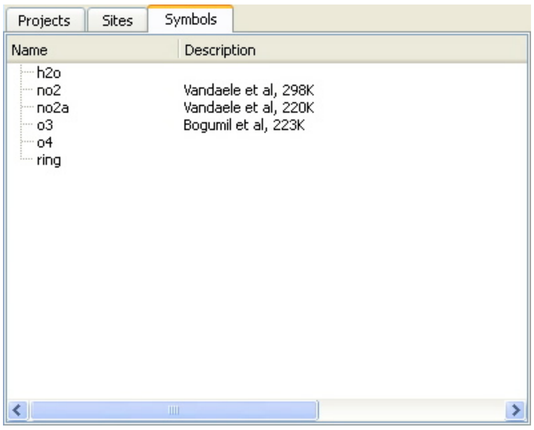
Source	Files

O_3	Bogumil et al. [4], 223 K	o3_223K_Bogumil.xs
NO_2	Vandaele et al. [26], 298 K et 220 K	no2_298K_vanDaele.xs no2a_220K_vanDaele.xs
O_4	Hermans et al.	o4_Hermans_web.xs
H_2O	From HITRAN data base	h2o_hitran.xs
Ring	Ratio of the rotational raman spectrum by the solar one, both convolved at the resolution of the instrument with the **Convolve Ring** option.	Ring_NDSC2003.xs

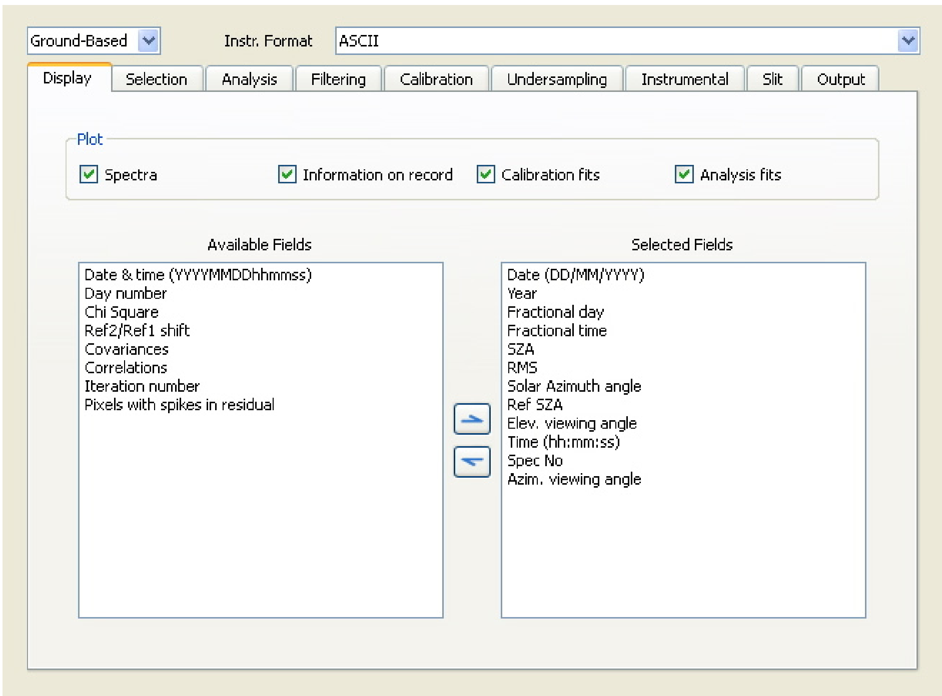
The cross sections are those recommended during the CINDI intercomparison campaign (see Roscoe et al. [21]).

Defining Symbols

The first thing to do is to define the cross-sections symbols according to the files names (see table above) : O3, NO2, NO2a, O4, H2O, Ring (the case is not important). A description can be added. QDOAS needs these symbols for internal use.



Projects Properties

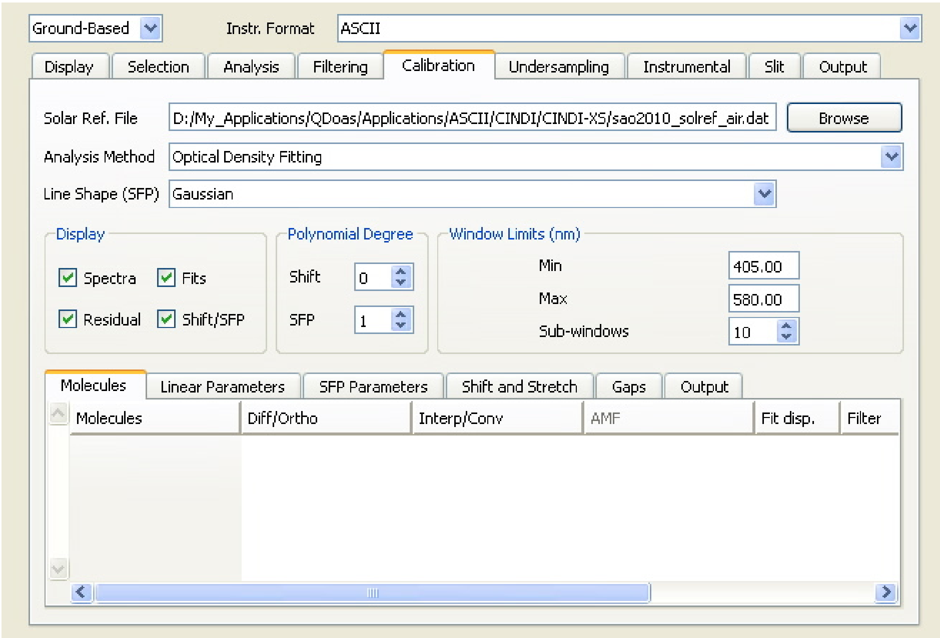


Go back to the **Projects tree** and right-click the **Properties** command from the MAXDOAS-VIS node to open the **Projects properties** dialog box. The **Display** tab page appears first. Some additional fields related to the analysis can be selected such as the **RMS** or the reference spectrum SZA (**Ref SZA**) :

Calibration Parameterisation

The wavelength calibration interval, specified by the **Window limits** fields, is subdivided in a number of equally spaced sub-windows. In each of these intervals, the shift and the **Slit Function Parameters (SFPs)** are fitted using a NLLS fitting procedure where a high-resolution solar atlas spectrum, degraded to the resolution of the instrument, is adjusted to the control spectrum. The shift values determined in all sub-windows are then used to reconstruct an accurate wavelength registration. Similarly, the wavelength dependent slit function is determined by polynomial fitting through individual SFP values. The resulting information is subsequently used in the programme, e.g. to convolve cross-sections.

In the example, the **Calibration** page is configured as follows :



Solar ref. file — use this button to locate the solar spectrum (in this case, a high-resolution one because the slit function is fitted; otherwise, a solar spectrum previously convolved at the resolution of the instrument;

Analysis Method — the fitting method used for wavelength calibration can be different from the one selected for spectra evaluation in the **Analysis tab page**;

Line Shape (SFP) — this button is checked in order to fit the resolution of the slit function; in this case, a Gaussian line shape is selected;

Display — check boxes in the frame to display the indicated graphs;

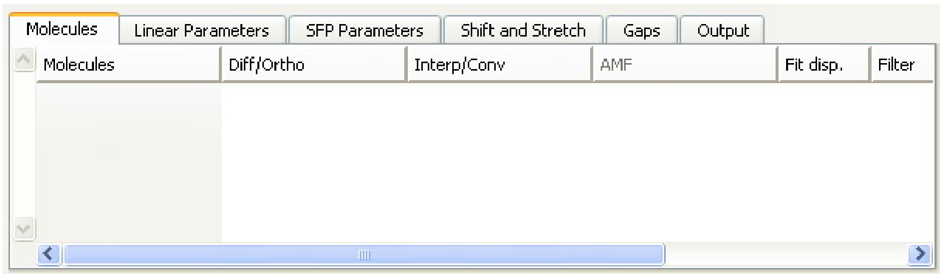
Polynomial degree the degree of the polynomial used in the final determination of the wavelength registration (shift) and the wavelength-dependent slit function (SFP);

Window limits the complete calibration interval;

Sub windows the number of calibration sub intervals;

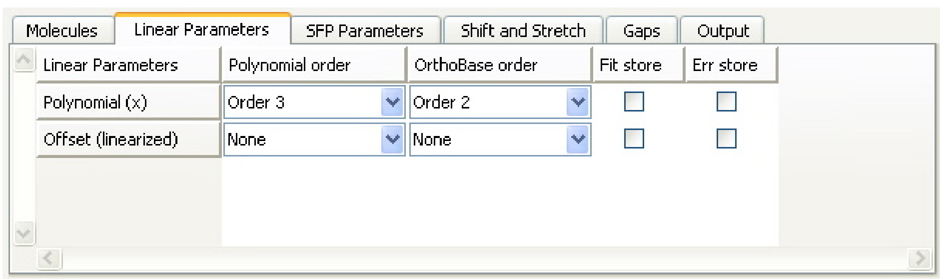
Options are also distributed in several pages. The four following ones are the most important for the wavelength calibration :

Molecules



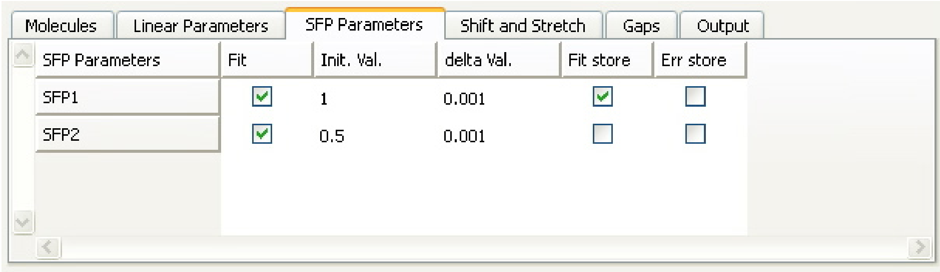
In these pages, we can specify absorption cross-sections to include in the fitting procedure (absorbing correcting terms). For best results (and given the usually limited information content over individual sub-windows), it is recommended to limit the number of parameters. In our example, we do not include cross-sections in the fit. In the UV region, it is sometimes necessary to add Ring and ozone. In this case, proceed as follows. First try and fit the cross-section term(s) freely, looking at the retrieved values in each interval. The usual situation is that spectral signatures are such that the information content largely differs from one interval to another. Look at results in the 'best windows', and fix the absorber amount to a mean value derived from these particular intervals. Although this way of working implicitly assumes that the molecule absorption is constant over the whole calibration interval (which is not necessarily true), this is usually the best compromise.

Linear Parameters



The smooth component of the differential absorbance is fitted by a polynomial. The degree of the polynomial may be adjusted according to the size of sub-windows and the quality of the fit. The orthogonal base is used to calculate differential cross-sections (not present in this example).

SFP Parameters

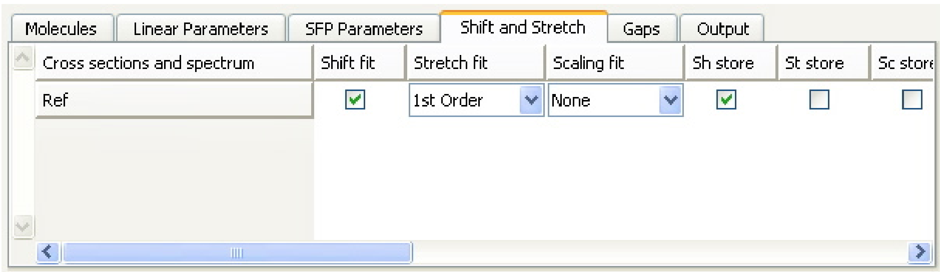


SFPs are defined in this page.

In the example, the selected line shape is a gaussian. The parameter to fit is the FWHM which is represented by SFP1. The other parameter SFP 2 is ignored for this type of line shape even though it is checked.

Again in this case, a better accuracy is obtained when limiting the number of free parameters according to the information content of spectra. For line shapes involving two parameters such as the error function, which is the convolution between a Gaussian (SFP 1) and a boxcar (SFP 2), it is recommended to fix the value of one (or several) parameters in order to optimize the algorithm. Several iterations may be needed.

Shift and Stretch

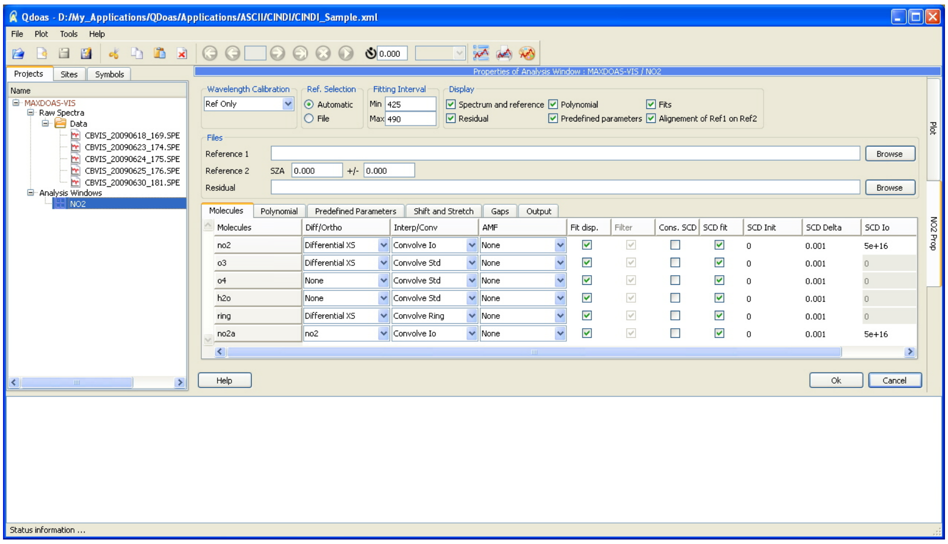


Shift (and stretch) can be applied either on the control spectrum (symbol **Spectrum** in this case) or on the solar spectrum (symbol **Ref** in this case). In order to avoid interpolating the control spectrum, we recommend to shift the high-resolution solar spectrum instead of the control one (see equation 3.36, section 3.3). *Note that, in this case, the cross-section(s) defined in the* ***Molecules*** *page must be shifted together with the solar spectrum.*

Right-click the **Insert** or **Modify** option to add a new item in the list or to modify a selection.

Analysis Window Properties

To create a 'new Analysis Windows' item in the **Projects** tree, select the predefined **'Analysis Windows'** node (or an existing analysis window to add the new one after) and right-click the **"New Analysis Windows..."** command. Give it a name and right-click the properties option from the new analysis windows item to have the following dialog box.



Analysis Windows Properties

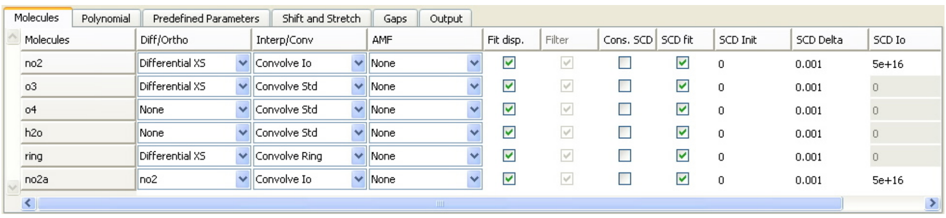
The recommended **fitting interval** for NO_2 in the visible region is 425-490 nm.

We have checked the option **Automatic** in the **Reference selection** frame. This means that a reference spectrum is automatically selected every day from the current data file. If both values are not zero, the spectrum will be different for each twilight. In the example, the spectrum measured at the minimum solar zenith angle of the day is selected.

The wavelength calibration is applied on the reference spectrum (here, **Reference 2**). If a file had also been specified in **Reference 1**, it would have had the priority for the wavelength calibration and the shift between both **Reference 1** and **Reference 2** would have been determined in order align cross-sections on **Reference 2** before the analysis of spectra.

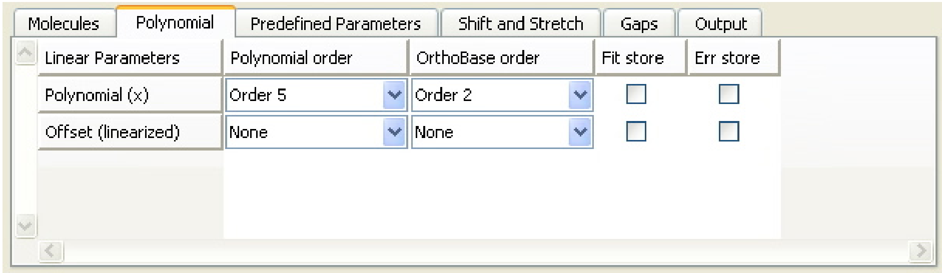
The structure of the **Analysis Windows Properties** pages is very similar to the one used for the calibration (and already defined above).

Molecules



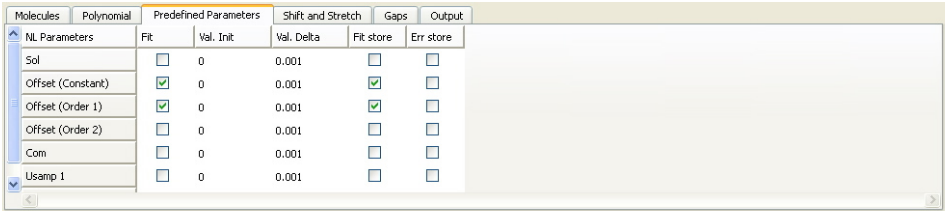
This page contains the absorption cross-sections needed for NO_2 retrieval (see the list, page 49). Differential cross-sections are generated by orthogonalisation to an orthogonal base defined in the **Polynomial** page. In order to avoid correlation between cross-sections (e.g. NO2 and NO2a) of similar shapes (e.g. when treating temperature effects by including two or several cross-sections of the same species), these cross-sections can be orthogonalised with respect to each other. High-resolution cross-sections are convolved using the information on the calibration and the slit function retrieved from the wavelength calibration procedure. NO_2 cross sections are convolved using I_0 correction (see page 49); a typical concentration of $5e16$ is used.

Polynomial



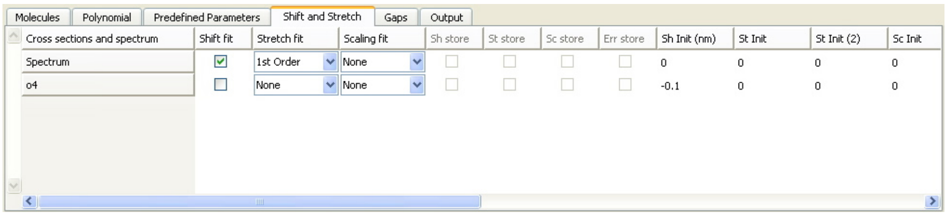
In this page, the polynomial used for fitting the smooth part of the absorbance is defined. An orthogonal base is built with the main components of the polynomial in order to calculate differential cross-sections.

Predefined Parameters



Predefined parameters page contains reserved symbols not defined by the user (for example, offset).

Shift and Stretch



Shift and stretch (1st order) applied to the spectrum are fitted here. In this page, a shift value is also applied (not fitted) to the O_4 cross-section. Note that several cross-sections can be grouped together. Right-click the **Insert** or **Modify** option to add a new item or to modify the selection.

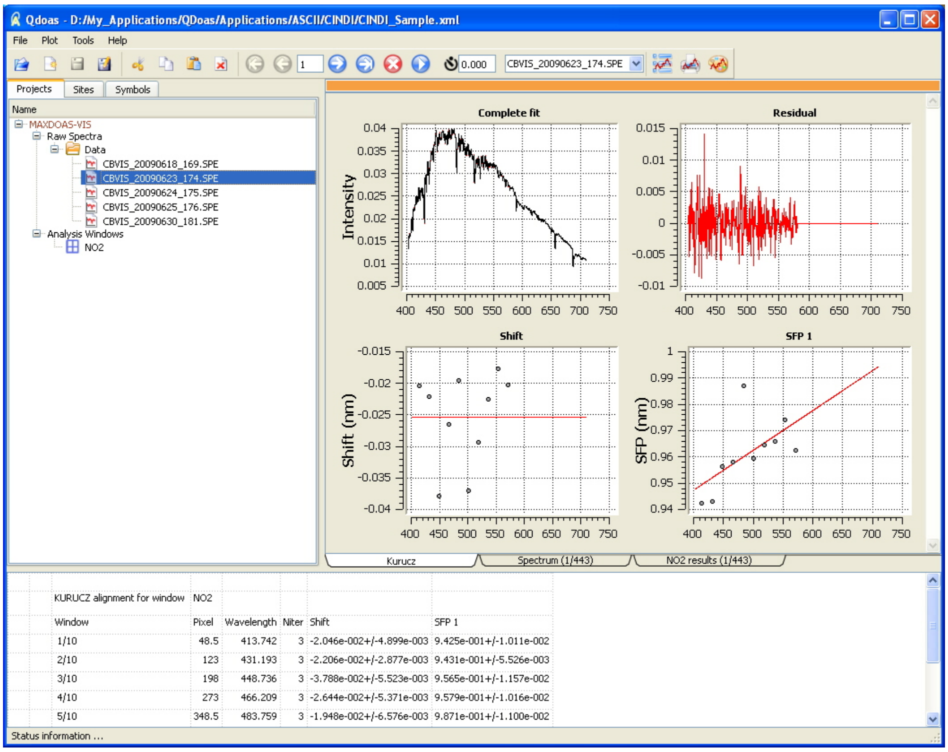
Running Analysis

To analyse a spectra file, select it in the **Projects** tree and right-click the **Run Analysis** command.

Note if you right-click **Run Analysis** command from a parent node (**Data** folder or **Raw Spectra**), the command will be applied on all spectra files defined in the selected project.

The analysis of a record is processed in one shot (even if several analysis windows are defined) and the results of the fit are plotted in different pages. The panel at the bottom of the user interface provides information related to the type of plot currently displayed.

Kurucz page



This page appears in front of the others when the first spectrum is processed. It contains the plots resulting from the wavelength calibration procedure :

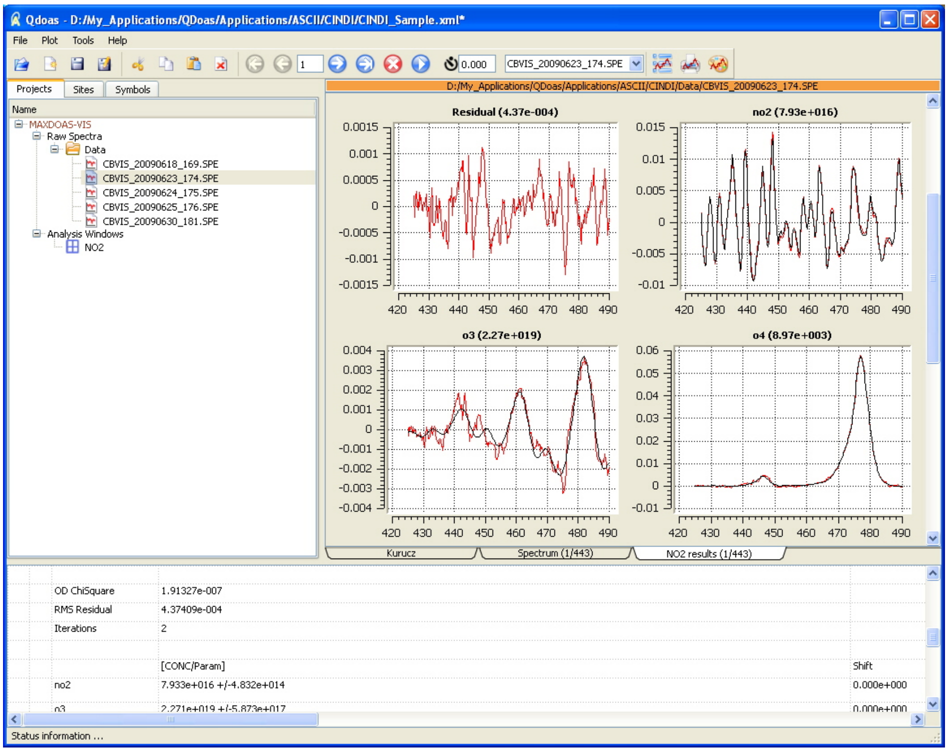
- ◇ **Complete fit** : the selected reference spectrum (in red) is compared to the high-resolution solar spectrum convolved with the calculated resolution of the instrument (in black); if you zoom in the plot, you can check if structures match. The wavelength calibration is the new calculated one. It can be saved by right-clicking on the **Save As** option in order to be associated to another reference spectrum.
- ◇ **Residual** : the normalised residual;
- ◇ **Shift** : the calibration error;
- ◇ **SFP 1** : the variation of the FWHM of the Gaussian with the wavelength.

The red line represents the polynomial that fits individual points calculated in each sub-windows (black dots). The whole detector wavelength range is covered. All this information can be saved in a file using the **Save As** option. A file with four columns is created (new wavelength calibration, polynomial fitting the individual points, wavelength at the centre of each sub-window and the calculated value for this sub-window. Columns 3 and 4 are completed with "0" values in order to have the number of points of the detector.

Spectrum page

The currently analyzed spectrum is displayed in this page. The panel at the bottom of the user interface provides information on the record according to the selection made in the **Selection page** of **Projects Properties**.

NO2 page



The information on the calibration and the resolution of the instrument retrieved from the wavelength calibration procedure are used to convolve cross-sections on the correct grid. The cross-sections respectively measured (the optical thickness after removal of the contribution of all molecules excepted one) and calculated (the remaining cross-section multiplied by the calculated slant column density) are displayed.

Output

To save the results, stop the current analysis using the red button in the toolbar, open **Projects Properties**, and go to the **Output** page. In order to save results, check “Analysis” and choose the location and format of the output file(-s). Check “Calibration” to save reference spectrum calibration results as well. Still on the **Output** page, you may select various other fields to be saved to the output file. Next, go to the **Analysis Window Properties** to select molecule densities and other analysis results that should be saved to output. To select which calibration data should be saved, go to the **Calibration** page of the **Projects Properties** window.

5 Projects and Analysis Windows Properties

This chapter covers :

1. the configuration of projects;
2. the parameterisation of the analysis;
3. the parameterisation of the wavelength calibration.

5.1 Projects properties

The **Projects properties** dialog box resumes the general options to configure the application. These options are divided into the following categories :

Display selection of information to display with spectra;

Selection selection of spectra to browse or to analyse;

Analysis options specific to the analysis (analysis method, interpolation, convergence criterion, ...);

Filtering selection of a filtering method to apply on spectra and absorption cross-sections;

Calibration configuration of the wavelength calibration procedure;

Undersampling selection of a method to calculate undersampling cross-sections and to include them in the fit;

Instrumental options specific to the selected input file format;

Slit definition of a slit function or a method to convolve cross-sections before the analysis using the information generated by the wavelength calibration procedure;

Output selection of the information on the spectra that should be saved in the output file after the analysis.

The creation of a new project always starts with the definition of the measurement type (satellite or ground-based) and the selection of the spectra file format.

Before browsing spectra, options in the **Instrumental page** and in the **Display page** should be checked. Options in the other pages of the **Project properties** concern the analysis of spectra and the configuration of the output. They have to be completed with the creation of cross-sections symbols and the settings in the **Analysis Windows properties** dialog boxes (definition of the spectral interval, specification of the reference spectrum, selection of parameters to include or not in the DOAS fit, . . .).

Display Page

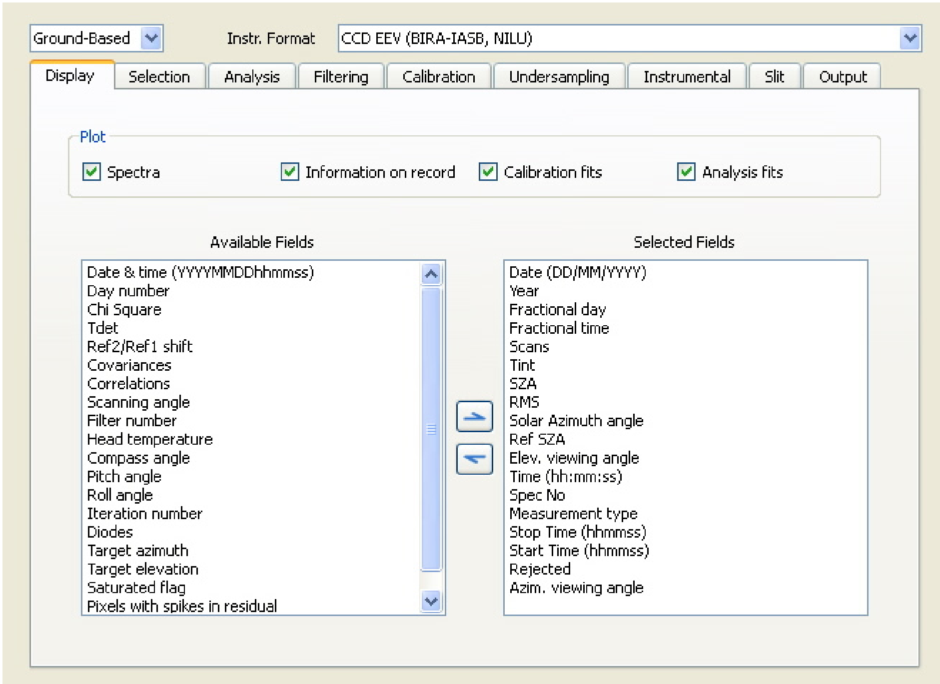


Figure 5.1.: Projects properties : Display page

The analysis of spectra can be performed in a non-stop way. Disabling the plot of spectra and fits during the analysis makes the processing significatively faster although the use of the command line tool **doas_cl** is recommended in this case. If the **Spectra** button is unchecked, the state of the **Data** button has no effect. If the **Calibration fits** button is unchecked, this will disable the display of the calibration plots whatever the state of the buttons in the **Display frame** of the **Calibration page**.

Selection Of Fields To Display

The content of this frame is similar to the one in the **Output** page. Information related to the measurements (e.g. date and time, viewing angles, geolocation coordinates, . . .) can be selected in this page and will be completed with analysis results according to buttons checked in the **Display** frame of the **Analysis windows properties** dialog box. The user-defined instrument or file format determines the list of fields available for display or output. A non-exhaustive list of fields available for ground-based and satellite measurements is given in appendix **B**.

Selection Page

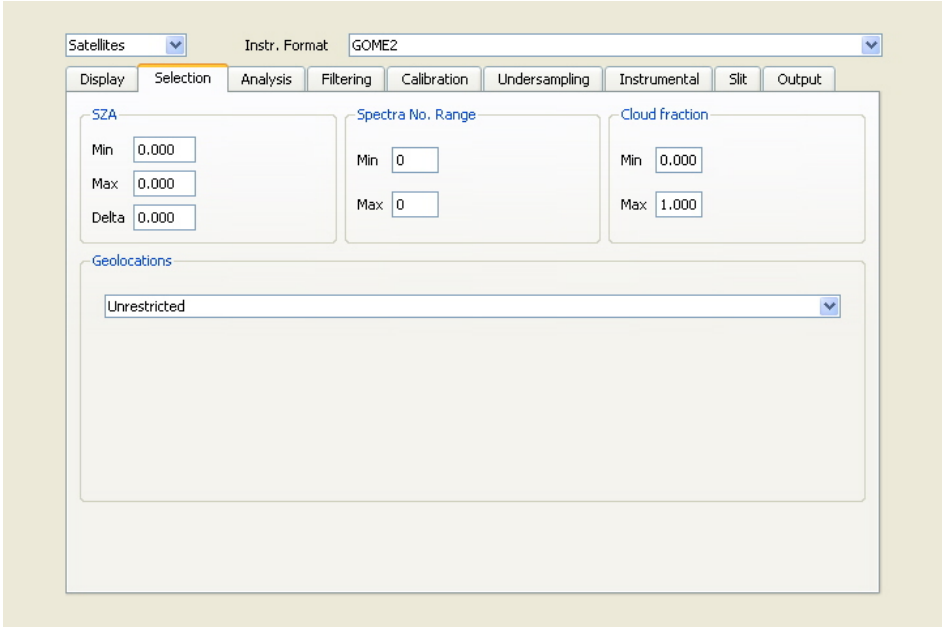


Figure 5.2.: Projects properties : Selection page

Spectra selection

This page is dedicated to the selection of spectra to browse or to analyse. The selection of spectra can be made on :

- **SZA** — specify a range of solar zenith angles and a step in degrees;
- **Spectra No** — specify a range of record numbers;
- **Cloud fractions** — for satellite measurements, specify a range of cloud fraction (0..1). Until now, only the GOME-2 file format includes information on the cloud fraction.
- **Geolocations** — for satellite measurements, selection of pixels based on the geolocation of measurements

To browse or to analyse all spectra of a file without any constrain, keep the fields initialized as shown in the figure above (default options).

Geolocation

Some applications just need satellite overpasses over a list of ground-based stations or above specific regions (satellite validation activities for example). The geolocation frame gives three possibilities to select pixels over specific locations :

- **Circle** — select pixels within a circle whose the radius is given in kilometers and whose the center could be the position of a station defined by its latitude and longitude;
- **Rectangle** — select pixels above a specific region bounded by the limits in longitude and latitude given in degrees (-180..180° or 0..360° for the longitude according to the satellite file format);

Sites select pixels within multiple circles with radius given in kilometers and center position determined by the longitude and the latitude of the observation sites defined in the **Sites tab page** (see the **Output page**, page 72, for the automatic creation of the output file name).

Analysis Page

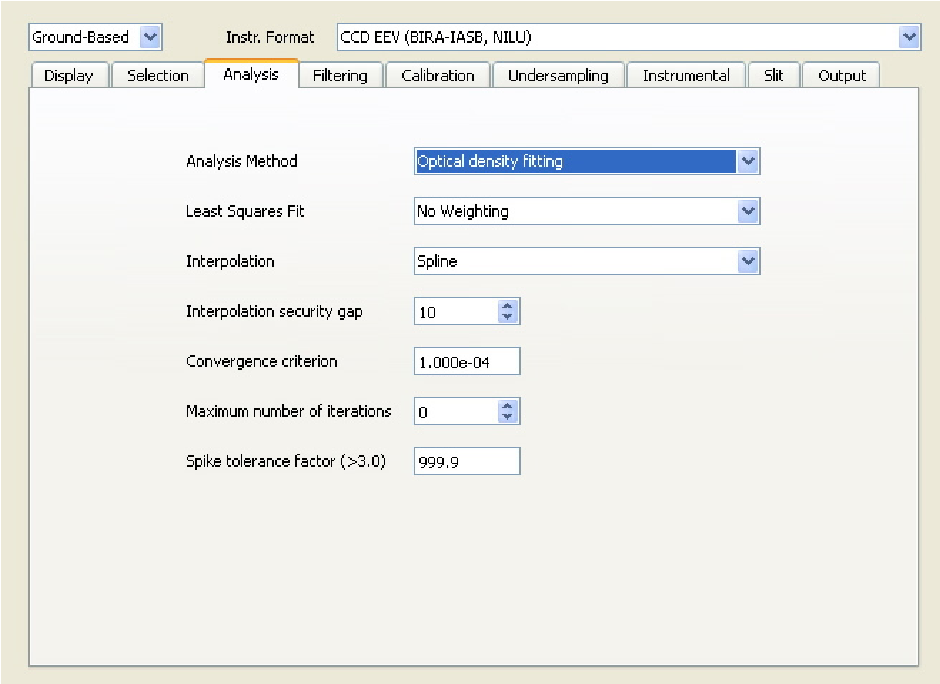


Figure 5.3.: Projects properties : Analysis page

Default options of this page are valid for all applications. Expert users can change them to perform some tests. Further details on the retrieval algorithms can be found in the **Description of Algorithms** chapter.

The Analysis Method Available retrieval method are :

- ◇ Optical density fitting;
- ◇ Intensity fitting (Marquardt-Levenberg+SVD).

These methods differ by the way the Beer-Lambert equation is expressed and resolved. Usually the **Optical density fitting** is preferred to analyze spectra.

Least-Squares Fit The fit can be weighted if instrumental uncertainties on measurements are known.

Interpolation **Linear** and **cubic Spline** interpolations are implemented. **Spline** interpolation is recommended

Interpolation Security Gap Convolution/filtering/interpolation operations could introduce edge effects if cross-sections are strictly defined on the different analysis spectral intervals. In order to avoid that, it is recommended to add some extra pixels on both sides of the final grid. The security gap determines this number of pixels. If the selected filter requires a larger number of additional pixels, the gap is recalculated by QDOAS.

Convergence Criterion

As explained in the description of the Marquardt-Levenberg Algorithm in section 3.2, the NLLS algorithm uses the convergence criterion to determine when it has arrived at a solution.

Usually a value of 1e-3 or 1e-4 is selected for the convergence criterion. For higher values of ϵ, the algorithm will use less iterations, but the accuracy of the results could be affected.

Maximum Number of Iterations

The number of iterations needed to analyze a spectrum is determined by the convergence speed of the Marquardt-Levenberg algorithm for this spectrum. For some tests, it is sometimes useful to limit it. A value of "0" doesn't limit the number of iterations.

Spike Tolerance Factor

QDOAS can try to automatically remove bad data points, such as satellite measurements affected by the South Atlantic Anomaly, from the fit. To do this, QDOAS calculates the average magnitude of the residuals after the fit. If pixels are found with a residual exceeding this average by more than the spike tolerance factor, QDOAS will remove these pixels from the analysis and calculate a new fit. This procedure is applied iteratively until no residuals exceed the average by more than the given tolerance factor. The analysis results contain a list of all pixels that were removed. This feature should be used with caution, as choosing a too low tolerance factor might exclude valid data points from the fit.

Filtering Page

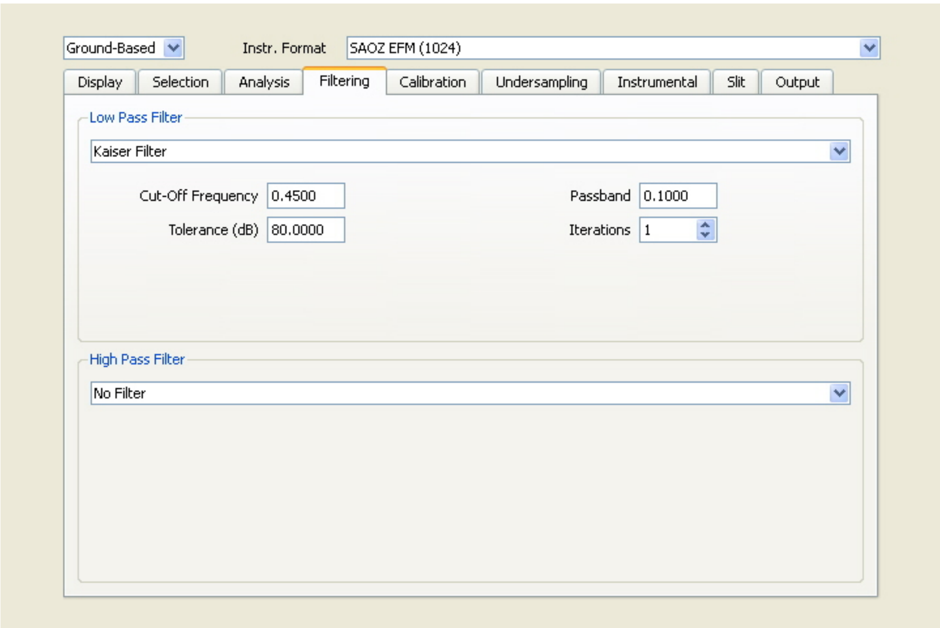


Figure 5.4.: Projects properties : Filtering page

Filtering attenuates components in the spectra with frequencies higher (low-pass filtering) or lower (high-pass filtering) than a given cut-off frequency. This simple method can improve the analysis of noisy spectra but may lead in the other hand to a loss of spectral information and should be used very carefully. Filtering corresponds to a convolution in the pixels domain. The most common filter functions are implemented. Further details can be found in the literature.

Kaiser correction using the algorithm described in Kaiser and Reed [12];

Boxcar convolution with a rectangle function; this filter consists in averaging the spectrum over several spectral points;

Gaussian convolution with a Gaussian function;

Triangular convolution with a triangle function;

Savitzky-Golay this filter uses a least-square linear regression fit of a polynomial of degree k over at least $k + 1$ data points around each point in the spectrum;

Binomial convolution with a filter function formed with the binomial coefficients calculated using the recursive Pascal's triangle algorithm;

Odd-even pixels smoothing obtained by averaging spectra interpolated on odd and even pixels.

According to the selected filter, different fields have to be completed. Select filter type **No Filter** if you want to disable spectra and cross-sections filtering.

Filtering is applied after interpolation of the original spectra or cross-sections on the final grid.

Low-Pass Filtering

Low-pass filtering is applied to the spectra and to the cross-sections. Nevertheless, the filtering of cross-sections could be disabled individually in the **Analysis windows properties** dialog box.

High-Pass Filtering

Cross-sections are filtered by subtracting (optical density fitting) or dividing (intensity fitting) a fitted polynomial or a smooth spectrum calculated by filtering the original cross-sections a high number of times. This can be an alternative to the Gram-Schmidt algorithm to calculate differential cross-sections.

For the moment, high-pass filtering is supported only in optical density fitting mode. It can be applied during the phase of calibration and/or during the analysis of spectra.

Calibration Page

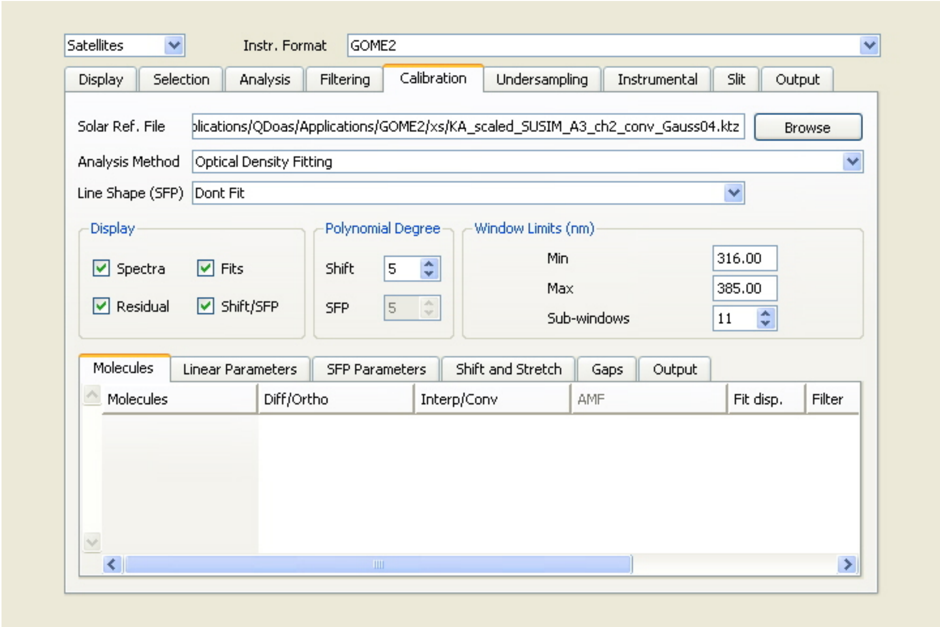


Figure 5.5.: Projects properties : Calibration page

Wavelength Calibration And Slit Function Characterization

The wavelength calibration procedure developed in QDOAS is based on a NLLS fitting approach where the shift between the spectrum to calibrate and a high-resolution solar atlas spectrum degraded to the resolution of the instrument is determined on a series of equally spaced short intervals. The **Analysis Method** (optical density fitting or intensity fitting) can be different from the one selected for the analysis of spectra in the **Analysis page**. The procedure also allows characterising the instrumental slit function, through fitting of user-defined Slit Function Parameters (**SFP**), either the FWHM of a analytical line shape (see the **Analytical line shapes**, page 40) or two different stretch factors applied on the grid of a user-defined function (option **File**). If the slit function is not fitted during the wavelength calibration procedure, the solar spectrum and the instrumental line shape to use for convolutions are defined in the **Slit page**, page 71.

Window Limits

The wavelength interval used for the calibration must be specified in the **Window limits (nm)** frame. It should cover all the spectral analysis windows defined under the **Analysis Windows** node of the projects tree. This calibration interval is divided in a number of equally spaced **sub-windows** and, the shift and the SFPs are fitted using the NLLS approach in each interval.

Polynomial Degree

The shift values determined in all sub-windows are then used to reconstruct an accurate wavelength calibration. Similarly, the wavelength dependent slit function is determined by polynomial fitting through individual SFP values. A different **polynomial degree** can be specified for the shift and for the slit function. The two information (wavelength calibration and variation of the slit function) are subsequently used e.g. to convolve high resolution cross-sections before the analysis of spectra and to build under-sampling cross-sections.

Solar Reference File

There are two cases to consider :

1. the slit function of the instrument is known and there is no need to characterise it once again (**line shape** not fitted). Then the **Solar Ref. File** in this page is disabled; it should be given in the **Slit page** with the instrumental line shape.
2. the slit function of the instrument need to be characterized (selection of a **analytical line shape**); then the **Solar Ref. File** should contain a high-resolution solar spectrum. Because QDOAS uses the Fourier transform in order to make the NLLS algorithm fast enough, a high-resolution solar spectrum sampled on a constant grid is expected.

Fitting Parameters

The wavelength calibration uses the same property sheet as the **Analysis windows properties**. The configuration of these pages is usually limited to the specification of the degree of the polynomial to use in the DOAS equation (different from the polynomial used to build the final grid from the individual values of the shift resulting from the fit as described above), the slit function parameters to fit according to the selection of the line shape and the shift between the spectrum to calibrate and the solar spectrum. But the algorithm can take also atmospheric absorption, Ring effect and offset correction into account.

Display

When the calibration procedure is applied, a page named "Kurucz" appears in the plot area of the program except if the **Calibration fits** button is unchecked in the **Display page**. This page includes four kinds of plot :

Spectra the complete fit between the observed and the calculated spectra;

Fits fit of the Ring effect and/or atmospheric absorptions if any;

Residual the residual of the fit;

Shift/SFP the wavelength dependency of the shift and the slit function parameters over the whole detector.

Undersampling Page

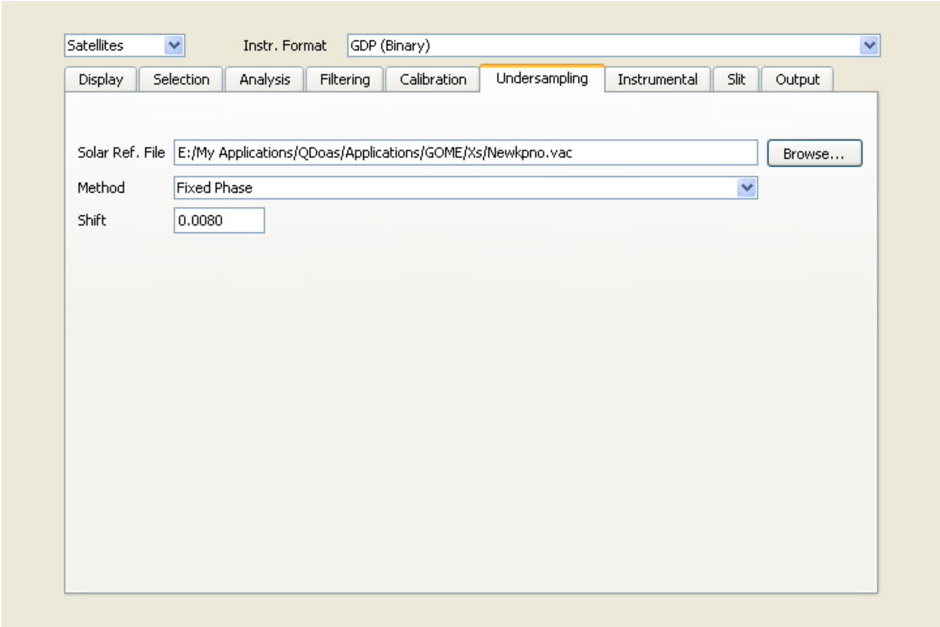


Figure 5.6.: Projects properties : Undersampling page

The undersampling is a well-known problem of GOME onboard the satellite ERS-2. It arises from the poor sampling ratio of the GOME instrument (2 to 3 pixels/FWHM of the resolution of the spectrometer) which results in a lost of spectral information when interpolating earthshine spectra during the DOAS fitting process. The problem can be corrected using ad-hoc cross-sections obtained by simulating the effect from a high-resolution solar reference. Undersampling cross-sections can be pre-calculated using the **The undersampling tool (usamp)** or they can be calculated in real time, just after the wavelength calibration procedure using the corrected grid and the determined slit function.

By default, no undersampling correction is applied.

Method

Different methods for the calculation of the undersampling correction are available.

From file	Undersampling cross-sections are provided in files like usual cross-sections. These files might be created using the **The undersampling tool (usamp)**. The files have to be provided in the **Analysis windows properties** (**Molecules** or **Predefined paremeters** page according to the selected analysis method).
Fixed phase	QDOAS uses the information derived from the calibration procedure to create the undersampling cross-sections, with a fixed value of the shift. The selection of this method is recommended.

Automatic phase The undersampling cross-sections are calculated at each iteration of the analysis procedure, using the fitted value for the shift between the reference and the measured spectra. This method is rather time consuming and only applicable for testing purposes.

Solar ref. file

In **Fixed phase** and **Automatic phase**, undersampling cross-sections are calculated from a high resolution solar spectrum convolved on an oversampled and an undersampled grid with the instrument slit function (according to **calibration options**, the slit function characterized by the calibration procedure or a slit function provided by the user in the **slit page** of **Projects properties**).

Shift

The **Shift** field operates only in **Fixed phase** method.

Instrumental Page

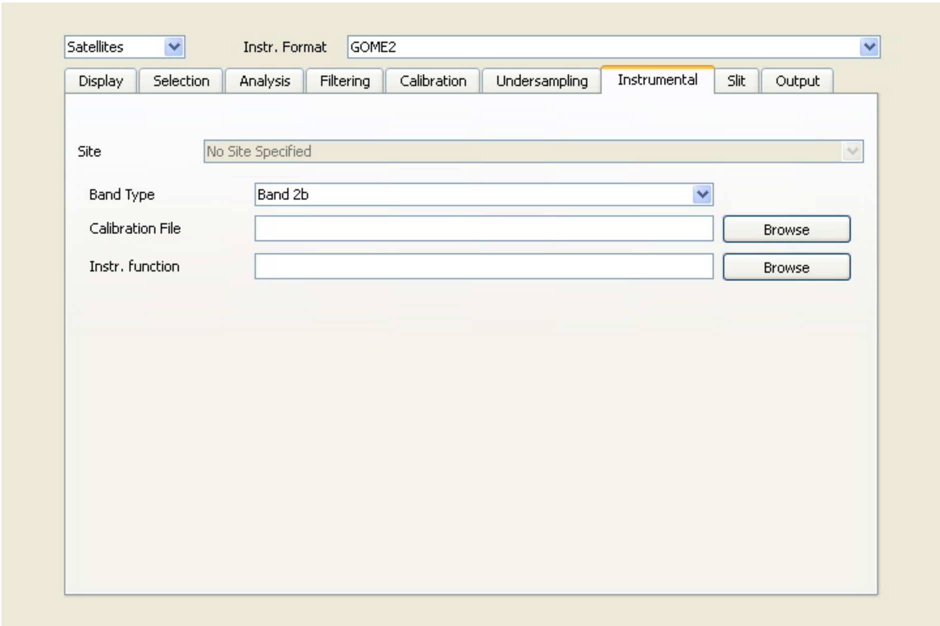


Figure 5.7.: Projects properties : Instrumental page

Except the observation **Site**, the **Calibration File** and the **Transmission file**), the fields that appear in this page depend strictly on the format of spectra files to process.

Calibration File And Instrumental Corrections

A preliminary wavelength calibration is necessary to browse spectra. If the wavelength calibration is coded in the spectra file, it is recommended to use it by keeping the field **Calibration File** empty.

For the analysis of spectra, the wavelength calibration of the reference spectrum always has the priority over the spectra ones. It is important to select this file very carefully mainly when browsing spectra to save a new reference spectrum.

Some instrumental corrections can be applied on spectra. For example, a transmission function previously determined in laboratory with calibrated sources can be specified in the **Transmission file** field. A two columns ASCII file is expected (wavelength calibration and transmission function) and spectra will be divided by this curve before the wavelength calibration procedure.

Dark current correction is also possible according to the file format. The selected file format determines how dark currents are provided and how spectra are corrected. See below for **Dark Current And Offset Correction For The MFC STD Format**.

For satellite measurements, the wavelength calibration of earthshine spectra and irradiances is provided in the files and no transmission file is needed. Both fields should then be kept empty. The only information to provide should be the spectral region to process : the band type (for GOME and GOME2) or the channel and the clusters (for SCIAMACHY).

Dark Current And Offset Correction For The MFC STD Format

According to the file format, measured dark current are available and subtracted from spectra just before the analysis. QDOAS supports the MFC STD format, an ASCII spectra file format produced by the well-known DOASIS program designed in Java by the atmospheric research group at IUP Heidelberg, Germany and largely used in the DOAS community :

https://doasis.iup.uni-heidelberg.de/bugtracker/projects/doasis/

For this format, spectra can be corrected by dark current and offset. The dark current should be a spectrum measured with a large integration time (typically 30 sec) and the offset should be the average of a large number of spectra measured with a very small integration time (typically 1000 x 3 ms).

Application of the offset correction :

$$spe = spe - offset * (spe\_scans/offset\_scans)$$
$$drk = drk - offset * (drk\_scans/offset\_scans)$$

where spe_scans, drk_scans and $offset\_scans$ are respectively the number of scans for the spectrum, the dark current and the offset.

Correction of spectra with the dark current (previously corrected by offset) :

$$spe = spe - spe\_scans * drk * spe\_et/(drk\_et * drk\_scans)$$

where spe_et and drk_et are respectively the exposure time of the spectrum and the dark current and drk_scans is the number of scans of the dark current.

For SO_2 retrieval, the stray-light can be problematic. Even if it can be attenuated by subtracting from the spectra, the average of the signal measured in the UV region (below 300 nm if possible), it is recommended to characterize it in laboratory.

The Observation Site The information on the observation **Site** is used to (re)calculate solar zenith angle from geolocation coordinates given for this site in the **Sites** sheet. This can be useful for example if the solar zenith angles saved in the files are not reliable enough. The abbreviation of the observation site is also used to build automatic output file names (see the **Output Page**, page 72).

OMI Options QDOAS provides some specific options to handle OMI files. To make optimal use of these options, refer to the detailed description of the OMI L1B data in the OMI IODS [16].

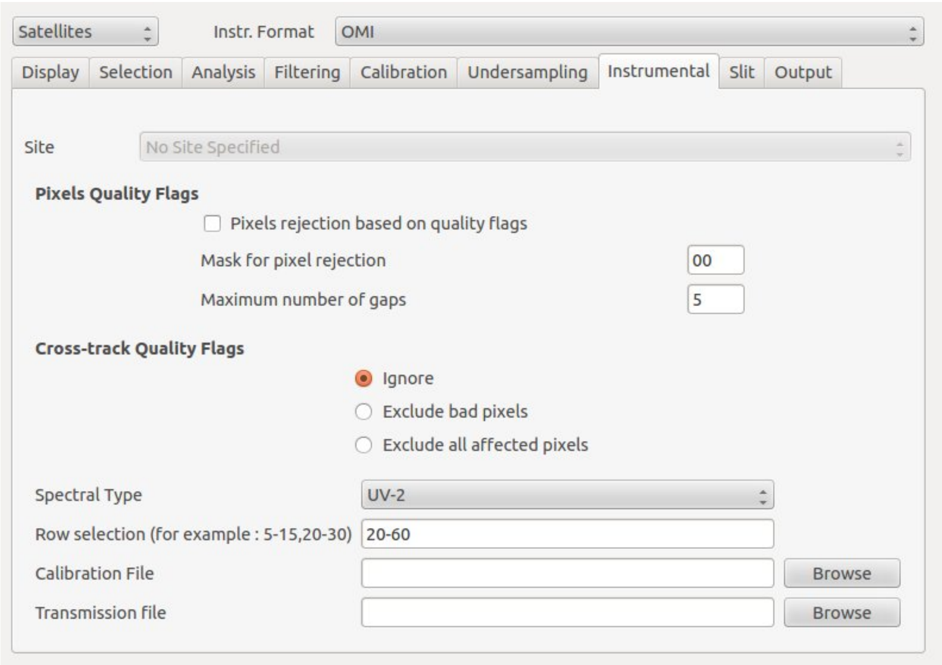


Figure 5.8.: Projects properties : Instrumental page for OMI.

Pixel Quality Flags These flags indicate if a wavelength pixel was affected by measurement problems such as dark current, stray light or saturation. Using this setting, QDOAS can exclude single pixels from the fitting procedure if certain flags are set.

To use the flags, check “Pixel rejection based on quality flags”.

The field “Mask for pixel rejection” should contain a hexadecimal number indicating which flags should lead to rejection. For example, to exclude pixels with flags 0, 1 and 3 set, one would choose a mask

$$2^0 + 2^1 + 2^3 = 11 = \mathrm{B}_{16}\,.$$

to reject all flags, one would choose the mask

$$2^0 + 2^1 + \ldots + 2^{15} = 65535 = \mathrm{FFFF}_{16}\,.$$

For a full description of the 16 PixelQualityFlags in the OMI L1B data, refer to the OMI IODS [16].

The value “Maximum number of gaps” indicates the maximum number of pixels that should be excluded from the spectrum.

Cross-track Quality Flags Cross-track Quality Flags describe the so-called "row anomaly" affecting the OMI data. These flags apply to a complete spectrum and indicate how badly the spectrum is affected. QDOAS provides three options for the handling of these flags (see [16]):

Ignore Use all spectra, disregarding the quality flags.

Exclude bad pixels Only exclude rows flagged as 'Affected, Not corrected, do not use' in the L1B data.

Exclude all affected pixels Only use rows flagged as 'Not affected'.

Spectral Type OMI measurements contain data from three spectral bands: UV-1, UV-2 and VIS.

Row selection This option allows the user to select a subset of the 60 detector rows for the analysis, by providing a list of ranges from 1 to 60.

Slit Page

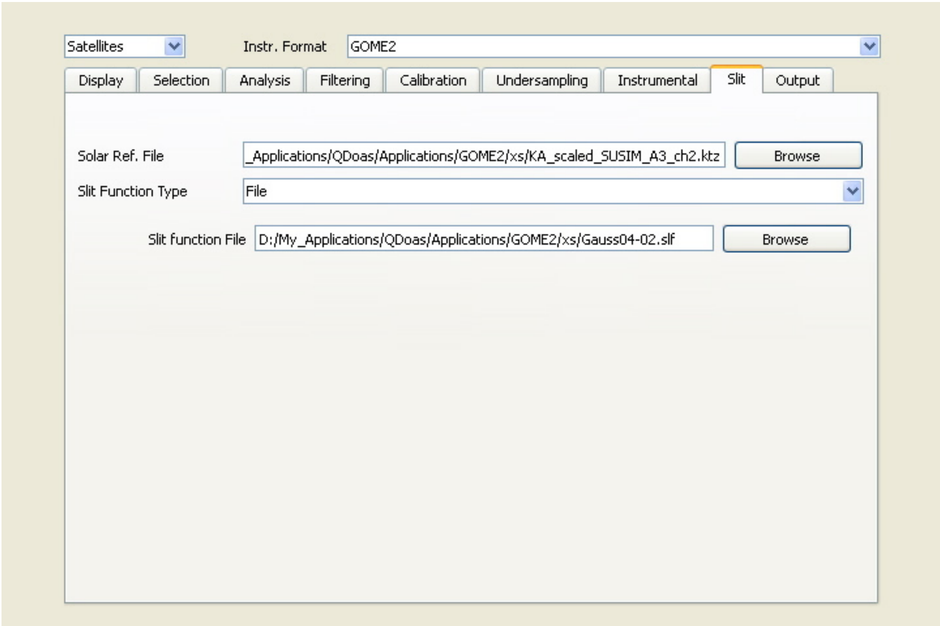


Figure 5.9.: Projects properties : Slit page

Input cross-sections have to be degraded to the resolution of the instrument before the analysis. This can be done using the **convolution tool**. However the programme also authorizes the direct use of high-resolution cross-sections which will be convolved in real time using information provided in this page **if and only if** the slit function is not characterized by the **wavelength calibration procedure**.

Slit Function Type

Several analytic line shapes are proposed including line shapes supported by the **wavelength calibration procedure** (gaussian, lorentzian, error function, voigt and asymmetric line shapes). Different fields have to be completed according to the selected slit function. ASCII file is requested for slit functions measured in laboratory (option **File**) or when the "Wavelength dependent" button is checked (analytical line shapes).

◇ Slit functions measured in laboratory : the first column should be the wavelength grid of the line shape; the maximum of the line shape is expected around 0 nm; look-up tables can be specified for line shapes defined at different wavelengths (in this case, the first line gives the individual wavelengths).

◇ Wavelength dependent analytical slit functions : the input file should contain the FWHM variation with the wavelenth calibration; at a given wavelength, cross-sections will be convolved with the appropriate resolution.

◇ Wavelength dependent stretch factors on a user-defined slit function : in addition to the slit function file, a three columns file is expected, giving the variation of a different stretch factor to apply on each side of the grid of the slit function. Such a file can be obtained by merging in one file the parameters SFP1 and SFP2 resulting of the wavelength calibration (use the **Save As** option from the title of the plots to save the curves in an ASCII file).

Solar Reference File

A high-resolution solar spectrum is expected to replace the solar spectrum of the **Calibration page** if the slit function is not characterized during the calibration procedure and solar spectrum and cross sections have to be convolved with the line shape specified in this page. Otherwise, if the slit function type of this page is **None**, preconvolved solar spectrum (in this page) and cross sections (in **Analysis windows properties**) are expected.

Output Page

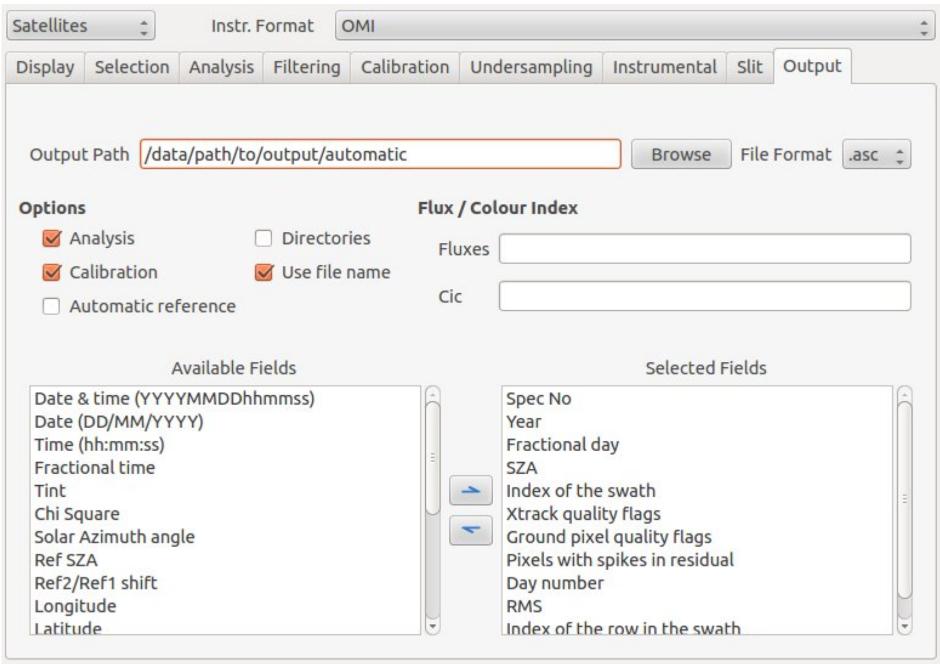


Figure 5.10.: Projects properties : Output page

This page is dedicated to the selection of information on analyzed records to write in the output file after calibration and/or analysis of spectra. When the **Analysis button** is checked, all the fields in this page are enabled and it is also possible to select the fit results that should be saved in the **Analysis windows properties** pages.

When the user selects chooses ".asc" as the file format, the program produces ASCII files with tab-separated columns for all selected output fields. These files may be loaded in spreadsheets such as Excel. The first line of the analysis output starts with a hash (#) character and is used to print the column titles. When the **Calibration button** is checked, wavelength calibration results are saved before the analysis results. Lines with calibration output start with a semicolon (;). **If an ASCII output file already exists at the specified location, QDOAS appends the new results to the existing file.** In this case, column titles and calibration information are not repeated. Therefore, it is best to avoid writing to existing files, unless exactly the same analysis and output configuration is used to produce the new data. To replace the content of an existing output file, the file must first be deleted manually.

When the user selects the file format ".he5", QDOAS produces HDF-EOS5[1] output files. The resulting files can be used in programming environments such as Matlab or IDL, or using the application hdfview. In HDF-EOS5 output mode, QDOAS saves data either as a "geolocation field" or as a "data field", depending on the kind of information contained in the field. In contrast to ascii mode, where results of multiple processing runs can be appended to a single output file, QDOAS reports an error if the chosen HDF-EOS5 output file already exists, and the results will not be saved.

QDOAS always saves all the output from a single input file in one shot, either when it has processed the last spectrum of an input file, or when the analysis is stopped using the **stop button**.

Automatic Creation Of The Output File Name

The path and the name of the output file can be specified in the **Output Path** field. If "automatic" is used as a file name, QDOAS will generate the name of the output file automatically, using the user-defined output path as a base.

For ground-based measurements, the **Directories** and **Automatic reference** buttons have no effect. The original file name is always used (but the file extension is changed in **".asc"**) except if the **Use file name** button is unchecked and an observation site has been specified in the **Instrumental page**. In this case, the output file name is built as follows :

<output path>/XXYYYYMM.ASC

Where :

- **output path** is the user-defined path;
- **XX** is the abbreviation of the observation site selected in the **Instrumental** tab page; if no observation site is specified, the original file name is used;
- **YYYY** is the year of measurement;
- **MM** is the month (zeros padded) of measurement;
- **ASC** is the default file extension for ASCII files;

[1] HDF-EOS5 is a binary output format based on the HDF5 format see `http://www.hdfeos.org`.

For satellite measurements, the **Use file name** button has no effect. If overpasses calculation is requested (option **Sites** in the **Geolocation** frame of the **Selection** page), then the output file name is determined as above (<output path>/XXYYYYMM.ASC where XX is the abbreviation of the station). Otherwise, for SCIAMACHY files, the output file name automatically created has the syntax SCIA_YYYYMMDD_NNNN.ASC where YYYYMMDD is the date of measurement (year, month, day) and NNNN the orbit number. For other satellite formats, the original file name is used (but with the file extension **".ASC"**). Files are distributed in a year/month/day folder structure if the **Directories** button is checked.

Fluxes and Colour Indexes

The **flux** is the value of the signal averaged over seven pixels around the specified wavelength. Divided by the exposure time, this can be used to check a relative intensity. To calculate and save fluxes in the output file, specify the central wavelengths separated by the semicolon (;) character. For example, to get fluxes at 330 nm, 350 nm and 380 nm, enter :

330; 350; 380;

The **colour index** is the ratio of two fluxes. To output different colour indexes (Cic), write the ratios separated by the semicolon (;) character as in the example below :

380/330; 380/350;

Selection Of Fields To Output

The content of this frame is similar to the one in the **Display page**. In QDOAS, the output is fully configurable. Information related to the measurements (e.g. date and time, viewing angles, geolocation coordinates, . . .) can be selected in this page. The selection of analysis results (e.g. slant column densities, fitted non-linear parameters, . . .) is made individually in the **Analysis windows properties** pages. The selected instrument or file format determines the list of fields available for output. For example, information on cloud fraction and cloud top pressure is available only for satellite instruments. A non-exhaustive list of fields available for ground-based and satellite measurements is given in appendix **B**.

5.2 Analysis windows properties

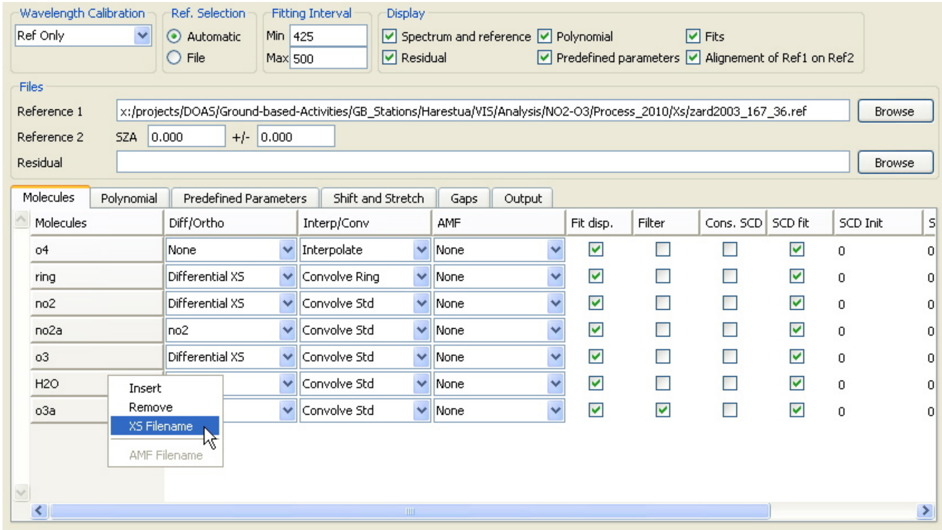


Figure 5.11.: Analysis windows properties

This dialog box completes the **Projects properties** for the configuration of the analysis of spectra. Several analysis windows can be defined under a same project. Next section will guide you in the definition of parameters to fit.

Fitting interval The fitting interval is the first option to specify when a new analysis window is created. It depends on the region covered by the spectrometer and the trace gases to retrieve. According to the molecules to focus on, some baseline recommendations can be found in the literature.

Reference Spectra In the DOAS technique, spectra are always analyzed with respect to a reference spectrum. This could be the irradiance spectrum of the current satellite file, any other reference spectrum provided in an ASCII file or a daily reference spectrum selected on a solar zenith angle criterion. The **Ref. Selection** box proposes to choose between the modes **File** (irradiance of the file for satellites measurements or an external reference spectrum) and **Automatic** (reference spectrum selected on specific criteria).

In addition, QDOAS gives the possibility to define two reference spectra (**Reference 1** and **Reference 2**). **Reference 1** is always a file; according to the **Ref. Selection mode**, **Reference 2** can be the name of an ASCII file or a spectrum automatically selected by the program. These options determines on which reference spectrum the wavelength calibration procedure is applied :

- If only one reference spectrum is specified (**Reference 1** or **Reference 2**), it is used as control spectrum i.e. the I_0 spectrum in the Beer-Lambert law. The wavelength calibration procedure is applied on this spectrum and the cross-sections are re-interpolated on the new calculated grid before the analysis of spectra.
- If two reference spectra are given, the wavelength calibration is applied only on the first one (**Reference 1**); the shift between both reference spectra is then determined (using a NLLS fitting approach)

in order to align cross-sections on the second reference spectrum (**Reference 2**) and spectra are analysed w.r.t. **Reference 2**.

Automatic Reference Selection

The information on the SZA is present in most ground-based file formats. According to the SZA range, a reference spectrum with the SZA the closest to the given value is selected for each twilight or the spectrum with the minimum SZA of the day is selected (both values initialized to 0 or the SZA range below all SZA values of the file). For MAXDOAS measurements, it is also possible to select the zenith spectrum of the scan if the scan button is checked/

For satellite measurements, if no **Reference 1** is specified (field kept empty), the irradiance of the current file is always implicitly used. This means that if a **Reference 2** is provided, the wavelength calibration is applied on the irradiance spectrum (**Reference 1**) of the file and the control spectrum (**Reference 2**) will be aligned on the irradiance before the analysis of earthshine spectra. For satellite measurements, the **Reference 2** spectrum could be an average of spectra selected in a specific region given by its minimum and maximum latitudes and longitudes. Other information such as the cloud fraction (GOME2) could also be used to refine the reference selection.

Wavelength Calibration

The quality of the fit results largely relies on a very accurate determination of the wavelength calibration of the reference spectrum. The wavelength calibration procedure developed in QDOAS allows correcting the preliminary grid of the reference spectrum using a high-resolution solar atlas spectrum degraded to the resolution of the instrument (see the **Calibration page**, page 65 of **Projects properties**). The information on the shift and eventually the slit function retrieved from this procedure are used to convolve/interpolate the cross-sections before the analysis. The wavelength calibration is always applied in priority on the **Reference 1** (the irradiance spectrum for satellite measurements). If two reference spectra are provided, **Reference 2** is aligned on **Reference 1** using the same non linear least-square algorithm as the one used for the analysis of spectra w.r.t. the control spectrum.

If the wavelength calibration of the reference spectrum is assumed to be accurate enough, the option **None** can be used instead of **Ref Only**. The option **Spectra only** is useful for some particular applications (for example, long paths measurements for which the reference spectrum is a lamp measurement).

The option **Ref+spectra** allows applying a calibration correction on both reference spectrum and spectra to analyze. This option has been designed to handle spectra recorded with unstable (unthermostated) instruments where the spectral resolution can vary a lot from one spectrum to another. In this case, the resolutions of both spectra are matched to the resolution of the less resolved spectrum, and the absorption cross-sections can be convolved in real-time to the same effective resolution. This option is time consuming and should be used carefully.

Display After the processing of a spectrum, QDOAS can plot for each spectral analysis window :

- ◇ the spectrum and the reference in the fitting interval;
- ◇ the residual of the fit (the difference between the observed and the calculated);
- ◇ the continuum part of the spectrum fitted by a polynomial;
- ◇ the fit obtained for each species
- ◇ the predefined parameters (offset, undersampling);
- ◇ in the case two reference spectra have been selected, these two spectra after the alignment correction.

The appropriate buttons are checked according to the graphs to plot. An individual selection of the cross-sections and the predefined parameters can still be performed in the dedicated tab pages.

Residuals In the tips and trick box, it is possible to save some residuals to realize further studies or to create a synthetic cross-section that could be introduced carefully in the fit in case systematic structures are identified. If a **"Residual"** file name is given, the calculated residuals will be saved in an ASCII file. There is one line per processed record and the three first numbers starting a line are respectively the record number, the solar zenith angle and the decimal time (see example below). The first line of the file should be the wavelength calibration. As the fits are always appended, the size of the file could increase significantly and it is recommended to disable this option by emptying the **"Residual"** file name field when it is not necessary anymore.

```
0 0 0 4.25848e+002 4.25689e+002...  4.99708e+002 5.00065e+002
16 81.024 7.2989 -3.992e-004 -3.021e-004...  -6.663e-005 2.460e-004
17 80.668 7.3006 3.584e-004 1.262e-004...  1.611e-004 9.982e-004
18 80.396 7.3019 2.594e-004 -1.683e-004...  7.704e-005 9.206e-004
```

Fitting Parameters The user must define the fitting parameters in the appropriate pages of the property sheet at the bottom of the dialog box. The different pages are :

Molecules	definition and configuration of the list of cross-sections to fit;
Polynomial	specification of the degree of the polynomial fitting the continuous component of the absorbance;
Predefined Parameters	this page proposes several predefined parameters such as offset, undersampling, . . . ;
Shift and Stretch	shift and stretch can be applied to any spectral item;
Gaps	gaps can be introduced in the fitting window (e.g. to eliminate bad pixels);
Output	selection of the calculated column densities and associated errors that should saved in the output file.

According to the associated type of parameters, the selected page proposes several columns of options to fill in, to check or to select from a multiple choice. The conviviality of the analysis parameterisation is enhanced by the use of right-click shortcut menus to handle the lists of items in the different tab pages. Because of the complexity of the whole set of options, the structure is detailed page after page in the following section.

5.3 Configuration of the fitting parameters

The Molecules Page

This page contains options for defining and configuring the list of cross-sections to fit (see figures below) :

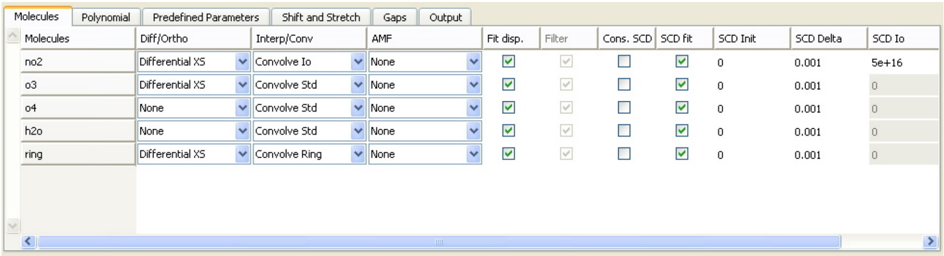


Figure 5.12.: Analysis Windows Properties : Molecules Page

Molecules are characterized by their cross-section. They are represented by symbols previously defined in the **Symbols** page of the user interface. QDOAS needs these symbols for internal use : to create lists of available molecules for specific options (for example : in the **Differential cross-sections** column or in the **Shift and stretch** page) and to build cross-section files filters.

- ◇ **For internal needs of the program, cross-section files names must imperatively start with the symbol name as prefix followed by the underscore character !**
- ◇ There is no constraint on the cross-section file extension; the default one used by QDOAS for creating cross-sections files filters starts with "xs".

Right-click and select **Insert**, **Remove** or **XS Filename** options in the contextual menu respectively to insert a new molecule in the list, to delete an existing one or to modify the file associated to a cross-section. The **Remove** option is disabled for a symbol if another cross-section is orthogonalised to the selected one or if the selected symbol is used in the **Shift and Stretch** pages.

Differential cross-sections

Differential cross-sections can be generated by orthogonalisation or high-pass filtering according to the definition of an orthogonal base formed with the component vectors (generally, a base of order 2) of the polynomial defined in the **Polynomial** page. Refer to the **Description of Algorithms** chapter for further details. Three options are available :

None the original cross-section is used;

Differential XS — a differential cross-section is generated either :

1. by orthogonalisation if an orthogonal base is defined in the **Polynomial** page (Gram-Schmitt algorithm);
2. using high-pass filtering options defined in the **Filter** tab page of **Projects properties** otherwise.

a cross section in the proposed list — the selected cross-section is orthogonalised to the orthogonal base (if defined) and to another cross-section defined in the list (orthogonalisation in cascade is allowed).

The latter case prevents from possible correlation between two cross sections (for example, two O_3 cross sections measured at different temperatures typically to separate contributions from the stratosphere and the troposphere or cross sections with strongly correlated absorption structures, eg. BrO and H_2CO). The list of available cross sections includes all cross section symbols defined in this page except the one selected. It is updated as cross-sections symbols are added to or removed from this page.

Interpolation/Convolution

Cross-sections should be defined on the grid of the control spectrum before the analysis. This column describes the action to perform on the selected cross-section :

None — the selected cross-section is assumed to be correctly aligned on the reference spectrum grid; so, no action will be performed on the cross-section (for example, a user-defined undersampling cross-section in optical density fitting);

Interpolate — the selected cross-section will be interpolated on the grid of the reference spectrum; a cross-section already pre-convolved at the resolution of the instrument is expected in input.

Convolve Std — this option gives the possibility to convolve a high-resoluted cross-section in real-time using either the information on the calibration and the slit function provided by the **wavelength calibration procedure** or the user-defined slit function specified in the **Slit Function page** of **Projects properties**. If the wavelength calibration procedure is applied on both the control spectrum and spectra to analyse, the cross-section is convolved with the poorest resolution;

Convolve I_0 — the cross-section is convolved with I_0 correction using the concentration defined in the column *SCD* I_0 (this is the slant column density of the cross-section used to calculate the theoretical optical depth in convolution with I_0 correction (see Aliwell et al. [1]);

Convolve Ring — in the same way, the program can generate a Ring cross-section; the expected input file must be a Ring cross-section pre-calculated by the **QDOAS Ring tool** on a high-resoluted grid;

Convolving cross-sections in real time is a comfortable option that avoid the pre-convolution of all cross-sections with respect to the selected reference spectrum and the calibration options.

AMF

Usually, it is better to calculate vertical columns out of QDOAS using appropriate radiative transfer model (e.g. LIDORT, DISORT). Nevertheless, QDOAS gives the possibility to calculate vertical columns or to correct a cross section using pre-calculated AMF through options proposed in the **AMF** column :

SZA — vertical columns are calculated using AMF depending only on the solar zenith angle;

Climatology — vertical columns are calculated using climatological air mass factors; the AMF depends on the solar zenith angle and the calendar day;

Wavelength — before the analysis, the selected cross-section is corrected using wavelength dependent AMF (modified DOAS).

Additional option **AMF Filename** is proposed in the contextual menu to complete with the name of the file containing the AMF (see the requested file format according to the selected AMF option in appendix **A**).

Control Of Parameters To Fit

QDOAS minimises residuals of the DOAS equation using a Marquardt-Levenberg NLLS fitting algorithm. The method implements a gradient-expansion algorithm, which is based on the iterative combination of a steepest-descent method (suitable for approaching the minimum from far away) and a linearisation of the fitting function.

- In “optical density fitting”, slant column densities of the molecules are fitted linearly and the **SCD Init**, **SCD Delta**, **SCD min** and **SCD max** buttons are ignored. Nevertheless, if the **SCD Fit** button is unchecked, the weight of the selected cross-section in the optical density is fixed at the concentration value given in the **SCD Init** column.
- In “intensity fitting”, the slant column densities of the molecules are non linear parameters. The initial concentration value and the initial

delta value used by the non-linear algorithm to calculate numerically partial derivatives of the fitting function are respectively given by **SCD Init** and **SCD Delta**. The **SCD Delta** default value shouldn't be modified except if the system seems not to converge. **SCD min** and **SCD max** can be used to constrain the concentration of the molecules within a given interval even if it is not recommended to do that.

The selection of the analysis method is made in the **Analysis page** of **Projects properties**. Further details on the retrieval algorithms can be found in the **Description of Algorithms** chapter.

For advanced users : it is possible to constrain the slant column density of a molecule to the value calculated in the previous analysis window.

If the **Cons SCD** button is checked, the **SCD Fit** button is unchecked and the **SCD Init** value is 0., the slant column density of the selected molecule is not fitted but initialized to the value calculated in the previous analysis window if any.

Fit display

This column is active only if the **Fits** button is checked in the **Display** frame of the current dialog box. It allows selecting which cross-sections fits will be displayed. Note that the display of the fits of all spectral analysis windows could be disabled from **Display Page** of **Projects properties**.

Filter

This column is active only if a low-pass filter has been selected in **Filtering Page** tab page of **Projects properties**. It allows defining individually which cross-sections are to be filtered.

The Polynomial Page

The degree of the polynomial (usually a polynomial in x) fitting the continuous part of the spectra is specified in this page.

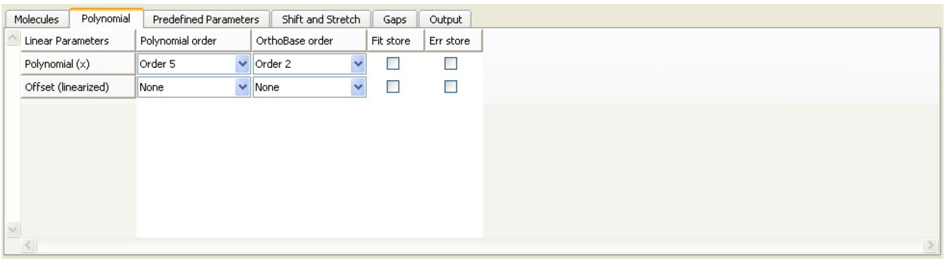


Figure 5.13.: Analysis Windows Properties : Polynomial Page

The values of the fitted coefficients account for the normalization applied on both the spectrum and the reference. **Differential cross-sections** can be generated by orthogonalisation according to the definition of an orthogonal base formed with the component vectors (generally, a base of order 2) of the polynomial. The **OrthoBase** order column specifies the degree of this orthogonal base.

The correction of instrumental and/or atmospheric straylight or residual dark current signal requires the introduction of an offset parameter that is usually fitted as a non linear parameter in the **Predefined Parameters** page. In some specific cases (typically, in the near UV, around 300 nm), the signal of the spectrum is very low and in order to avoid systematic logarithm errors in DOAS fitting when resolving the DOAS equation, the fit of a linear offset is preferred. The equation is just a little bit different :

$$\log(I(\lambda)) = \log(I_0(\lambda)) - \sum \sigma_i c_i + \frac{\text{offset}(\lambda)}{I(\lambda)} \tag{5.1}$$

Note that a linear offset and a non linear offset should not be fitted in the same spectral analysis window.

The Predefined Parameters Pages

This page proposes different parameters that can be fitted linearly or non linearly according to the fitting method :

- scaling factor for the control spectrum (**Sol**);
- offset;
- common residuals (**Com**).
- undersampling (**Usamp1** and **Usamp2**);
- synthetic cross section to fit very small differences in the resolution between the spectrum and the reference (**Resol**)

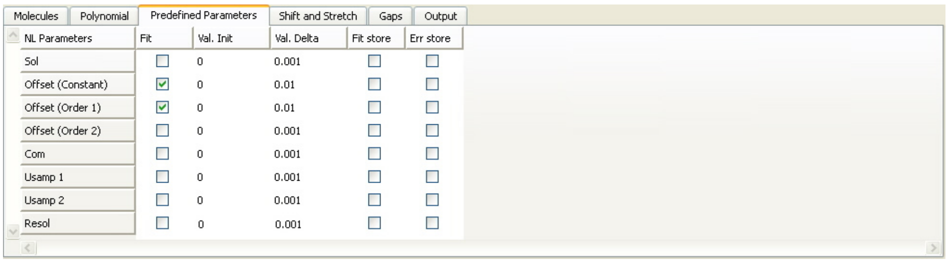


Figure 5.14.: Analysis Windows Properties : Predefined Parameters Page

A cross section file is always expected for **Com** parameter. A cross section file is expected for **Usamp1** and **Usamp2** parameters if the method **"File"** has been selected in the **Undersampling** page of **Projects properties**. To specify the name of the cross section file, right-click the **"Select File"** option from the parameter line.

Val init and **Val delta** are respectively the initial value and convergence factor, two parameters used by the NLLS algorithm. In general, the default values should not be modified, except in case of convergence problems. **Fit store** and **Err store** columns are enabled only if the **Analysis button** is checked in the **Output** tab page of **Projects properties**.

Offset

An ideal spectrometer in an ideal atmosphere would measure the part of the sunlight that has been elastically scattered by air molecules and particles in the zenith direction. In a real experiment however a number of possible additional sources of signal may add up to the ideal Rayleigh/Mie contribution leading to "offset" the measured intensity by a certain amount. In addition to the Ring effect, which is to a first approximation a natural source of offset, instrumental sources of offset also need to be considered like stray light in the spectrometer and dark current of the detector. This is the purpose of the offset parameter which is better described in the **Description of Algorithms** chapter. The offset is normalized w.r.t. the intensity of the spectrum.

In some specific cases (typically, in the near UV, around 300 nm), the signal of the spectrum is very low and in order to avoid systematic logarithm errors when resolving the DOAS equation, the fit of a linearized offset is preferred (see the **Polynomial** page). Note that a linear offset and a non linear offset should not be fitted in the same spectral analysis window.

Common residual

When systematic structures appear in the residuals, it is sometimes useful to eliminate them using a synthetic cross section obtained by averaging some of such residuals (cfr the **"Residual"** field in the **Files** frame of this dialog box). In DOAS fitting, this cross section can be introduced either in the **Molecules** page with a user-defined symbol or in this page with the predefined symbol "**Com**". In intensity fitting, it is recommended to use the predefined symbol **Com** that is always fitted linearly whatever the analysis method.

Undersampling

The undersampling is a well-known problem of GOME onboard the satellite ERS-2. It arises from the poor sampling ratio of the GOME instrument (2 to 3 pixels/FWHM of the resolution of the spectrometer) which results in a lost of spectral information when interpolating earthshine spectra during the DOAS fitting process. The problem can be corrected using ad-hoc cross-sections obtained by simulating the effect from a high-resolution solar reference. Undersampling cross-sections can be pre-calculated using the **QDOAS undersampling tool**.

Resol synthetic cross section

This cross section is built automatically by dividing the selected reference spectrum with itself but convolved with a gaussian with a FWHM of 0.05 nm. It allows accounting for very small differences in the resolution of the reference spectrum and the spectrum to analyze.

The Shift and Stretch Page

Shift and stretch parameters allow correcting for possible misalignment between the various spectral items involved in the data evaluation (i.e. measured and reference spectra as well as absorption cross-sections). The equation below gives the wavelength transformation to apply when a shift and a stretch order 2 are fitted :

$$\Delta = a + b.(\lambda - \lambda_0) + c.(\lambda - \lambda_0)^2 \quad (5.2)$$

Less used, the scaling parameter consists in a wavelength dependent scaling factor to apply to a cross-section. It can also be order 1 or order 2.

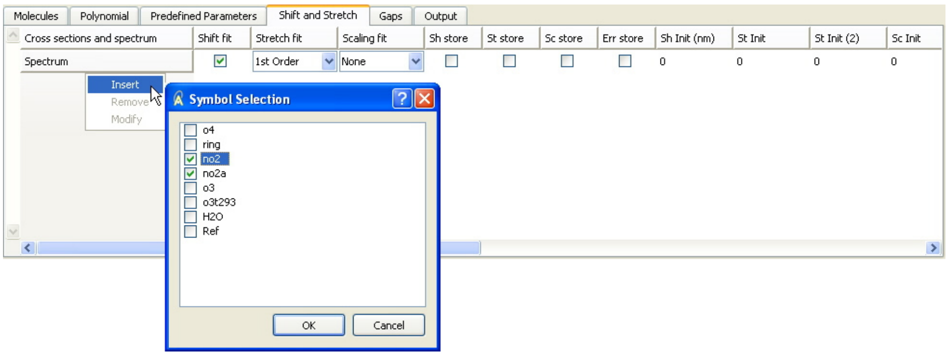


Figure 5.15.: Analysis Windows Properties : Shift and Stretch Page

To add an item to shift, stretch or scale, right-click the **Insert** option to open a dialog box with the list of available symbols (all cross-sections defined in the **Molecules** page and completed with **Spectrum** and **Ref** symbols). It is possible to select only one or several symbols. In the latter case, the same shift and stretch parameters will be applied to all items of the selection (in the example above, the same shift and stretch will be applied on both NO_2 cross-sections). After the validation of the selection, QDOAS automatically updates the list of available symbols so that a symbol can not be selected twice.

Note that a symbol can not be removed from the ***Molecules*** *page as long as it is used in the* ***Shift and Stretch*** *page.*

Output

Buttons in the **Sh store**, **St store** and **Sc store** columns are enabled only if the **Analysis** button is checked in the **Output page** of **Projects properties**. They allow saving respectively the fitted values for the shift, the stretch and the scale. If buttons in the **Err store** column are checked, the standard deviations of the fitted parameters are also saved in the output file.

Initial and delta values

The shift, stretch and scale parameters are fitted non linearly by the Marquardt-Levenberg NLLS algorithm. This iterative method needs to start from an initial solution given by **Init** values of parameters to fit. The convergence parameters **Delta** are used by the algorithm to numerically calculate partial derivatives of the fitting function and to determine the direction of the steepest descent to approach the solution. There is one **Init** column and one **Delta** column for each parameter to fit (shift, stretch order 1, stretch order 2, scaling order 1 and scaling order 2).

Convergence control

In case of convergence problems or for safety reasons, the range of values allowed for the shift can be limited to a specified interval (**Sh Min** and **Sh Max**).

The Gaps Page

Gaps can be introduced in order to eliminate bad pixels from the fitting interval.

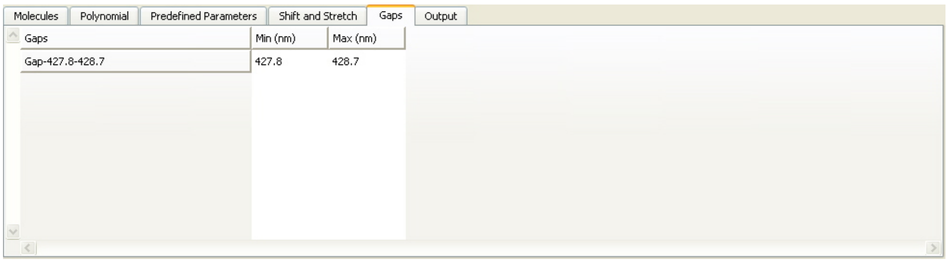


Figure 5.16.: Analysis Windows Properties : Gaps Page

Insert a gap To insert a gap, right-click the **Insert** option and complete the **Min (nm)** and **Max (nm)** columns with the limits given in nanometers. The first column is automatically updated after validation of the entry fields.

Remove a gap To remove a gap, select it in the **Gaps** column and right-click the **Remove** option.

The Output Pages

For each cross-section defined in the **Molecules** page, this page proposes to select the analysis results to save in the ASCII output file(s). Columns are enabled only if the **Analysis** button is checked in the **Output page** of **Projects properties**.

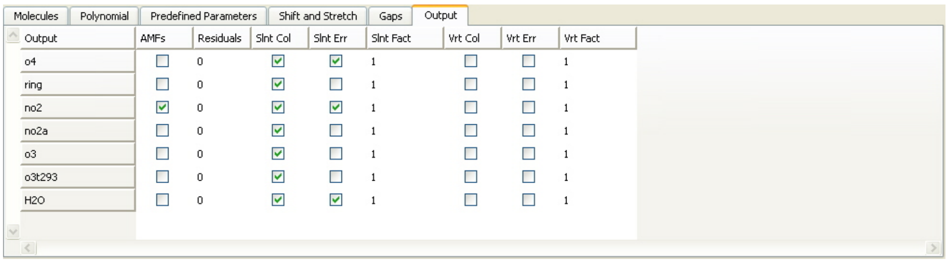


Figure 5.17.: Analysis Windows Properties : Output Page

QDOAS calculates and saves vertical columns if an AMF dependency has been selected in the **Molecules** page. The **Residuals** column gives the possibility to specify a value for the residual column amount of the selected species in the reference spectrum.

In the output file, slant columns and vertical columns (and their respective errors) can be divided by a scaling factor using **Slnt Fact** and **Vrt Fact** edit controls.

In the output file, the title of columns with the retrieval results always starts with the name of the analysis window. Slant columns are indicated by **SlCol**, standard deviations by **SlErr**, vertical columns by **VCol**, air mass factors **AMF**, etc. . . For example, if the application contains two analysis windows (no2 and o3), no2.slcol(o3) and o3.slcol(no2) refer to the column titles for respectively the slant columns of O3 in the no2 window and NO2 in the o3 fitting window.

Examples of output generated by QDOAS can be found in appendix **B**.

5.4 Configuration of the wavelength calibration procedure

The wavelength calibration facility developed in QDOAS is based on a NLLS fitting procedure where the shift between the spectrum to calibrate and a highly accurate solar reference spectrum is determined on a series of equally spaced short intervals. The procedure also allows characterising the instrumental slit function, through fitting of user-defined SFPs. The wavelength calibration can be applied to any kind of spectrum (the reference spectra or spectra to analyze).

The wavelength calibration can be configured in the **Calibration tab** of the **project properties**. It uses the same property sheet as the one described in the **Analysis windows properties**. The previous section (5.3) gives a detailed description of options, page per page. This section describes aspects particular to the parameterisation of the calibration.

The Molecules page

The **Molecules** page allows introducing correcting absorbers that may optimise the accuracy of the wavelength calibration, e.g. the Ring effect (when calibrating a scattered-light spectrum) and O_3 absorption can be taken into account in the fit.

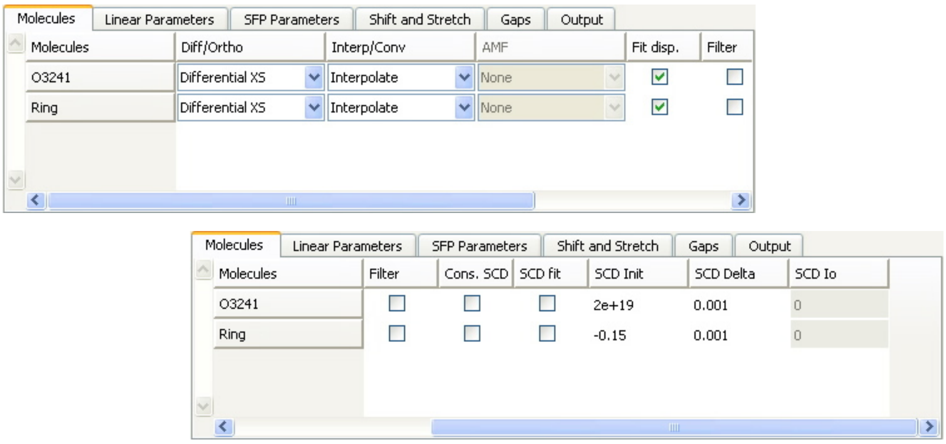


Figure 5.18.: Calibration Properties : Molecules Page

To generate differential cross-sections (column **Diff/Orthog**), see page 78. The **Fit display** column is activated only if the **Calibration** button is checked in the **Display** page of **Projects properties** (see page 60) and if the **Fits** button is checked in the **Display** frame of the **Calibration** page (see page 65). The selected cross-section are usually pre-convolved with the resolution of the instrument and interpolated on the grid of the control (reference) spectrum.

In order to optimise the accuracy of the calibration (and given limitations inherent to the method), it is recommended to limit the number of parameters to fit and to constrain the slant column density of molecules. This can be done in two passes :

- in the first pass, the column density is fitted (**SCD Fit** button is checked) over the whole calibration interval; a mean value of the concentration is then determined from the sub intervals where the fitting of the cross-section has a sense (where the spectral information is largest);

- in the second pass, the concentration is fixed at the mean value determined at the previous pass.

See previous section (5.3) for a complete description of the columns in this page.

The Linear Parameters Page

In this page, you define the polynomial fitting the continuous component of the spectrum to calibrate. To generate differential cross-sections by the orthogonalisation method, don't forget to build an orthogonal base (see page 78).

The Predefined Parameters Page

The SFPs can be fitted in this page.

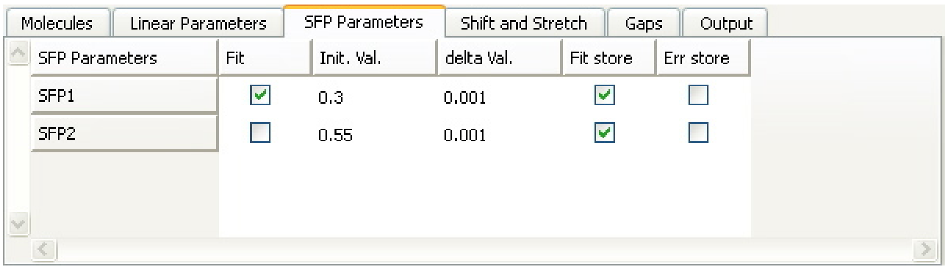


Figure 5.19.: Calibration Properties : Predefined Page (Parameterisation for an error function line shape)

There are two predefined items for SFP : SFP 1 and SFP 2. According to the line shape selected in the **Calibration page** of **Projects properties** (see page 65), these parameters are used or ignored. Note that if you do not want to fit the slit function during the wavelength calibration procedure, select the slit function type **None** in this page and give a solar reference spectrum and line shape in the **Slit Page** of **Projects properties** (see page 71).

For analytical line shapes :

SFP 1 is generally used for fitting the FWHM of the selected line shape. The Voigt profile function is the convolution of a Gaussian and a Lorentzian line shapes. The second parameter is the Lorentz/Gauss ratio. Asymmetric line shapes can be fitted by introducing an asymmetry factor in the Gaussian formula. For two-parameter line shapes, it is generally recommended to fix one of the parameters to an estimated value in order to avoid numerical instabilities.

	SFP 1	**SFP 2**
File	Stretch factor (negative wavelengths)	Stretch factor (positive wavelengths)
Gaussian	FWHM	Ignored
Error function	FWHM	Boxcar width
2n-Lorentz	FWHM	Ignored
Voigt profile	FWHM (Gaussian)	Lorentz/Gauss ratio
Asymmetric line shape	FWHM (Gaussian)	Asymmetry factor

The Shift and Stretch Pages

For the configuration of these pages, refer to the previous section (5.3, page 83). In order to avoid the interpolation of the spectrum to calibrate, it is recommended to fit the shift of the high-resolution solar spectrum, represented by the symbol **Ref**.

In this case, all cross-sections defined in the ***Molecules*** *page have to be shifted with the solar spectrum.*

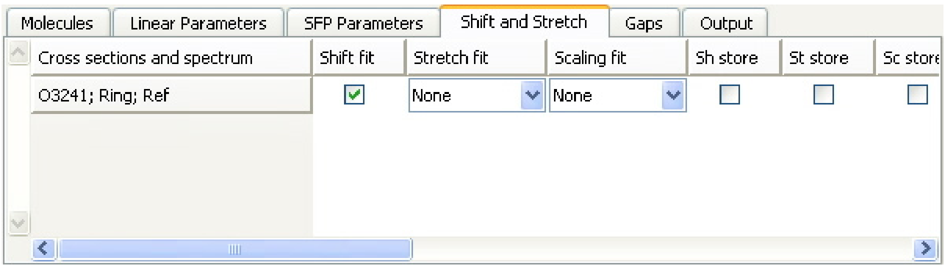


Figure 5.20.: Calibration Properties : Shift Page (The O_3 and Ring cross-sections defined in the **Molecules** page are shifted with the solar spectrum.)

Output

Fitted slant column densities and non linear parameters are saved in the output file if the **"Calibration"** button is checked in **Output Page** of **Projects properties**. This is particularly useful if a **Run Calibration** is performed on all spectra of the file.

6 The QDOAS Tools

QDOAS is delivered with four off-line modules :

- ◇ **convolution** : a convolution/filtering tool;
- ◇ **Ring** : a tool to create Ring effect cross-sections;
- ◇ **usamp** : a tool to create undersampling cross-sections;
- ◇ **doas_cl** : a command line tool for batch processing.

The three first ones were already in WinDOAS. If they can still be called from the QDOAS user interface, they are separate executables with their own user interface, menu options and XML configuration files.

6.1 The convolution/filtering tool (convolution)

The **Convolution/Filtering** tool gives the possibility :

- ◇ to convolve spectra and cross-sections;
  - user-defined slit functions and analytical line shapes are accepted;
  - convolution with I_0 correction is supported;
- ◇ to shift the calibration grid before convolution;
- ◇ to create an effective slit function taking into account the (finite) resolution of the source spectrum (using a FT deconvolution method);
- ◇ to apply a low-pass or a high-pass filter to the convolved cross-section before saving it.

Convolution/Filtering tool options are distributed in three pages :

General	general options (convolution type, input/output files...);
Slit	selection and parameterisation of the slit function;
Filtering	selection and parameterisation of the filter;

The General Page

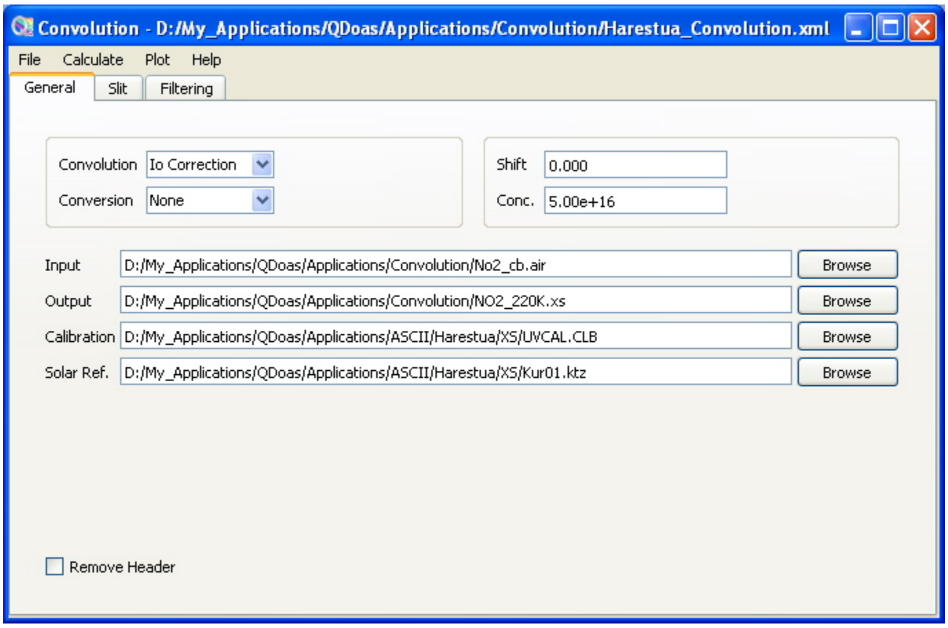


Figure 6.1.: Convolution/Filtering Tool

The Convolution Type

QDOAS supports standard convolution and convolution with I_0 correction. The convolution integral is calculated using the method of trapezes. If **None** is selected, the cross-section is just interpolated on the final grid.

Conversion

Before the convolution, it is possible to convert the original wavelength calibration of the input cross-section file from the air to the vacuum or inversely, from the vacuum to the air.

Requested Files Names

Input file the name of the high resolution cross-section file to interpolate or convolve;

Output file the name of the resulting interpolated or convolved cross-section file;

Calibration the final grid on which the original cross-section (input file) must be interpolated or convolved;

Solar ref. the high-resolution solar spectrum requested only if the convolution with I_0 correction is selected;

The format of input and output files is described in appendices **A** and **B**. The resulting cross-section file can be used as input for the retrieval. It is then better to give the name of the output file in the format imposed by QDOAS : **cross-section files names must imperatively start with the symbol name as prefix followed by the underscore character!**

Shifting the Convolved Cross-section

A shift in nm can be applied to the convolved cross-section. In order to avoid interpolation after convolution, this shift is applied on the calibration grid before convolution.

I_0 correction

The fields **Solar Ref.** and **Conc** are respectively the name of the high resolution solar spectrum file and the scaling column density of the concerned molecule. Both are used for calculating the synthetic optical density in the formula of I_0 correction convolution. These fields are ignored if I_0 correction is not used.

The Slit Function Page

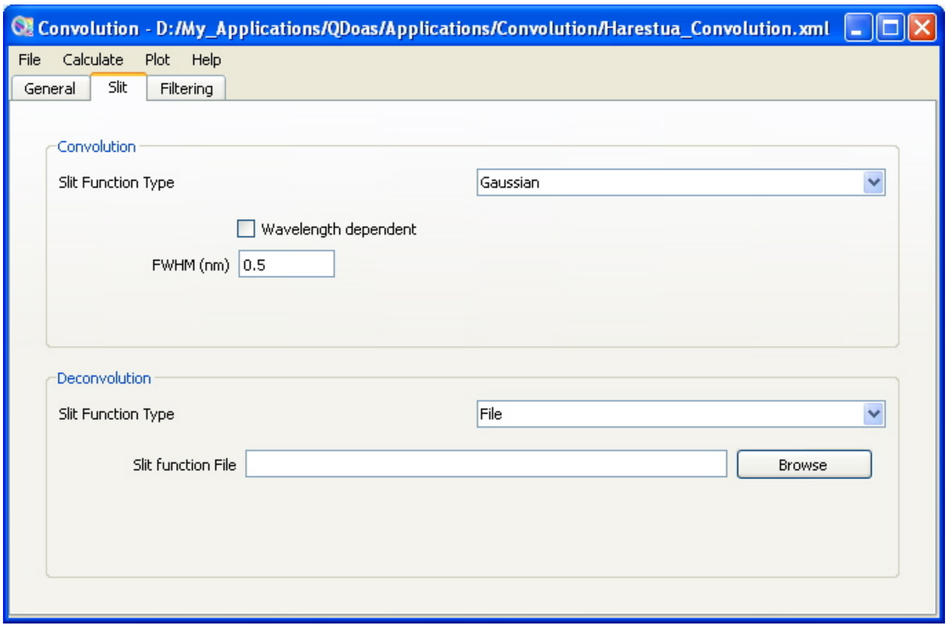


Figure 6.2.: Convolution/Filtering Tool: Slit Function page

This page is dedicated to the selection and the parameterisation of the convolution slit function. Different analytical line shapes (Gaussian, Lorentzian, Voigt, error functions, asymmetric gaussian) are supported. The wavelength dependency of the slit function parameters characterized by the wavelength calibration procedure can be saved from the plot page in order to be accounted for the convolution. Check the **Wavelength dependent** button to enter files instead of numbers. Refer to the section **Analytical line shapes** on page 40, for further information on the supported analytical line shapes.

The use of arbitrary slit functions is possible with **File** option. Look up table of slit functions defined at specific wavelengths is accepted. If the **Wavelength dependent** button is checked, a three columns file is expected giving the variation of two different stretch factors to apply on the grid of the slit function. Such a file can be obtained by merging in one file the SFP1 and SFP2 parameters resulting from the wavelength calibration procedure.

See file formats in **Input file format Annex**.

Deconvolution

A deconvolution slit function can also be defined. In this case, the high resolution cross-section is convolved using an effective slit function obtained from the FT of convolution and deconvolution slit functions. This feature doesn't work if a wavelength dependent slit function is selected. By default, no deconvolution is applied.

The Filtering Page

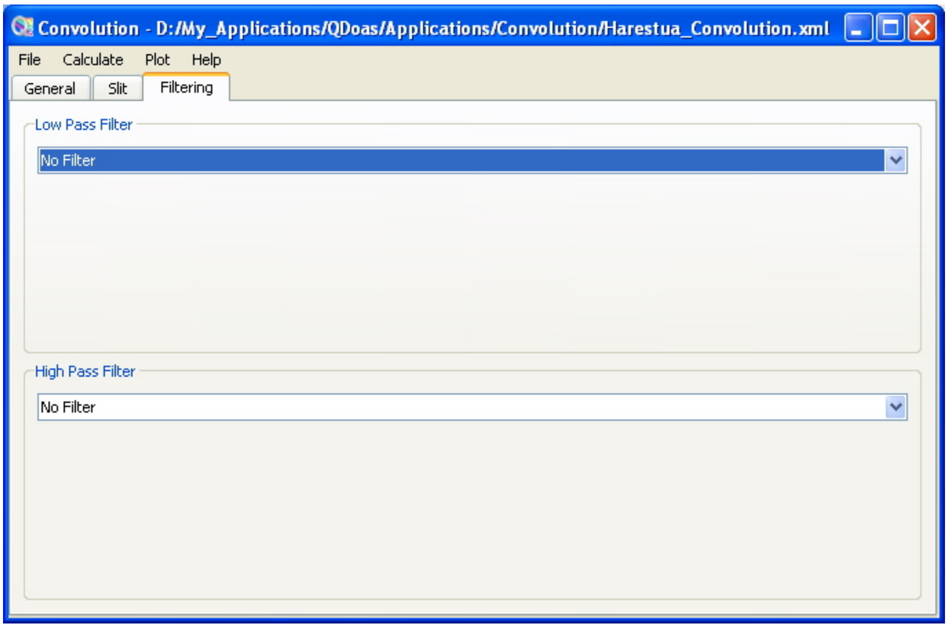


Figure 6.3.: Convolution/Filtering Tool: Filtering page

After convolution, a low-pass and/or a high-pass filtering can be applied on the cross-section. By default, no filtering is applied. The presentation of this page is the same as the **Filtering** one of **Projects properties**. According to the selected filter type, the requested information can be different.

The original spectrum can be divided by the smoothed one or the smoothed spectrum can be subtracted from the original one. The second feature is useful to create differential cross-sections.

The Convolution

Once the parameters specified, the convolution is performed using the **Calculate** → **Run Convolution** option from the menu bar. The original cross section and the convolved one (respectively in black and in red on the plot below) are displayed. In order to avoid edge effects, the convolution has been performed on a larger interval but only the part of the convolved spectrum defined on the final grid is output. If a filtering has been applied, another plot follows, with the original cross section and the resulting one after convolution and filtering.

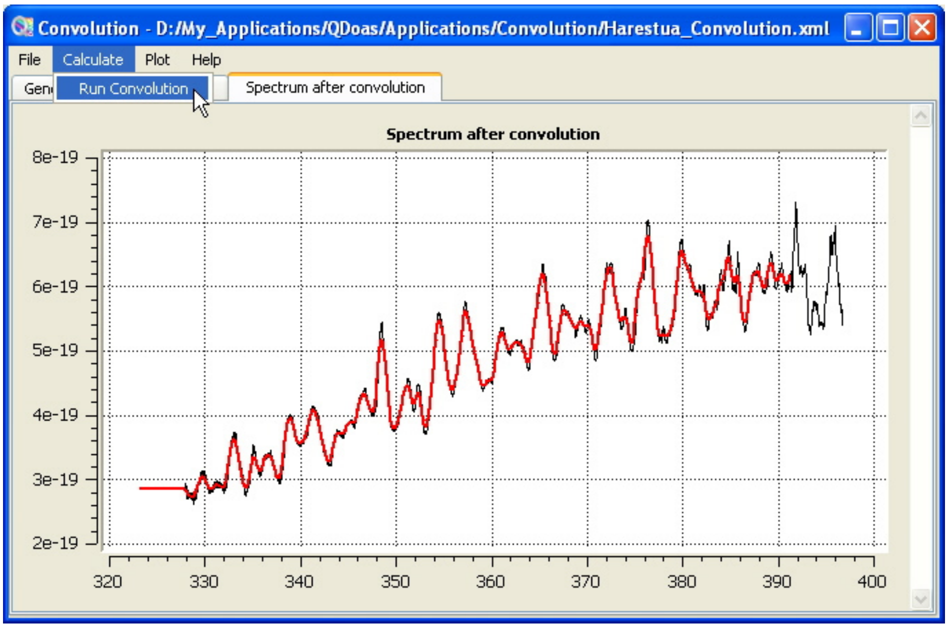


Figure 6.4.: Convolution with I_0 correction of a NO_2 cross-section with a Gaussian (FWHM : 0.5 nm) [26]

6.2 The Ring tool (ring)

The so-called Ring effect arises in the atmosphere due to inelastic scattering processes (mainly RRS by molecular O_2 and N_2). Roughly speaking, it manifests itself by a broadening of the solar and atmospheric spectral features present in measured spectra. This broadening typically reduces the depth of thin solar and atmospheric absorption features by several percents. Hence, it has a strong impact on spectroscopic measurements using the DOAS method and requires appropriate correction to be implemented in retrieval algorithms. This is especially true for minor absorbers like BrO or OClO, for which weak absorption features can be completely masked by Ring structures.

In DOAS, the Ring effect is usually accounted for as an absorber. The QDOAS Ring tool calculates Ring cross-sections using a simple method described by Chance and Spurr [8]. See the **Description of Algorithms** chapter, page 33 for further information on the Ring effect.

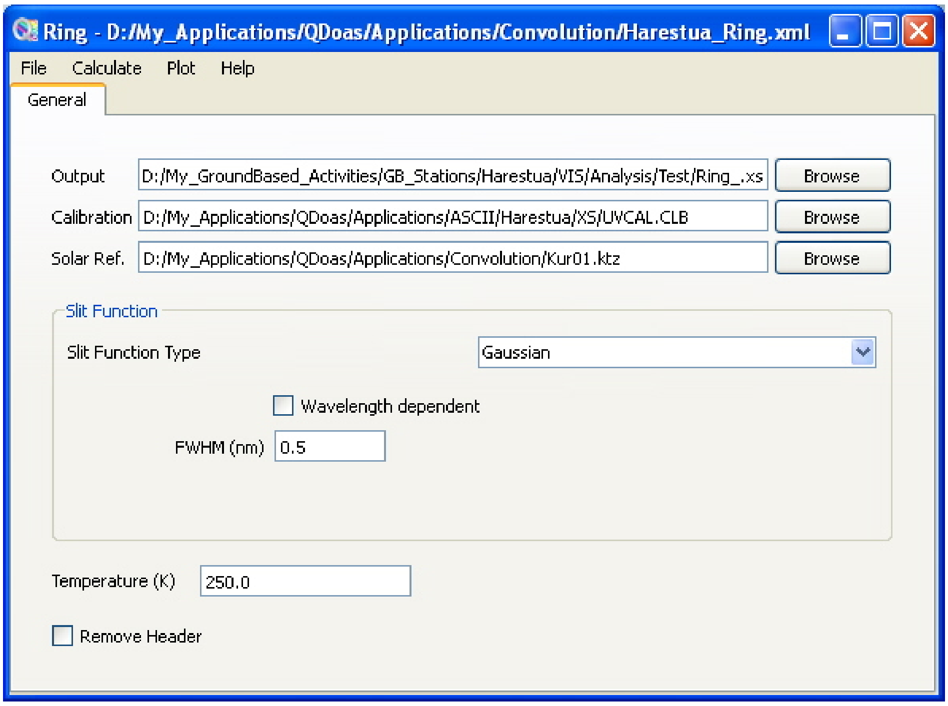


Figure 6.5.: The Ring Tool

Input QDOAS requires :

1. the final grid on which the Ring cross-section must be calculated;
2. a high-resolution solar spectrum;
3. the slit function to use for the convolution : user-defined slit functions and analytical line shapes (Gaussian, Lorentzian, Voigt and error functions) are accepted. The wavelength dependency of the line shape (Gaussian or error function) characterized by the wavelength calibration procedure can be saved from the plot page in order to be accounted for the convolution.

Output As the calculated Ring cross-section is accounted as an absorber, it is recommended to give the name of the output file in the format imposed by QDOAS : **cross-section files names must imperatively start with the symbol name as prefix followed by the underscore characters!**

The Ring cross-section is calculated as the ratio of the rotational Raman spectrum by the solar spectrum (R/S). The output file is an ASCII file with four columns :

- the input wavelength calibration;
- the calculated Ring cross-section;
- the interpolated Raman spectrum;
- the convolved solar spectrum.

When this file is used as cross-section for spectra analysis, QDOAS loads only the two first columns except if the **Convolve Ring** action is requested (see the **Molecules page** of **Analysis windows properties**). In this case, the program uses the information on the slit function retrieved from the wavelength calibration procedure or from the slit function page to convolve separately the Raman and the solar spectra then the calculated ratio is introduced in the fit.

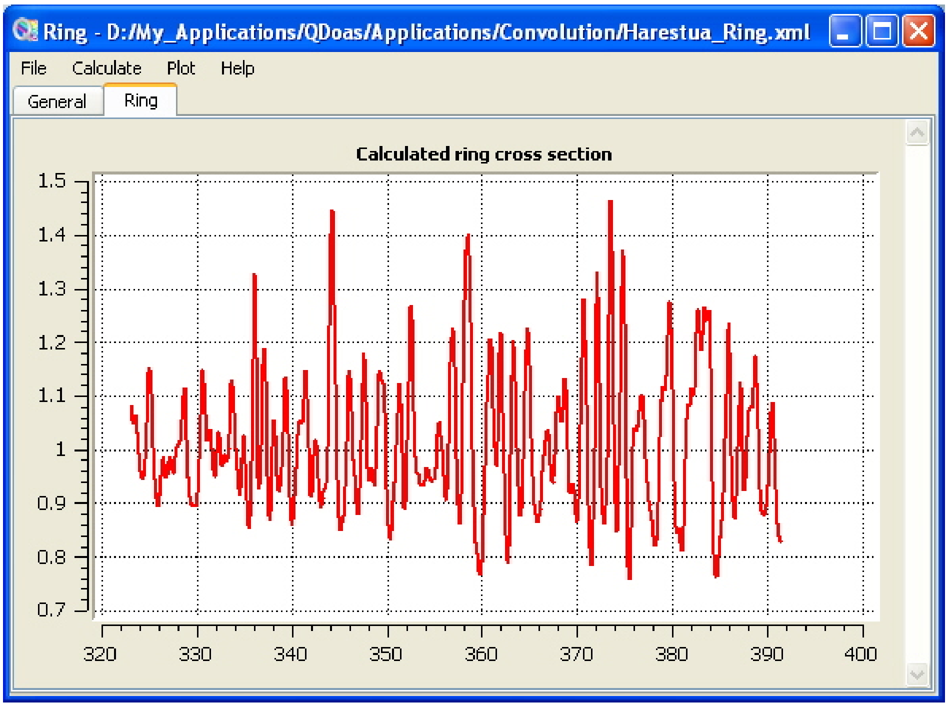


Figure 6.6.: Ring cross section generated with he Ring Tool

6.3 The undersampling tool (usamp)

The undersampling is a well-known problem of GOME onboard the satellite ERS-2. It arises from the poor sampling ratio of the GOME instrument (2 to 3 pixels/FWHM of the resolution of the spectrometer) which results in a lost of spectral information when interpolating earthshine spectra during the DOAS fitting process. The problem can be corrected using ad-hoc cross-sections obtained by simulating the effect from a high-resolution solar reference (see Chance K., 1998 [6]).

The approach consists in building two spectra (an oversampled one and an undersampled one) from the high resolution solar spectrum and according to the selected analysis method, to calculate the ratio (DOAS fitting) or the difference (Intensity fitting) in order to simulate the interpolation error. Two undersampling cross-sections are generated (the first one using the instrument grid and the second one using the instrument grid with a small shift applied).

See the **Description of Algorithms** chapter, page 33, for further information on the undersampling.

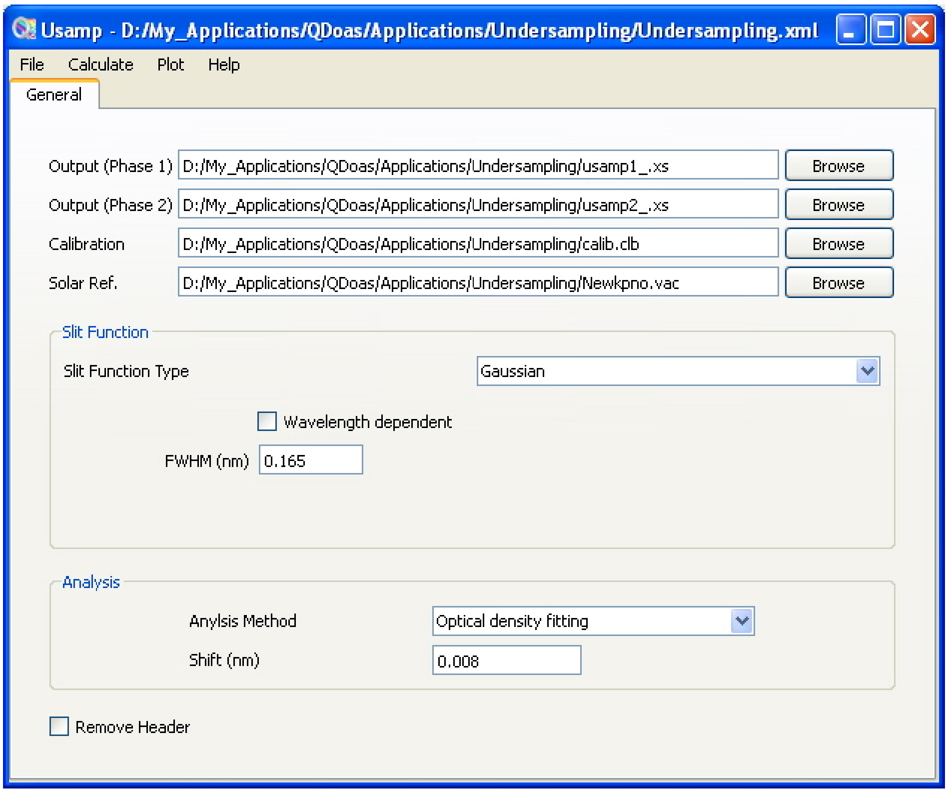


Figure 6.7.: The Undersampling Tool

Input QDOAS requires :

- the final grid on which the undersampling cross-sections must be calculated;
- a high-resolution solar spectrum;
- the slit function to use for the convolution : user-defined slit functions and analytical line shapes (Gaussian, Lorentzian, Voigt and error functions) are accepted. The wavelength dependency of the line shape (Gaussian or error function) characterized by the wavelength calibration procedure can be saved from the plot page in order to be accounted for the convolution.
- the shift to apply to oversampled and undersampled spectra in the calculation of undersampling;
- the analysis method that determines the relation between oversampled and undersampled spectra;

Output Two undersampling cross-sections are generated by the procedure. It is recommended to give the name of the output files in the format imposed by QDOAS : **cross-section files names must imperatively start with the symbol name as prefix followed by the underscore character !**

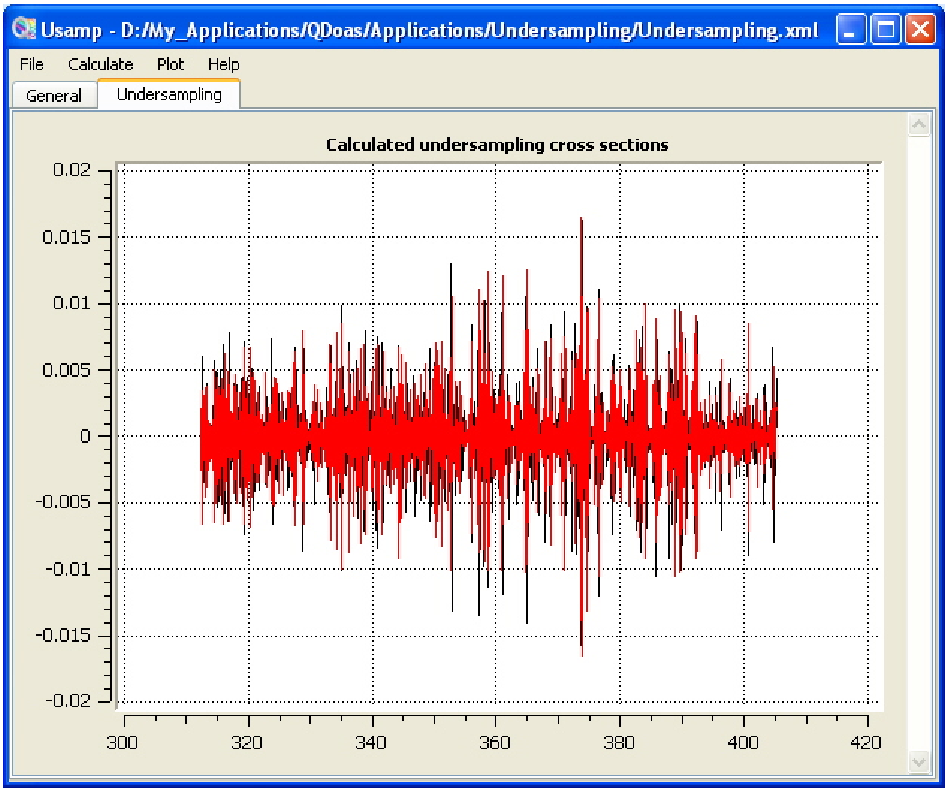


Figure 6.8.: Undersampling cross-sections generated with the Undersampling Tool

6.4 The command line tool (doas_cl)

The QDOAS package includes a very powerful command line tool : doas_cl. It consists in a separate module to load from the command line with a xml configuration file (a QDOAS application or the configuration file built from the convolution/filtering, Ring or undersampling tool).

To see the syntax, just run doas_cl without arguments :

```
doas_cl -c <config file> [-a/-k <project name>] [-o <output>] [-f <file>] ...

    -c <config file>    : A QDoas, convolution, [Ring or usamp] config file.
                          The tool to invoke is determined from the type of
                          configuration file specified;

    -a <project name>   : for QDoas, run analysis on the specified project
    -k <project name>   : for QDoas, run calibration on the specified project

    -v                  : verbose on (default is off)

    -xml <path=value>   : advanced option to replace the values of some options
                          in the configuration file by new ones.
------------------------------------------------------------------------------
doas_cl is a tool of QDoas, a product jointly developed by BIRA-IASB and S[&]T
Last version : Qdoas version 2.1 - 20 December 2012
```

doas_cl is useful to process large amount of files (for example satellite data). It applies on spectra and directories. An output file name different from the one given in the **Output** page of **Projects properties** can be specified.

Example of doas_cl command included in a bash file :

```
/usr/local/bin/doas_cl -c "$HA_pathAnalysis/QDOAS_Harestua.xml" \
-a "Harestua" -o "$HA_pathAnalysisOutput/$year/automatic" -f "$HA_fileToProcess"
```

This command uses the QDOAS_Harestua.xml file previously generated by QDOAS. It loads the project "Harestua" (important to specify if several projects exist in the application). The output file name is generated automatically (see the **Output page** of **Projects properties**).

Important : always use slash as path separator for doas_cl file arguments (input and output) even if you work under Windows.

For the convolution tool, the switch -f applies only to one file but the command can be called several times from a batch. For the **Ring tool**, the switch -f modifies the final calibration grid. To change other parameters, it is better to write a piece of code to modify the xml file.

-xml switch In batch processing or in the frame of specific tests, it can be useful to modify slightly the original options of the configuration file. For example, use another reference spectrum, shift slightly a spectral window,...

The xml configuration file is structured with blocks of options delimitated by start/end tags.

```
<qdoas>
  <paths>
   ...
  </paths>
  <symbols>
   ...
  </symbols>
  <project name="MAXDOAS-VIS" disable="false">
    ...
    <analysis_window name="NO2" disable="false" kurucz="ref"
                     refsel="auto" min="425.000" max="490.000" >
      <display spectrum="true" poly="true" fits="true" residual="true"
               predef="false" ratio="true" />
      <files refone=""
             reftwo=""
             residual=""
             szacenter="0.000" szadelta="0.000" minlon="0.000" maxlon="0.000"
             minlat="0.000" maxlat="0.000" refns="0"
             cloudfmin="0.000" cloudfmax="0.000"
             maxdoasrefmode="sza"
             east="false" center="false" west="false" backscan="false" />
       ...
    </analysis_window>
    <raw_spectra>
      ...
    </raw_spectra>
  </project>
</qdoas>
```

Options related to a project are given within tags <project ...> and </project>. A project includes one or several <analysis_window ...> and </analysis_window> blocks with analysis windows properties.

Given this structure, an option can be easily reached by building a "path" with the tags of the successive blocks it belongs to. For example, the option **Reference 1** of the **Analysis windows properties** can be reached by :

```
/project/analysis_window/files/refone
```

To use a reference file other the one specified in the xml file, the switch -xml in the doas_cl command can be used as follows :

```
-xml "/project/analysis_window/files/refone=<new file>"
```

It is recommended to quote the whole command. If the name of the analysis window is specified, the changes are applied only on this window. Otherwise, they will be applied to all analysis windows of the project.

To modify the spectra range of the analysis window named NO2, two successive switches are used :

```
doas_cl <...> -xml "/project/analysis_window/NO2/min=450"
              -xml "/project/analysis_window/NO2/max=490"
```

If the xml command is recognized, the following lines should be displayed on the console :

```
/project/analysis_window/NO2/min : 425.00 replaced by 450 (NO2)
/project/analysis_window/NO2/max : 490.00 replaced by 500 (NO2)
```

All options of the configuration file can not be modified yet. doas_cl will indicate if a field can not be changed.

A Input file format

Spectra Files

Used in	Projects properties, Instrumental page
File name	no restriction;
File extension	**spe** by default, but it is not restrictive;
Format	Specific to the different institutes that developed them.
Example	See below for ASCII format

ASCII Spectra File Format

If a format is not supported by QDOAS, it should be possible to convert the files in ASCII. When the ASCII format is selected, spectra can be provided in the file one record per line (**line format**) or one spectral value per line (**column format**). The size of the detector has to be specified. Then, according to the checked flags in the **Instrumental page** of **Projects properties**, the following information are expected strictly in the given order :

- ◇ Solar Zenith Angle
- ◇ Azimuth Viewing Angle
- ◇ Elevation Viewing Angle
- ◇ Date in the DD/MM/YYYY (day, month, year) format
- ◇ Fractional time

Example of records in an ASCII file in **line format** with solar zenith angle, date and fractional time options checked :

```
78.417543 29/02/2000 8.181111 5504.343400...  25379.428769
77.426307 29/02/2000 8.356389 7568.723923...  25736.597692
76.444749 29/02/2000 8.536944 8371.684631...  27477.536662
                              <----- spectra values ----->
```

In the column format, **angles have to be given on the same line** and a wavelength calibration can be provided with spectra. Example of records in **column format** with solar zenith angle, elevation viewing angle and fractional time options checked :

```
59.7336 1                  <- SZA and elevation viewing angle
16.0452752135897           <- fractional time
  415.53904  4.1053669e+005
  415.57920  5.1616777e+005
  ...                        Wavelength and spectra values
  456.10521  5.0256531e+005
  456.14444  4.9851523e+005
58.6879 5                  <- record number 2
15.953346969803
  415.53904  5.1705925e+005
  415.57920  6.5113944e+005
  ...
```

```
  456.10521  6.4016200e+005
  456.14444  6.3482669e+005
60.4205 10                 <- record number 3
16.1055305555417
  415.53904  5.2111045e+005
  415.57920  6.5623468e+005
  ...
  456.10521  6.4077000e+005
  456.14444  6.3549114e+005
```

Calibration

Used in	Projects properties Tools
File name	no restriction;
File extension	**clb** by default, but it is not restrictive;
Format ASCII	**Column 1** : the wavelength calibration;
Example	ANYTHING.CLB

Cross-sections

Used in	Analysis windows properties Tools
File name	For cross-sections implied in the definition of analysis windows, the file name must start by the user defined relevant symbol followed by an underscore; this restriction does not apply to input cross-sections in QDOAS tools.
File extension	**xs*** by default, but it is not restrictive;
Format ASCII	**Column 1** : the wavelength calibration **Column 2** : the cross-section
Example	BrO_W228.XS

Solar Spectrum

Used in	Projects properties Tools
File name	no restriction;
File extension	**ktz** by default, but it is not restrictive;
Format ASCII	**Column 1** : the wavelength calibration **Column 2** : the solar spectrum
Example	KUR_01.KTZ

Reference spectrum

Used in	Analysis windows properties
File name	no restriction;
File extension	**ref** by default, but it is not restrictive;
Format ASCII	**Column 1** : the wavelength calibration **Column 2** : the reference spectrum
Example	80302191.REF

Instrumental function

Used in	Project properties
File name	no restriction;
File extension	**ins** by default, but it is not restrictive;
Format ASCII	**Column 1** : the wavelength calibration **Column 2** : the transmission function (spectra will be divided by this curve before the wavelength calibration procedure).
Example	Transmission.ins

Dark current and Offset (ex : MFC)

Used in **Projects properties**. Dark currents and offset are corrections specific to the selected instrument, so they have to be provided in the original format.

AMF

Used in Analysis windows properties

File name The name of AMF file associated to cross-sections implied in the definition of analysis windows must start by the user defined relevant symbol followed by an underscore;

File extension AMF_SZA for SZA dependent AMF;
AMF_CLI for climatology dependent AMF;
AMF_WVE for wavelength dependent AMF;

AMF_SZA Format **Column 1** : SZA
Column 2 : AMF

AMF_CLI Format

0	(JD-1)/365
SZA	AMF

Climatology dependent AMF have to be provided in a matrix whose first column is SZA grid and first line, day number grid.

AMF_WVE Format

0	λ
SZA	AMF

Interpolation is made in a 2-dimension matrix (first column is SZA grid and first line, some wavelengths).

Example BrO_W228.AMF_SZA

Slit functions

Used in	Analysis windows properties
File name	no restriction;
File extension	**slf** by default, but it is not restrictive;
Format ASCII	**Column 1** : the wavelength calibration **Column 2** : the line shape The slit function has to be provided with a wavelength calibration around 0 nm. For wavelength dependent slit function types, the second column is the parameter dependent on the wavelength. Since QDOAS version 2.00, lookup tables of wavelength dependent slit functions can be provided. In this case, the number of columns depends on the available slit functions. Wavelengths are specified in the first line of the file.

Example

```
 0                        340                     380
 -1.00  2.9802322387695299e-008  7.8886090522101049e-031
 -0.98  5.9192925419630987e-008  1.2276631396533808e-029
 -0.96  1.1594950525907111e-007  1.8074887363782194e-028
 -0.94  2.2399967890119956e-007  2.5176165401687836e-027
 ...
 -0.04  9.7265494741228542e-001  8.9502507092797223e-001
 -0.02  9.9309249543703593e-001  9.7265494741228542e-001
  0.00  1.0000000000000000e+000  1.0000000000000000e+000
  0.02  9.9309249543703593e-001  9.7265494741228542e-001
  0.04  9.7265494741228542e-001  8.9502507092797223e-001
...
  0.94  2.2399967890119956e-007  2.5176165401687836e-027
  0.96  1.1594950525907111e-007  1.8074887363782194e-028
  0.98  5.9192925419630987e-008  1.2276631396533808e-029
  1.00  2.9802322387695299e-008  7.8886090522101049e-031
```

Specific case : For wavelength dependent arbitrary slit function files (including lookup tables of slit functions), the variation of the two stretch factors to apply on the grid of the line shape is given in a three-columns file.

B Output

Information related to the measurements (e.g. date and time, viewing angles, geolocation data, ...) can be selected in the **Display** and the **Output pages** of **Projects properties**. The selected instrument or file format determines the list of fields available in this page. For example, information on cloud fraction and cloud top pressure is available only for satellite instruments. A non-exhaustive list of fields available for ground-based and satellite measurements is given in figure B.1.

In ASCII output files, columns are separated using tab characters and it is normal that they are not aligned with the column titles when the file is loaded in a simple text editor. Figure B.2 provides an example. For this application, the **calibration button** is checked and results of the calibration procedure precede the analysis results. The Root Mean Square (RMS), the shift between the reference spectrum and the solar spectrum and the calculated value of the FWHM of the fitted line shape (Gaussian in this application) for each of the sub-windows of the wavelength calibration interval are saved (see the **Calibration page** of **Projects properties** for further details).

The output in figure B.2 contains the following fields:

1. The record number (Spec No)
2. The year of measurements
3. The fractional calendar day
4. The fractional time
5. The number of scans
6. The exposure time (Tint)
7. The solar zenith angle (SZA)
8. The shift calculated between the spectrum and the reference in the no2 analysis window (no2.RefZm)
9. The RMS of the fit in the ? “no2” analysis window (no2.RMS)
10. The slant column of NO_2 calculated in the ”no2” analysis window (no2.SlCol(no2))
11. The error on the slant column of NO2 (no2.SlErr(no2))
12. The slant column of O_3calculated in the “no2” analysis window (no2.SlCol(O3))
13. ...

Field name	Description	Ground-based measurements	Satellite measurements
Altitude	the altitude of the instrument during the measurement	Available in some file format	
Azim. viewing angle	the azimuth viewing angle	According to the type of measurements	LoS Azimuth at point B
Chi Square	the χ2, the sum of square of residuals	x	x
Cloud fraction	the cloud fraction		GOME ERS2 and GOME2
Cloud Top Pressure	the cloud top pressure		GOME ERS2 and GOME2
Compass angle	compass angle for airborne measurements	Airborne measurements only	
Cooler status	the status of the cooling system	BIRA-IASB file format only	
Date & time (YYYYMMDDhhmmss)	measurement date and time in the specified format	x	x
Date (DD/MM/YYYY)	measurement date	x	x
Day number	the day number of measurement (integer from 1 to 366)	x	x
Earth radius	the radius of the earth		x
Elev. viewing angle	the elevation viewing angle	According to the type of measurements	LoS ZA at point B
Filter number	the filter number	Available in some file format	
Fractional day	the fractional day number	x	x
Fractional time	the fractional time	x	x
GDP NO2 VCD	the NO2 vertical column retrieved from the GOME Level-2 files		GOME GDP format
GDP O3 VCD	the total ozone column retrieved from the GOME Level-2 files		GOME GDP format
Head temperature	the temperature in the optic head	BIRA-IASB file format only	
Index coeff	the coefficients used to calculate the wavelength calibration		GOME GDP format
Iterations number	the iteration number	x	x
Latitude	the latitude of the instrument during the measurement	Available in some file format	x
Longitude	the longitude of the instrument during the measurement	Available in some file format	x
LoS Azimuth	the line of sight azimuth angle		given at points A, B, C
LoS ZA	the line of sight zenith angle		given at points A, B, C
Measurement type	the measurement type	Available in some file format	
Mirror status	the status of the mirror	BIRA-IASB file format only	
Name	the record name	Available in some file format	
Orbit number	the orbit number		x
Pitch angle	pitch angle for airborne measurements	Airborne measurements only	
Pixel number	the pixel number		GOME GDP format
Pixel type	the pixel type		GOME GDP format
Ref SZA	solar zenith angle of the reference spectrum	x	
Ref2/Ref1 shift	shift between Ref1 and Ref2 when two reference spectra are selected	x	x
Rejected	the number of rejected scans	Available in some file format	
RMS	the root mean square or the square root of the chi square	x	x
Roll angle	roll angle for airborne measurements	Airborne measurements only	
Satellite height	the satellite height		x
Scanning angle	the scanning angle	Available in some file format	
Scans	the number of scans	all except ASCII format	
SCIAMACHY Quality Flag	quality flag for SCIAMACHY measurements		SCIAMACHY only
SCIAMACHY State Id	state id for SCIAMACHY measurements		SCIAMACHY only
SCIAMACHY State Index	state index for SCIAMACHY measurements		SCIAMACHY only
Solar Azimuth angle	the solar azimuth angle	x	given at points A, B, C
Spec No	the record number	x	x
Start Date (DDMMYYYY)	date at the beginning of measurements	University of Toronto only	
Start Time (hhmmss)	time at the beginning of measurements	Available in some file format	
Stop Date (DDMMYYYY)	date at the end of measurements	University of Toronto only	
Stop Time (hhmmss)	time at the end of measurements	Available in some file format	
SZA	the solar zenith angle	x	given at points A, B, C
Tdet	the temperature of the detector	Available in some file format	
Time (hh:mm:ss)	measurement time	x	x
Tint	the exposure time	all except ASCII format	all except GDP format
Year	the year of measurement	x	x

Figure B.1.: A list of some of the output fields available in QDOAS.

```
; Calib.RMS Calib.SFP 1 Calib.Shift(Ref)
;  6.3281e-003  1.7772e+000  5.0290e-002
;  1.0623e-002  1.6887e+000  1.4931e-001
;  4.7789e-003  1.7718e+000  9.7033e-002
;  4.1439e-003  1.8126e+000  2.5568e-001
;  2.7647e-003  1.5897e+000  7.8512e-002
;  5.4757e-003  1.6247e+000  1.2608e-001
;  3.4599e-003  1.5409e+000  1.3272e-001
;  6.6463e-003  1.4055e+000  1.2555e-001
;  3.3634e-003  1.3380e+000  1.1108e-001
;  2.0073e-003  1.1712e+000  9.4016e-002
# Spec No Year Fractional day Fractional time Scans Tint SZA no2.RefZm no2.RMS no2.SlCol(no2) no2.SlErr(no2) no2.SlCol(o3) ...
   3 2010  16.284769    6.834444444444444     1   370.000000    93.455956   67.472  1.6204e-003  4.2013e+016  2.2423e+015  ...
   4 2010  16.288345    6.920277777777778     1   190.000000    92.671356   67.472  1.2127e-003  3.4127e+016  1.6782e+015  ...
   5 2010  16.292743    7.025833333333333     1    72.000000    91.715622   67.472  1.0063e-003  2.9196e+016  1.3926e+015  ...
   6 2010  16.294722    7.073333333333333     1    52.000000    91.288940   67.472  9.8481e-004  2.6081e+016  1.3628e+015  ...
   7 2010  16.296227    7.109444444444445     1    52.000000    90.966019   67.472  8.7168e-004  2.4254e+016  1.2063e+015  ...
   8 2010  16.296991    7.127777777777778     1    37.000000    90.802559   67.472  9.7069e-004  2.1932e+016  1.3433e+015  ...
   9 2010  16.298299    7.159166666666667     1    37.000000    90.523460   67.472  8.7238e-004  2.2109e+016  1.2072e+015  ...
  10 2010  16.298970    7.175277777777778     1    37.000000    90.380585   67.472  8.9183e-004  2.1461e+016  1.2341e+015  ...
  11 2010  16.299641    7.191388888888889     1    37.000000    90.237968   67.472  9.0008e-004  2.0794e+016  1.2456e+015  ...
  12 2010  16.300417    7.210000000000000     2    27.000000    90.073555   67.472  8.2671e-004  1.9166e+016  1.1440e+015  ...
  13 2010  16.302257    7.254166666666666     2    27.000000    89.684776   67.472  8.3183e-004  1.7197e+016  1.1511e+015  ...
  14 2010  16.303229    7.277500000000000     2    27.000000    89.480194   67.472  8.8032e-004  1.7134e+016  1.2182e+015  ...
  15 2010  16.304109    7.298611111111111     3    19.000000    89.295593   67.472  8.2983e-004  1.6257e+016  1.1483e+015  ...
  16 2010  16.305810    7.339444444444444     3    19.000000    88.939850   67.472  8.2490e-004  1.4891e+016  1.1415e+015  ...
  17 2010  16.306678    7.360277777777778     3    19.000000    88.759033   67.472  8.1263e-004  1.4015e+016  1.1245e+015  ...
  18 2010  16.307546    7.381111111111111     3    19.000000    88.578682   67.472  8.2421e-004  1.3783e+016  1.1406e+015  ...
  19 2010  16.308414    7.401944444444444     4    14.000000    88.398804   67.472  7.9733e-004  1.3064e+016  1.1034e+015  ...
  21 2010  16.319444    7.666666666666667     6    10.000000    86.155655   67.472  8.6106e-004  7.6774e+015  1.1916e+015  ...
  22 2010  16.321308    7.711388888888889     8     7.200000    85.784805   67.472  9.0389e-004  7.0009e+015  1.2508e+015  ...
  23 2010  16.322998    7.751944444444445     8     7.200000    85.450623   67.472  8.8281e-004  6.5996e+015  1.2217e+015  ...
  24 2010  16.323877    7.773055555555556     8     7.200000    85.277466   67.472  9.1311e-004  6.2825e+015  1.2636e+015  ...
  25 2010  16.324757    7.794166666666667     8     7.200000    85.104866   67.472  9.3670e-004  6.1341e+015  1.2962e+015  ...
  26 2010  16.325637    7.815277777777778     8     7.200000    84.932823   67.472  9.2760e-004  5.6908e+015  1.2836e+015  ...
  27 2010  16.326516    7.836388888888889     8     7.200000    84.761353   67.472  9.2331e-004  5.5878e+015  1.2777e+015  ...
  28 2010  16.327396    7.857500000000000     8     7.200000    84.590446   67.472  9.0594e-004  5.5403e+015  1.2537e+015  ...
  29 2010  16.328275    7.878611111111111     8     7.200000    84.420113   67.472  9.1884e-004  4.9534e+015  1.2715e+015  ...
  30 2010  16.329155    7.899722222222223     8     7.200000    84.250359   67.472  9.2554e-004  5.1407e+015  1.2808e+015  ...
  31 2010  16.330035    7.920833333333333     8     7.200000    84.081184   67.472  9.6229e-004  4.8166e+015  1.3317e+015  ...
  32 2010  16.330914    7.941944444444444     8     7.200000    83.912598   67.472  9.4661e-004  4.9410e+015  1.3099e+015  ...
  33 2010  16.331794    7.963055555555556     8     7.200000    83.744606   67.472  9.4779e-004  4.4337e+015  1.3116e+015  ...
  34 2010  16.333623    8.006944444444445    11     5.200000    83.397255   67.472  9.6634e-004  4.0186e+015  1.3373e+015  ...
  35 2010  16.335313    8.047499999999999    11     5.200000    83.078598   67.472  1.0075e-003  4.0440e+015  1.3942e+015  ...
```

Figure B.2.: Example of ASCII output generated by QDOAS.

Information on the measurement					Results in the no2 analysis windows			Results in the o3 analysis windows			
Fractional day	Fractional time	SZA	Tint	Scans	no2.RMS	no2.SlCol(no2)	no2.Shift(Spectrum)	o3.RMS	o3.SlCol(no2)	o3.SlCol(o3)	o3.Shift(Spectrum)
121.110926	2.662222	94.264435	30	10	1.3507E-03	9.7441E+16	-4.4727E-03	1.4278E-03	9.9785E+16	2.3290E+20	-7.2725E-03
121.118692	2.848611	93.191666	300	1	1.4670E-03	8.9633E+16	-5.3057E-03	9.7118E-04	8.9410E+16	2.3735E+20	-7.8688E-03
121.125012	3.000278	92.291199	175	1	1.0263E-03	7.8968E+16	-5.7724E-03	7.9208E-04	7.8775E+16	2.2592E+20	-8.0405E-03
121.132558	3.181389	91.185425	75	4	6.4970E-04	6.4068E+16	-5.6592E-03	6.3902E-04	6.4525E+16	1.9791E+20	-7.4061E-03
121.136921	3.286111	90.531677	55	6	5.3305E-04	5.6060E+16	-5.6395E-03	5.9283E-04	5.6766E+16	1.7931E+20	-7.0787E-03
121.141181	3.388333	89.883873	40	7	4.0971E-04	4.8983E+16	-5.5500E-03	6.0563E-04	5.0389E+16	1.6208E+20	-6.7385E-03
121.146111	3.506667	89.122551	30	12	3.3785E-04	4.1753E+16	-5.8020E-03	6.1831E-04	4.3728E+16	1.4350E+20	-6.6600E-03
121.150231	3.605556	88.477341	20	18	3.5418E-04	3.6562E+16	-5.5562E-03	6.3690E-04	3.8874E+16	1.3007E+20	-6.4225E-03
121.154005	3.696111	87.879639	15	18	3.5597E-04	3.2664E+16	-5.3633E-03	6.2127E-04	3.4858E+16	1.1796E+20	-6.1987E-03
121.158368	3.800833	87.180603	10	30	2.9240E-04	2.8658E+16	-6.0796E-03	5.2140E-04	3.0385E+16	1.0331E+20	-6.5743E-03
121.162558	3.901389	86.501846	10	30	2.6022E-04	2.5524E+16	-6.8018E-03	4.6458E-04	2.7132E+16	9.2917E+19	-7.1440E-03
121.168519	4.044444	85.524200	7.5	39	2.2336E-04	2.1845E+16	-6.9571E-03	4.2663E-04	2.3320E+16	8.1449E+19	-7.4855E-03
121.174525	4.188611	84.525635	5.5	53	2.3448E-04	1.8586E+16	-7.9820E-03	3.0474E-04	1.9696E+16	6.9258E+19	-8.2730E-03
121.180544	4.333056	83.512787	5.5	53	2.2280E-04	1.6013E+16	-8.1626E-03	3.1061E-04	1.7167E+16	6.0824E+19	-8.5144E-03
121.186435	4.474444	82.510422	5.5	53	2.0947E-04	1.3857E+16	-7.8369E-03	3.3111E-04	1.4940E+16	5.3602E+19	-8.1247E-03
121.192188	4.612500	81.522194	4	72	2.1789E-04	1.2035E+16	-8.0944E-03	2.6116E-04	1.2840E+16	4.6788E+19	-8.2143E-03
121.197975	4.751389	80.519478	4	72	2.0444E-04	1.0608E+16	-7.9407E-03	3.0132E-04	1.1501E+16	4.2303E+19	-8.0659E-03
121.203819	4.891667	79.499039	4	77	2.0458E-04	9.6225E+15	-7.9556E-03	3.1058E-04	1.0758E+16	3.8465E+19	-8.0567E-03
121.209352	5.024444	78.526909	2	137	1.8826E-04	8.2901E+15	-7.0092E-03	2.0252E-04	9.1008E+15	3.3766E+19	-7.3214E-03
121.215116	5.162778	77.508568	2	146	1.9988E-04	7.5296E+15	-7.3432E-03	2.4012E-04	8.6531E+15	3.0690E+19	-7.6187E-03

Example of output generated by QDOAS and loaded using Excel.
In this example, only the fractional date and time, the solar zenith angle (SZA), the exposure time (Tint) and the number of scans have been selected in the **Output page** of **Projects properties**. The application contains two analysis windows (no2 and o3). In this example, the NO2 column has been retrieved from both no2 and o3 windows. The column title starts with the name of the analysis window. Slant columns are indicated by **SlCol**; errors on slant columns by **SlErr** (not present in this example).

# Date & time (YYYYMMDDhhmmss)	Latitude(1)	Latitude(2)	Latitude(3)	Latitude(4)	Latitude (pixel center)	Longitude(1)	Longitude(2)	Longitude(3)	Longitude(4)	Longitude (pixel center)	SZA(A)	SZA(B)	SZA(C)
20081101005057.400000	-85.546806	-86.130089	-85.292442	-85.772873	-85.788170	-52.098881	-52.269180	-30.390318	-27.930834	-40.250431	78.919197	79.260002	79.876480
20081101005057.600000	-85.546806	-86.130089	-85.491753	-86.034256	-85.829269	-52.098843	-52.269138	-41.490208	-40.181370	-46.468582	78.919197	79.148293	79.387756
20081101005057.800000	-85.504166	-86.052078	-85.321762	-85.816452	-85.699341	-42.647118	-41.484276	-32.738930	-30.496643	-36.741394	79.336899	79.564804	79.797203
20081101005058.000000	-85.345139	-85.845619	-85.046555	-85.487846	-85.454216	-33.699413	-31.544424	-24.657108	-21.857054	-27.798925	79.751816	79.984985	80.213982
20081101005058.200000	-85.077072	-85.523720	-84.683258	-85.071953	-85.108315	-25.421968	-22.662062	-17.544973	-14.515321	-19.884333	80.173485	80.402267	80.632378
20081101005058.300000	-84.717667	-85.110893	-84.253319	-84.594345	-84.684753	-18.138636	-15.119659	-11.485102	-8.447759	-13.156230	80.596146	80.822212	81.047653
20081101005059.100000	-82.706650	-82.942383	-82.079849	-82.289673	-82.511307	1.589660	4.153407	4.979877	7.347762	4.590302	82.276932	82.501884	82.721901
20081101005059.500000	-81.495354	-81.686485	-80.830109	-81.004822	-81.258324	7.577471	9.787894	10.061144	12.124291	9.931158	83.123260	83.347649	83.567696
20081101005059.800000	-80.217331	-80.380623	-79.527931	-79.681641	-79.954285	11.991574	13.947298	13.859651	15.723614	13.901634	83.969322	84.193123	84.413368
20081101005103.200000	-84.990997	-85.481735	-83.871201	-84.204536	-84.751106	-32.677650	-30.600973	-11.110887	-8.301934	-19.372065	80.119469	80.776337	81.427582
20081101005103.400000	-85.202606	-85.785927	-84.966904	-85.452217	-85.448189	-52.025188	-52.157120	-31.816395	-29.671967	-41.078465	79.207077	79.548241	80.163574
20081101005103.600000	-85.202606	-85.785927	-85.150017	-85.693390	-85.485168	-52.025154	-52.157082	-42.126835	-40.989548	-46.789959	79.207077	79.438522	79.678085
20081101005103.800000	-85.161629	-85.710159	-84.991165	-85.489609	-85.362457	-43.202785	-42.191051	-33.984852	-32.032154	-37.770855	79.627213	79.855202	80.085922
20081101005104.000000	-85.013008	-85.516891	-84.730034	-85.177742	-85.131783	-34.886841	-33.012489	-26.282328	-23.805965	-29.376274	80.040497	80.277229	80.506210
20081101005104.200000	-84.758781	-85.211555	-84.388474	-84.786461	-84.805023	-27.008970	-24.571575	-19.511747	-16.791721	-21.841866	80.465714	80.692986	80.921761
20081101005104.300000	-84.421082	-84.823410	-83.976028	-84.327660	-84.402779	-20.085287	-17.378704	-13.572090	-10.802816	-15.331815	80.885506	81.113075	81.339851
20081101005104.500000	-84.010376	-84.365540	-83.511162	-83.821960	-83.940094	-14.018887	-11.248859	-8.485973	-5.786962	-9.770410	81.307281	81.531189	81.755417
20081101005104.700000	-83.545860	-83.859451	-82.998322	-83.273727	-83.429916	-8.833926	-6.127674	-4.087526	-1.521368	-5.041052	81.725945	81.950691	82.174507
20081101005105.300000	-81.905869	-82.128220	-81.269379	-81.470413	-81.698967	2.748437	5.010471	5.733624	7.843977	5.390619	82.991005	83.216759	83.437584

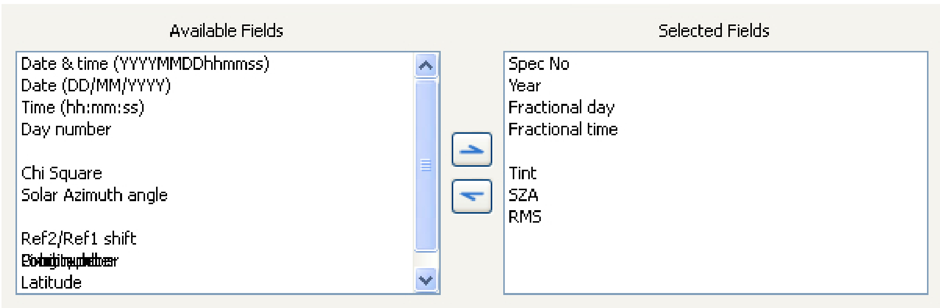
Example of output file generated by QDOAS and loaded using Excel.
This example has been generated from a satellite application (GOME-2). Results of the fit are not shown here. For satellite measurements, the accuracy of the measurement time is important. The format YYYYMMDDhhmmss (year, month, day, hour, minute, second accolated; milliseconds in the fractional part) is usually preferred to the fractional date and time. Geolocation coordinates are given at the four corners and at the centre of the pixel. Angles such as the solar zenith angles are given at the beginning, the middle and the end of the measurement.

C Troubleshooting

This section describes some problems that could be met with the user interface or some error messages displayed by QDOAS. Most of error messages come from a wrong configuration (calibration or analysis settings). If you can not solve a problem or if you have detected a bug, it's important to contact authors. The log file produced by QDOAS in the application directory is an important source of information for us. A small application with a detailed description of the trouble and the sequence of manipulations leading to it can help us to solve the problem quickly.

C.1 Known user interface problems

Refreshing Problem In The Projects Properties



In the **Display** and the **Output pages** of **Projects properties**, the list of available fields that can be selected for display or output depend on the file format. There is a problem with the refreshing of the list (missing fields or overwritten fields) after the selection of a new instrument or file format. The list is correctly refreshed after quitting the **Projects properties** dialog box on **OK** and load it again.

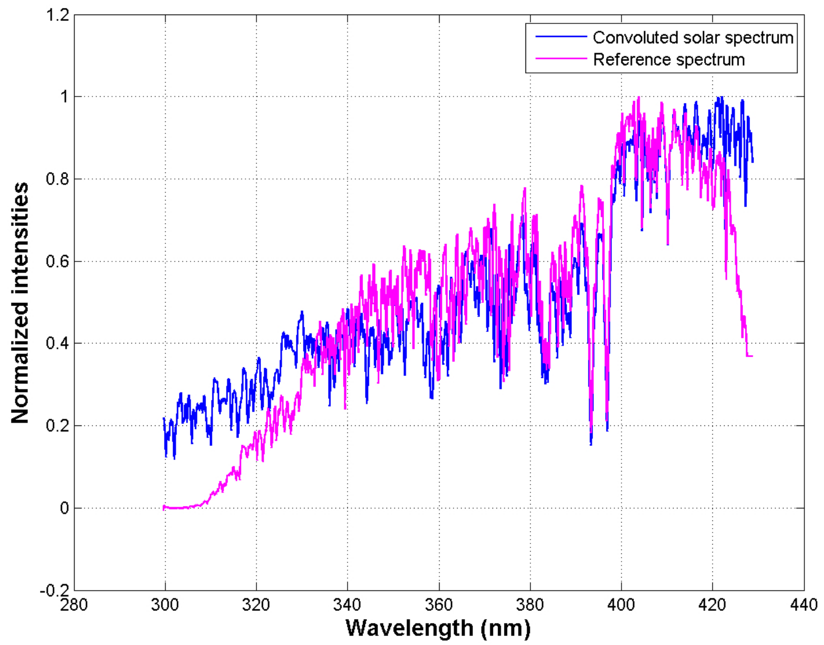
All selected fields in the output page will be in the **output file** but some selected fields in the **Display page** could still have no effect on the display in the **Data page**.

C.2 Analysis problems

Calibration problems

Most problems usually come from the original wavelength calibration of the reference spectrum. QDOAS corrects small shifts but the NLLS algorithm may not converge if the initial values are too far away from the solution (convergence to a local minimum of the chi-square). Before using

QDOAS, it is recommended to determine the preliminary wavelength calibration with a mercury lamp or to pre-convolve a solar spectrum at the resolution of your instrument, plot it with your spectrum and fit a polynomial through some pixels/nm couples set from the most representative Fraunhofer lines. In the example below, even if the calcium lines match between the reference spectrum and the solar spectrum convolved at the resolution of the instrument, we can see that the wavelength calibration is completely wrong below 380 nm. The differences are too large for QDOAS and it is better to correct that manually before running the calibration procedure.



Analysis error messages

Log error :

This message occurs mainly when the signal of the spectrum is too poor. Usually, the message can be ignored if the cause can be identified : poor light conditions during twilight... If this error is systematic, the fit of a linear offset can be preferred to a non linear one (see page 82) or the fitting interval can be adjusted to another region where the signal is higher.

Sqrt argument error :

Curfit error :

Ill-conditioned matrix :

These two messages are usually related to a problem with the configuration.
Check that all cross-sections are defined in the fitting interval. This can be done by right-clicking the **"View cross sections"** option from the analysis windows items.
Eventually, reduce the number of fitting parameters to the minimum (just the polynomial) and proceed step by step in order to identify the problem.
If the problem occurs during the calibration procedure, report to the section **"Calibration problems"** above.

Allocation error during the Kurucz procedure :

The degree of the polynomial fitting the continuous part of spectrum has not been defined in the **"Linear parameters page"** (see **Calibration page** of **Projects Properties**, page 65).

spline interpolation requests increasing absissae (...) :

The problem can come from a bad input file (preliminary wavelength calibration in the **"Instrumental page"** of **Projects properties**, cross-section, reference spectrum) or the wavelength calibration procedure doesn't succeed to correct the preliminary wavelength calibration (report to the section **"Calibration problems"** above).

Number of degree of freedom <= 0... :

Too many parameters are fitted w.r.t. the size of the fitting interval or the settings of the filter are not suitable. Reduce the number of parameters to fit, increase the fitting interval or adjust the size of the filter. Check also the calibration settings (Calibration page of Projects Properties).

Cross-section file is empty or not large enough :

Check that all cross-sections are defined in the fitting interval. This can be done by right-clicking the **"View cross sections"** option from the analysis windows items. Do not also forget the cross sections and the solar spectrum defined in the Calibration page of Projects Properties.

Glossary

AMF Air Mass Factor

ASCII American Standard Code for Information Interchange

BEAT Basic Envisat Atmospheric Toolbox

BIRA-IASB Belgian Institute for Space Aeronomy

Cic Colour Index

CINDI Cabauw Intercomparison Campaign of Nitrogen Dioxide measuring Instruments

CODA Common Data Access Toolbox

DISORT Discrete Ordinates Radiative Transfer program

DOAS Differential Optical Absorption Spectroscopy

DOASIS DOAS Intelligent System

ENVISAT Environmental Satellite

ERS European Remote Sensing Satellite

FFT Fast Fourier Transform

FWHM Full Width at Half Maximum

GDP Gome Data Processor

GOME Global Ozone Monitoring Experiment

GPL General Public License

GUI Graphical User Interface

HDF Hierarchical Data Format

HDF-EOS Hierarchical Data Format - Earth Observing System

HTML Hypertext Markup Language

JPG Graphics file format developed by the Joint Photographics Expert Group

LIDORT Linearized Discrete Ordinate Radiative Transfer Program

M-L Marquardt-Levenberg

MAXDOAS Multi-Axis DOAS

METOP Meteorological Operational satellite

NDACC Network for the Detection of Atmospheric Composition Change

NLLS Non-Linear Least Squares

OHP Observatoire de Haute Provence, France

OMI Ozone Monitoring Instrument

PDS Payload Data Segment (SCIAMACHY)

PNG Portable Network Graphics format

RMS Root Mean Square

RRS Rotational Raman Scattering

S[&]T Science and Technology `http://www.stcorp.nl`

SAOZ Système d'Analyse par Observation Zénithale

SCD Slant Column Density

SCIAMACHY Scanning Imaging Absorption spectrometer for Atmospheric Cartography

SFP Slit Function Parameter

SVD Singular Value Decomposition

SVN Subversion, software revision control system

SZA Solar Zenith Angle

VCD Vertical Column Density

XML Extensible Markup Language

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