LUFTBLICK
EARTH OBSERVATION TECHNOLOGIES

Manual for Blick Software Suite 1.8

Manual version 1.8-3, 28 Apr 2021

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Contents

Document Change Record

Issue	Date	Section	Modifications
1	21 Dec 2014	All	First version
2	25 Mar 2015	All	Started expanding L2Fit algorithm, several minor modifications
3	31 Jul 2015	All	Added several sections and applied corrections suggested by Thorsten Fehr and Stefano Casadio
4	30 Jan 2016	All	Expanded BlickF description, IO section and algorithm section; introduced s-, f- and r-codes
5	7 Aug 2016	All	Completed description of L0, L1, L2 files and Processing Setup
6	15 Jan 2017	All	All sections filled; first complete version
7	20 Apr 2017	IO	More description in IO section (calibration file, BlickP config-file)
8	28 Aug 2017	IO	Changes in calibration file
9	11 Dec 2017	IO	Changes in calibration file and data processing
10	18 Jun 2018	IO	Updated description of meta data information in data files, stray light parameters and data quality indices
11	21 Jan 2019	All	Update IO section and make a general review of the manual
1-7	24 Oct 2019	IO	Change manual versioning to match SW versioning, Update IO section, routine description, schedule description
1.8-1	29 Dec 2020	All	Updated convolution technique, Updated output data description, New uncertainty section, Updated ATBD, New section with climatologies
1.8-2	3 Mar 2021	All	Updated ATBD
1.8-3	28 Apr 2021	Setup	Updated routines and schedules sections

Acronyms and Abbreviations

2D	Two dimensional
LuftBlick	LuftBlick OG
AC	Alternating Current
AD	Analog-to-digital
AMF	Air mass factor
AOD	Aerosol Optical Depth
ASCII	American Standard Code for Information Interchange
AtmVar	Atmospheric Variability
AtmVar($L1_i$)	Atmospheric variability of level 1 data for pixel i
BC	Bright counts
BlickF	Blick file-transfer and operation-monitoring software
BlickO	Blick operating software
BlickP	Blick processing software
BlickSFA	Blick spectral fitting algorithm
CCD	Charge-Coupled Device
CMOS	Complementary Metal-Oxide–Semiconductor
COSPAR	Committee on Space Research
DC	Dark counts
DLL	Dynamic-link-library
DN	Digital number
DOAS	Differential Optical Absorption Spectroscopy
DQ	Data quality
DQ0	Data quality 0
DQ1	Data quality 1
DQ10	Data quality 10
DQ11	Data quality 11
DQ12	Data quality 12
DQ2	Data quality 2
DQ20	Data quality 20
DQ21	Data quality 21
DQ22	Data quality 22
DQF	Data quality flag
DU	Dobson Units
ESA	European Space Agency
FEL lamp	ANSI standard 1000 watt quartz halogen lamp
FOV	Field of View
FTP	File Transfer Protocol
FWHM	Full Width at Half Maximum
GPS	Global Positioning System
GUI	Graphical User Interface
HDF	Hierarchical Data Format
ICF	Instrument Calibration File
IOF	Instrument Operation File
IP address	Internet protocol address
ISO	International Organization for Standardization
JPEG	Joint Photographic Experts Group

L0	Level 0
L1	Level 1
L2	Level 2 files
L2	Level 2
L2*	Level 2Fit and L2 files
L2Fit	Level 2 spectral fitting results file
LZA	Lunar Zenith Angle
NASA	National Aeronautics and Space Administration
OD	Optical Depth
ODR	Optimized Dark Ratio
Pandora	Pandora spectrometer system
PAZ	pointing azimuth
PDF	Portable Document Format
PGN	Pandonia Global Network
PRNU	Pixel Response Non Uniformity
PZA	Pointing zenith angle
QA	Quality Assurance
QC	Quality Control
RAM	Random-access memory
rms	Root Mean Square
ROE	Readout electronics
RTC	Radiative Transfer Calculations
SI	International System of Units
SkyFOV	Field of view for sky observations
SNR	Signal to noise ratio
SunFOV	Field of view for direct sun observations
SZA	Solar Zenith Angle
U	Total uncertainty
U_C	Common uncertainty
U_I	Independent uncertainty
$U_I(L1_i)$	Independent instrumental uncertainty of level 1 data for pixel i
U_S	Structured uncertainty
USB	Universal Serial Bus
UT	Universal Time

1 Introduction

1.1 About this Manual

This manual is an official document of

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It describes the Blick Software Suite, which operates the Pandora spectrometer system (Pandora) and other similar instrumentation. It can be downloaded as PDF from `https://www.pandonia-global-network.org/home/documents/manuals/`. Note that hardware related information about Pandora such as instrument installation and maintenance is not described in this manual. For this refer to the "SciGlob Pandora Installation Manual" [3], which can be downloaded from the same site.

1.2 Overview

The Pandora project was initiated in 2006 at the Atmospheric Chemistry and Dynamics Laboratory, Code 614, at NASA Goddard Space Flight Center under principal investigator Jay Herman. NASA has continuously funded Pandora-related projects ever since. Since 2011 Pandora is manufactured by SciGlob Instruments and Services, Maryland, USA (see `http://sciglob.com/`). Starting in 2013, ESA started to fund Pandora-related projects under principal investigator Alexander Cede. LuftBlick is responsible for Pandora-related software development since 2010 with funding from NASA and ESA projects. This manual describes the Blick Software Suite version 1.8.

The main part of the software and the entire manual are written by Alexander Cede. Other team members, who have contributed to the Blick Software Suite, or this manual, are:

- Daniel Santana
- Elena Spinei
- Christian Posch
- Martin Tiefengraber
- Christian Retscher
- Nader Abuhassan

There are three separate pieces of software described in this manual:

BlickO
The Blick operating software reads the Instrument Operation File (IOF), connects to the instrument hardware, changes filterwheel positions, moves the tracker, operates the camera, controls the temperature box, takes spectroscopic measurements, saves the raw signals, called Level 0 (L0) data, and provides a graphical user interface (GUI) for the user to display current data and to operate Pandora.

BlickF
The Blick file-transfer and operation-monitoring software serves two purposes. One task is to automatically push files from a local directory to a remote directory at a user selected frequency. The other task is to monitor BlickO and restart it if needed.

BlickP
The Blick processing software reads the IOF and Instrument Calibration File (ICF), reads the L0 data and converts them into Level 1 (L1) data, which are corrected signals, i.e. all instrumental corrections applied on the L0 data. It also creates different types of Level 2 (L2) data (slant column amounts, vertical column amount, surface concentrations, etc.).

The Blick Software Suite is written in the open source programming language Python (`http://python.org/`). The Windows setup files and other necessary files are freely available from `http://pandonia.net/docs/`.

2 Software Installation

2.1 Computer Requirements

Although Python is a platform independent programming language, BlickO has to run on Windows NT or later for most Pandora systems, since most spectrometer types currently used are controlled through a manufacturer supplied Windows DLL. BlickF and BlickP are platform independent. No minimum requirements for RAM or processor speed are needed. In order to run a Pandora, the operating computer needs to have one USB connection for each spectrometer, one serial connection to control the head sensor and one serial connection for the temperature control.

2.2 Blick Software Suite Installation

If the user decides to run the Blick Software Suite on a Windows machine and does not intend to make modifications to the source code, it is not necessary to install the Python programming language. The Blick Software Suite can be installed from a setup file and run from the executable files (e.g. for BlickO the file `/bin/BlickO.exe`). The starting slash / stands for the installation directory, e.g. `C:/Blick/`. If the user wants to use another operating system (e.g. Linux) or make modifications to the source code, he first needs to install the Python programming language on his computer. Section 2.4 describes how to install Python with all the modules needed to run the Blick Software Suite. It is also useful to make some modifications on the computer running BlickO. In section 2.5 we give a list of recommendations for this purpose.

Here we explain how to install the Blick Software Suite on a Windows machine. On another platform the whole directory structure (except for `/bin/`) as described in section 2.3 has to be copied. We recommend installing the Blick Software Suite before connecting the USB or serial interfaces of a Pandora spectrometer system, since the necessary drivers are installed during the setup process (see also *Abuhassan et al.* [3]).

Execute the setup file `Blick-OPF-1.8.*_setup.exe`. Choose the directory for the installation (we recommend `C:/Blick/`). The chosen directory should NOT have write protection. When finished, icons for BlickO, BlickF and BlickP will be created on the desktop. To run any of the programs just double-click the respective icon or directly the executable file (`/bin/BlickO.exe`, `/bin/BlickF.exe` and `/bin/BlickP.exe` respectively).

If the Python programming language is installed on the computer, BlickO, BlickP or BlickF can also be started by double-clicking the Python files `blick_osmain.pyw`, `blick_filepush.py` or `blickp.py` respectively, which are all located in the source code directory `/src/`. Finally, one could also use a Python editor (e.g. the one listed in section 2.4) to load one of the above files, and then run or debug it. Only when source code modifications are made and the software is being debugged do we recommend using the last editor method. For operational use, this method has often caused the computer to "hang" after a while, since the editors usually have multiple additional threads running, which can cause loss of control.

When starting BlickO, a dialog appears saying "Choose an instrument operation file". For the first use of BlickO, you can choose Pandora 0, which is a virtual Pandora unit used for testing purposes, or you can click "Cancel" and then copy the IOF of the Pandora unit you want to run into directory `/data/operationfiles/` (see section 5.3).

To upgrade to a newer Blick Software Suite version, just execute the new setup file and choose the same software directory (allow it to overwrite). The source code, executables, routines, etc. will then be updated, while all data files such as alignment files, L0 files, etc. will be untouched. If the setup process stops, because a previously installed software version is write-protected, we recommend stopping the setup process, then uninstalling the previous version (execute file `/unins000.exe`), and then executing the setup file again.

To connect to the Pandora unit after successful installation of the Blick Software Suite, use the BlickO GUI "Connection buttons" as described in section 3.1.

2.3 Blick Software Suite Directory Structure

This section describes the directory structure of the Blick Software Suite, which is automatically created when installing from a setup file as described in section 2.2. In this case, the files `/unins000.dat` and `/unins000.exe` are also created in the installation directory. These files are used if the software is uninstalled or if a newer version is installed.

Below is a complete list of the directories used in the Blick Software Suite. Again, the starting slash / stands for the installation directory, which can be chosen by the user during the setup process (e.g. `C:/Blick/`).

/src

This directory contains the Python source code files (`blick_*.py`, `blick_*.pyw` or `blickp_*.py`) and possibly the compiled Python files (`blick_*.pyc` or `blickp_*.pyc`).

/lib

This directory contains subdirectories `/oslib`, `/pslib` and `/fslib`, which contain a variety of files needed to run BlickO, BlickP or BlickF respectively.

/lib/routines

This directory contains "routine files" (`XY.rout`, where XY is any two letter or one letter plus one number combination). A "routine" is a sequence of commands for a Pandora unit (e.g. direct sun observations SO). For more details see sections 3.1 and 4.1.

/lib/schedules

This directory contains "schedule files" (`*.sked`). A "schedule" is a sequence of routines to be executed over the course of the day. For more details see sections 3.1 and 4.2.

/log

This directory contains subdirectories `/oslog`, `/fslog` and `/pslog`, which will be filled by BlickO, BlickF or BlickP respectively with "error-log-files", "warning-log-files" and "info-log-files" (`*_errorlog.txt`, `*_warninglog.txt` and `*_infolog.txt`). Each time an error or warning occurs, an error-log or warning-log entry is added log-file. The info-log-file is filled in addition with information like "Started schedule XY", "Connected tracker", etc.

/data/tmp, /data/L0, /data/L1, /data/L2Fit, /data/L2

These directories contain temporary data files and L0, L1 and L2 data files respectively. Raw data files produced by BlickO go initially into directory `/data/tmp` and are then pushed to directory `/data/L0` once they are finished. Care should be taken when opening/reading these temporary files in directory `/data/tmp`, since they are currently in use and are permanently written on.

/data/operationfiles

Instrument operation files (`*_of.txt`) contain the hardware information for a specific Pandora unit (section 5.3). In order to run BlickO or BlickP, the IOF must be present.

/data/calibrationfiles

Instrument calibration files (`*_cf.txt`) contain the calibration data for a specific Pandora unit (section 5.11). In order to run BlickP the correct ICF must be present.

/data/alignments

This directory has the "alignment files" (`*_alignments.txt` or `*_alignments_YYYYMMDDTHHMMSSZ.txt`), which contain results of the "alignment routines". These routines are sun (or moon) scanning sequences that allow determining the exact pointing of the instrument towards the sun or moon. Some scanning routines also produce pictures, which are stored inside this directory in subdirectories `/figures` and `/figures_ddf`. More details can be found in section 5.16.

/data/diagnostic

This directory will be filled with diagnostic data (or figures) of a Pandora unit, e.g. the temperature evolution over a day or the count rate at a specific wavelength.

/config

This directory contains the "configuration files". These files list parameters, which are configured by the user to run BlickO, BlickF or BlickP, e.g. the size of the GUI window or the last location selected. For BlickO these settings can be changed during software operation. At the end of each BlickO session, the configuration file is updated. The configuration files are described in sections 5.4, 5.5, 5.6 and 5.9.

/doc

This directory contains documentation, e.g. this manual itself.

/bin

This directory contains the executable files `BlickO.exe`, `BlickF.exe` and `BlickP.exe` and many other files (mostly *.dll and *.pyd files). It is not needed if the software is run directly from the Python file in the source code.

2.4 Python Installation

If the user intends to make modifications to the source code of the Blick Software Suite it is necessary to install the Python programming language as described in this section. Note that such modifications are only allowed, if the license shown in section 1.1 is obeyed.

Python consists of a basic software package and additional modules for specific purposes. The step-by-step instructions below show how to download and install all modules needed for the current Blick Software Suite version 1.8. Note that before performing the steps below, the Blick Software Suite should be installed as described in section 2.2, i.e. in directory C:/Blick/.

Step 1: Program language "Python"

Download file `https://www.python.org/ftp/python/2.7.17/python-2.7.17.msi`
Execute the file using the default directory C:/Python27/

Step 2: Module for GUI functions "wxpython"

Download file `https://sourceforge.net/projects/wxpython/files/wxPython/2.8.12.1/wxPython2.8-win32-unicode-2.8.12.1-py27.exe/download`
Execute the file using default directory C:/Python27/Lib/Site-packages/

Step 3: Get remaining packages

Open an command window and run the following commands:

```
cd C:/Blick
C:/Python27/python.exe -m pip install -r requirements.txt
```

2.5 Recommended Computer Settings

This section contains recommendations, which we have found very useful, when running a Pandora spectrometer system. Although they are for Windows operating systems only, it might be useful to read them for other platform installations too in order to understand the basic concept behind them. The purpose of these settings is to keep routine computer operating system operations from interfering with Pandora operations.

Antivirus
Choose an antivirus program that does not ask you too frequently for restarts of your computer.

Firewall and updates
1) Turn on Windows Firewall (Control Panel – Windows Firewall - Turn Windows Firewall on or off)
2) Download all windows updates. Repeat the updating as often as needed until no updates are found.
3) Set automatic updates: Control Panel – Windows Update - Change Settings – Check "Download them but let me choose ...". Do Windows updates manually, preferably during night.

Windows 10 does not allow to disable windows updates. But this option could help to avoid having windows stuck in the blue login screen waiting for user actions, after it does a major update:
Go to Search - Notifications & Actions settings - disable this option: "Show me the windows welcome experience after updates and occasionally when I sing in to highlight what's new and suggested"

Power options
Go to Control Panel – Power Options - Change Plan Settings - Change advanced power settings - set options to...
... Hard disk: Turn off hard disk after: Never
... Sleep: Sleep after: Never, Hibernate after: Never
monitor after 15 minutes, never turn off hard disk or do standby
... Power buttons and lid: Lid close action: Do Nothing.
... Display: Dim display after: 5 min, Turn off display after: 10 min

Internet time
To keep the computer time correct in a controlled way, the open source software NetTime v3.14 can be used (`https://www.timesynctool.com/`). It is recommended to switch the primary synchronization server of the computer from "0.nettime.pool.ntp.org" to "time.windows.com", and configure it to synchronize the hour every 24h. When using this app, it is recommended to switch off the windows inbuilt option to synchronize the hour automatically. IN order to do this go to Control Panel - Clock and Region - Set the time and date - Internet Time - Change Settings - uncheck "Synchronize with an internet time server"

Windows sign-in credentials
Depending of the internet requirements of your institution, a windows sign-in password may be mandatory. If this is the case, then it is recommended to configure the computer to automatically log-in using the configured password, without the need of user intervention, if the computer is restarted by a windows update or by an unexpected power outage. Otherwise the instrument operation will be interrupted until the somebody notices this). To do this open a command window and run "netplwiz" - Uncheck the option "Users must enter a user name and password to use this computer" (the password will be requested to be able disabling this option).

Task manager
Go to Control Panel – Administrative Tools - Task Scheduler - Task scheduler library

Remove unnecessary tasks, especially those that say under "Triggers": "After triggered, repeat every XX:XX for a duration of YY." or even "...repeat indefinitely..." (e.g. Adobe Flash Player Updater)

3 Blick Software Suite Description

3.1 BlickO - Instrument Operation

3.1.1 BlickO Startup

When BlickO is started, the user is first asked to select an IOF in a file selection dialog (figure 1). If a different IOF is selected then at the previous use of BlickO, a warning message will appear in order to avoid that users unintentionally select a wrong IOF. Another warning message might appear, in the case the selected instrument is already in use. Note that this warning message can also appear in the case BlickO was not closed properly in the previous use of the software.

Then BlickO checks internet connections, power status etc. of the operating computer, which can take a few seconds. If the previous use of BlickO was at another IP address than the current one or has been more than a full day ago, another warning message appears to remind the user, that he might be at a different location now.

Note: BlickO also writes to and reads from the so-called "BlickO-BlickF Messenger File" `/log/Blick_message.txt` in order to communicate with BlickF. The meaning of this file is described in section 3.2.

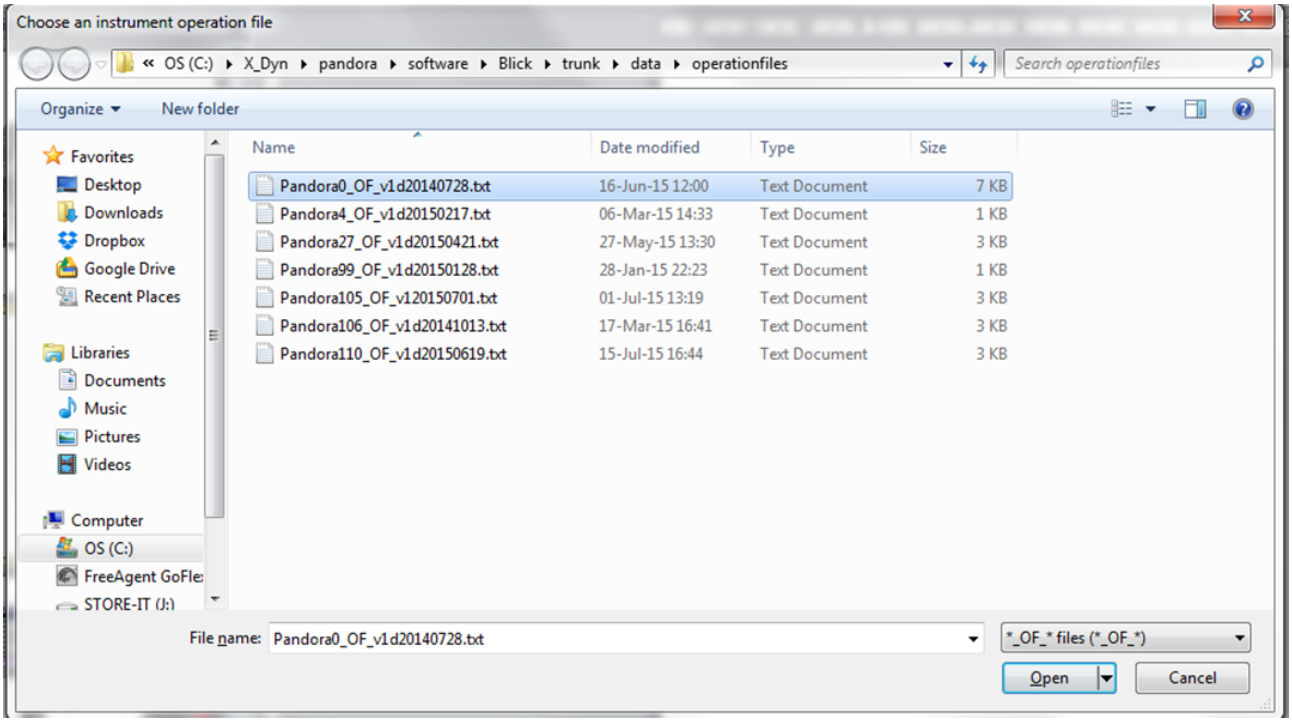


Figure 1: File dialog to select an IOF.

3.1.2 GUI Overview

Figure 2 shows the GUI screen as it appears after starting BlickO and selecting an IOF, in this case for Pandora 0. The different sections of the BlickO GUI (called GUI-sections) are marked by red numbers on figure 2 and are listed here:

1. Instrument + location label
2. Label with date, time, solar/lunar angles and time of local day progress bar
3. Connection status labels
4. Connection buttons for all interfaces
5. Auxiliary sensor readings display
6. Display of sun-search results (at software startup just contains an image of the sun)
7. Action logger
8. Figure showing current measurements for all spectrometers
9. Routine control, load schedule button, and reset button
10. Start-stop button
11. Spectrometer settings: repetition control, integration time control and cycles control for each spectrometer
12. Filterwheel settings: filterwheel 1 selection and filterwheel 2 selection
13. Tracker settings: zenith angle control, azimuth control, track-sun button and track-moon button
14. Save figure button, save comment button and exit button

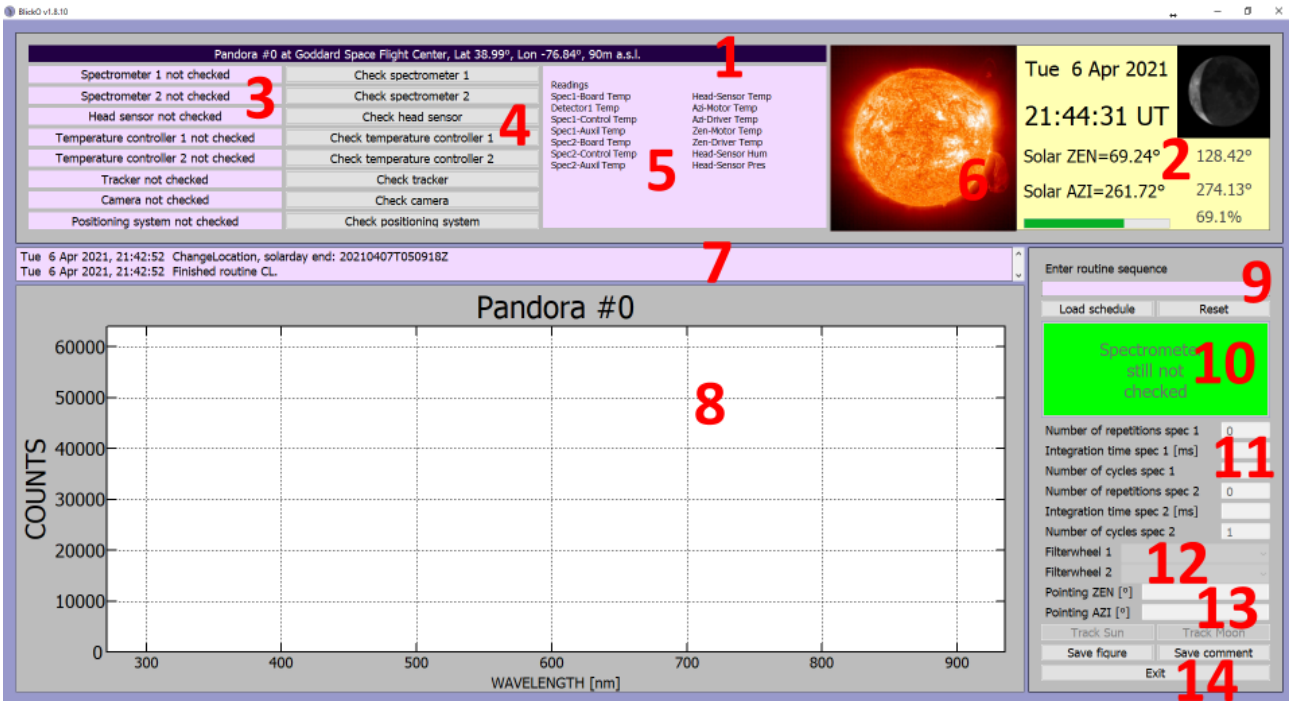


Figure 2: GUI of BlickO in real mode

3.1.3 Simulation mode

The purple background in figure 2 indicates that the "Instrument operation mode" for BlickO is set to "real mode", which means the connected hardware will "really" be accessed through the connection ports. BlickO can also be run in a "simulation mode", in which case the GUI would have a red background and the hardware connections will just be simulated (figure 3). The instrument operation mode is set in the BlickO Instrument Configuration File (section 5.5). A value of 1 means real mode with the instrument not in use, 2 means real mode with the instrument in use and 0 means simulation mode. So in order to change BlickO from real to simulation mode (simulation to real mode), the configuration file has to be manually edited and the line with "Instrument operation mode" has to be changed from 1 to 0 (0 to 1) before starting BlickO. In real mode, BlickO automatically changes the instrument operation mode to 2 at start-up and then back to 1 at program exit. This is to prevent the user from unintentionally trying to start BlickO on the same instrument twice.

All functions of BlickO can be tested in simulation mode. For users who want to modify the source code, it is recommended to test their modified code in the simulation mode first before proceeding to the real mode.

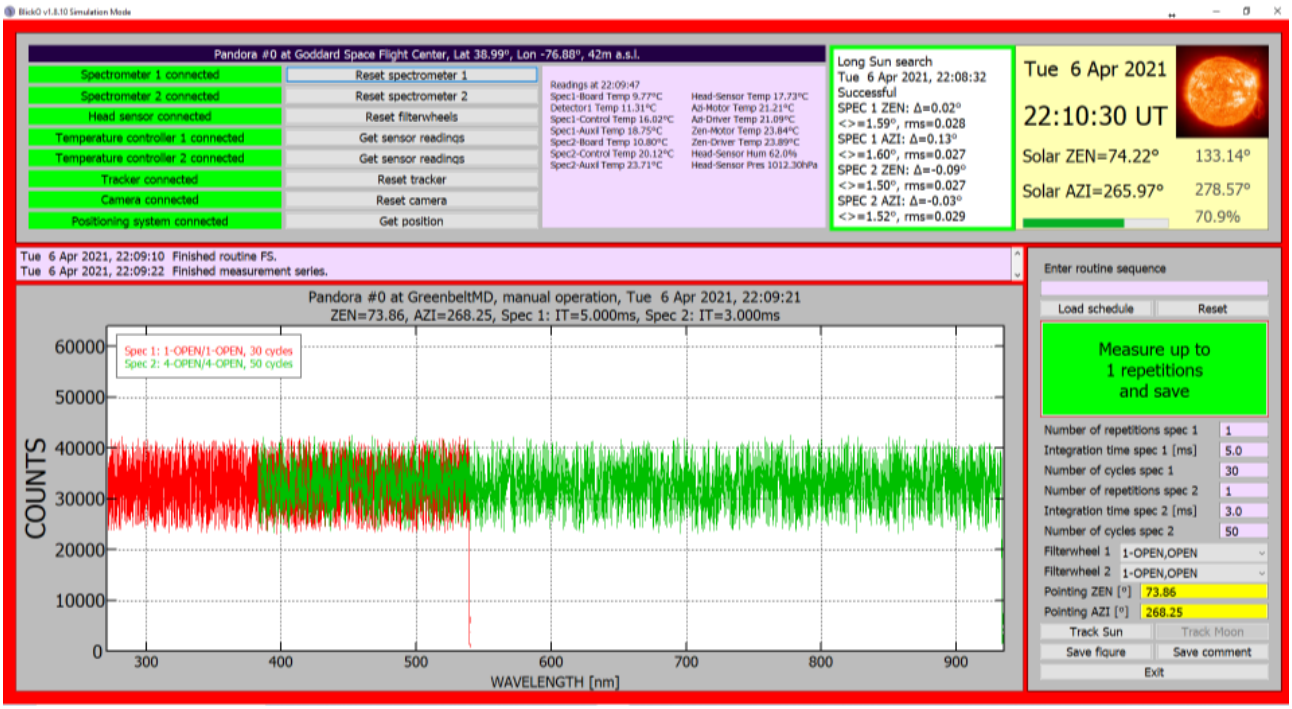


Figure 3: GUI of BlickO in simulation mode

3.1.4 Debug mode

One can also run the instrument in "Debug mode". For this purpose entry "Instrument operation mode" in the BlickO Instrument Configuration File (section 5.5) needs to be set to 3 before BlickO is started. BlickO then automatically changes the instrument operation mode to 4 at start-up and then back to 3 at program exit. The only difference between the real mode (Instrument operation mode is 1 or 2) and the debug mode (Instrument operation mode is 3 or 4) is that there are much more lines written in the info-log file (see 5.15). Note that it is not recommended to use this option for normal operation, since it slows down the system to some extent. It should only be used when trying to research why a specific functionality of the instrument is not working.

3.1.5 GUI sections

GUI-section 1 shows the instrument name and the name, latitude and longitude of the currently selected location.

GUI-section 2 shows the current date and time (UT) and the calculated solar and lunar angles based on the time and the instrument location coordinates. During daytime (between sunrise and sunset), an image of the moon is shown at the top right corner of GUI-section 2. During nighttime an image of the sun is shown.

BlickO reads the current time from the computer operating system. Hence if the time on the computer is not correct, then the solar/lunar angles will also not be correct, which causes pointing problems for the instrument. Therefore, we recommend the computer time be kept correct within ±10 s, preferably within ±1 s by periodic updating through the internet (see section 2.5). The computer running BlickO does not necessarily have to be in UT time-zone. As long as the computer-time and the time-zone match, BlickO will work fine.

At BlickO start, GUI-section 6 shows an image of the sun (daytime) or the moon (nighttime). Once a successful target search has been done, by either scanning the sun or the moon (see section 6.1) or by taking a picture with the camera, the result of this last target search is displayed.

Once the hardware is connected and powered on, the connection buttons (GUI-section 4) are used to establish connection with the hardware pieces (see section 3.1.6). While the connection is being established, the respective connection status label (GUI-section 3) turns yellow. After a successful connection it turns green (figure 3). Otherwise an error message will appear and the label turns red.

GUI-section 5 displays the last readings of Pandora's auxiliary data (currently only temperatures). The action logger (GUI-section 7) is permanently updated and displays the last action started by BlickO (e.g. "connected tracker" or "start tracking sun").

The figure (GUI-section 8) will display spectral measurements (in counts versus pixel number or wavelength) once they are taken. In the case there are more than one spectrometer in the Pandora unit, the panels can be arranged horizontally (as in figures 2 and 3) or vertically or the two spectra can be plotted in the same panel. This can be changed in the BlickO Instrument Configuration File (section 5.5). There are some mouse-click operations, which can be done on the figure:

- A right-click on the figure toggles the y-scale between "full range" (for measured spectra this is from 0 to the unit's effective saturation limit) and "optimized range" (from the minimum to the maximum of the measured counts with a little margin at both sides).
- The user can also zoom into the figure. This is done by a left-click of the mouse on a point of the figure, then dragging the mouse while the left button is pressed, and then releasing the mouse.
- If the figure has a legend, then a double-right-click on the figure moves the legend to different places on the figure (e.g. top left corner, top right corner, etc.).
- A double-left-click on a figure panel toggles between showing all figure panels or just one figure panel.
- A triple-right-click on a figure panel toggles between showing and not showing grid lines on this panel.

Pressing the "Exit" button (GUI-section 14) exits BlickO, after asking the user for confirmation. This is identical to pressing the "exit cross" on the top-right corner of the window. Pressing the "Save figure" button (GUI-section 14) opens a dialog allowing the user to choose a figure name and then saves the figure currently displayed in GUI-section 8. Pressing the "Save comment" button (GUI-section 14) opens a dialog allowing the user to enter a text line, which will then be saved in the L0 data file (section 5.7).

Pressing the "Track sun" button (GUI-section 13) will point the Pandora head sensor towards the sun, if the tracker is connected and if the sun is above the horizon. In the same way, pressing the "Track moon" button (GUI-section 13) will point the Pandora head sensor towards the moon, if the tracker is connected and if the moon is above the horizon. Entering a zenith angle or azimuth in the zenith angle control or azimuth control

box (GUI-section 13) will point the head sensor to the entered direction. The azimuth is counted clockwise starting at north. So 0° is north and 90° is east.

The combo-boxes filterwheel 1 and filterwheel 2 (GUI-section 12) can be used to select a specific filter.

Entering numbers in the spectrometer controls (GUI-section 11) will change the respective spectrometer setting. The integration time must be in ms between the minimum and maximum allowed values (listed in the IOF, see section 5.3). Number of cycles is the number of spectra to be averaged before being displayed on the figure. E.g. 10 cycles means that BlickO reads 10 spectra from the spectrometer, builds average and standard deviation and then displays the result in the figure. Number of repetitions says how many times a full set of cycles is measured, displayed and saved in the L0 data file. It can also be set to 0, in which case no repetitions are measured, or set to -1, in which case an unlimited number of repetitions is measured and the data are displayed, but not saved.

The Start-Stop-button (GUI-section 10) is used to start and stop Pandora actions. In case the routine control (GUI-section 9) is empty, the system is said to be in "manual mode". Then the Start-Stop-button simply starts or stops spectrometer measurements using the settings in the spectrometer controls (GUI-section 11). Since Start-Stop is a non-blocking function, any action can be stopped at any time. Spectra saved in the manual mode are marked by a "**" in the first column of the L0 data file (more in section 5.7).

The routine control (GUI-section 9) is used to enter a sequence of one or more two-character code routines (for more about routines see section 4.1). Pressing the "Load schedule" button (GUI-section 9) opens a dialog, which allows the user to select a schedule file (section 4.2).

The "Reset" button (GUI-section 9) simply deletes any text in the routine control and sets the spectrometer controls to -1 repetition (i.e. an unlimited number of repetitions is measured), minimum integration time and 1 cycle respectively. This brings the system back to "manual mode".

3.1.6 BlickO operations

Connect the Pandora system by pressing the connection buttons one after another. "Check spectrometer X" (X is the spectrometer number) is a blocking function, i.e. no other action can be performed on BlickO while the spectrometer connection is established, and takes a few seconds only. "Check head sensor" and "Check temperature controller X" are non-blocking functions, i.e. other actions can be performed on BlickO while the connection is established. They take only a few seconds each. "Check tracker" is a non-blocking function and takes up to 2 min, since it includes a full tracker reset. "Check camera" is a blocking function and takes a few seconds only.

If the connection to an interface could not be established, the user has to trouble-shoot. These are the ad-hoc procedures to be taken. If a procedure is not successful, then the user should proceed to the next point.

1. Make another attempt to connect by pressing the connection button again.
2. Exit and restart BlickO and try to connect again.
3. Exit BlickO and check, whether the respective device is listed in the computer's device manager. If it is not listed, then disconnect and reconnect the respective USB cable until it is listed. Then restart BlickO and try to connect again.
4. Exit BlickO, restart the computer and then restart BlickO and try to connect again.
5. Turn off the external power to the optical head or the entire system and then restart.

When text is entered in the routine control, the system is said to be in "routine mode". For example, writing "SOSU" in the control and pressing the Start-Stop button will cause it to first execute routine SO and directly afterwards routine SU (for "routines" see section 4.1).

If a positive integer <100 is written at the end of a routine sequence, the sequence is repeated that many times. E.g. "SOSU3" means the combination SO and then SU is repeated 3 times, i.e. it is the same as writing "SOSUSOSUSOSU". One is also allowed to use single () brackets in the routine sequence string. In this case the strings inside the brackets are "resolved" first and then combined to one long sequence. So e.g. "(SOSU3)SB" means first 3 repetitions of the combination SO plus SU are executed followed by routine SB.

A special command for the routine control is "?". In this case a dialog appears with a short description of each routine in directory `/lib/routines/` (section 4.1).

When pressing the "Load schedule" button (GUI-section 9), a file dialog opens, where the user can choose a schedule (figure 4). After a schedule file is selected, it will be displayed in the routine control after the characters "->". In this case the system is said to be in "schedule mode". After pressing the Start-Stop-button, BlickO will execute the routines listed in the selected schedule.

The user can also combine a sequence with a schedule. E.g. if the string in the routine control is "SOSU -> sun-1S.sked", then BlickO will first execute "SOSU" and then start schedule "sun-1S.sked".

While a change of the instrument is only possible at the start of BlickO, a change of the location can be done typing "CL" in the routine control (GUI-section 9) and then pressing enter or the Start-Stop-Button (GUI-section 10). A dialog appears allowing to select a different location. If the desired location is not listed, then the locations file has to be edited and the desired location has to be added (see section 5.2). Then BlickO has to be restarted and the location can be selected as described above.

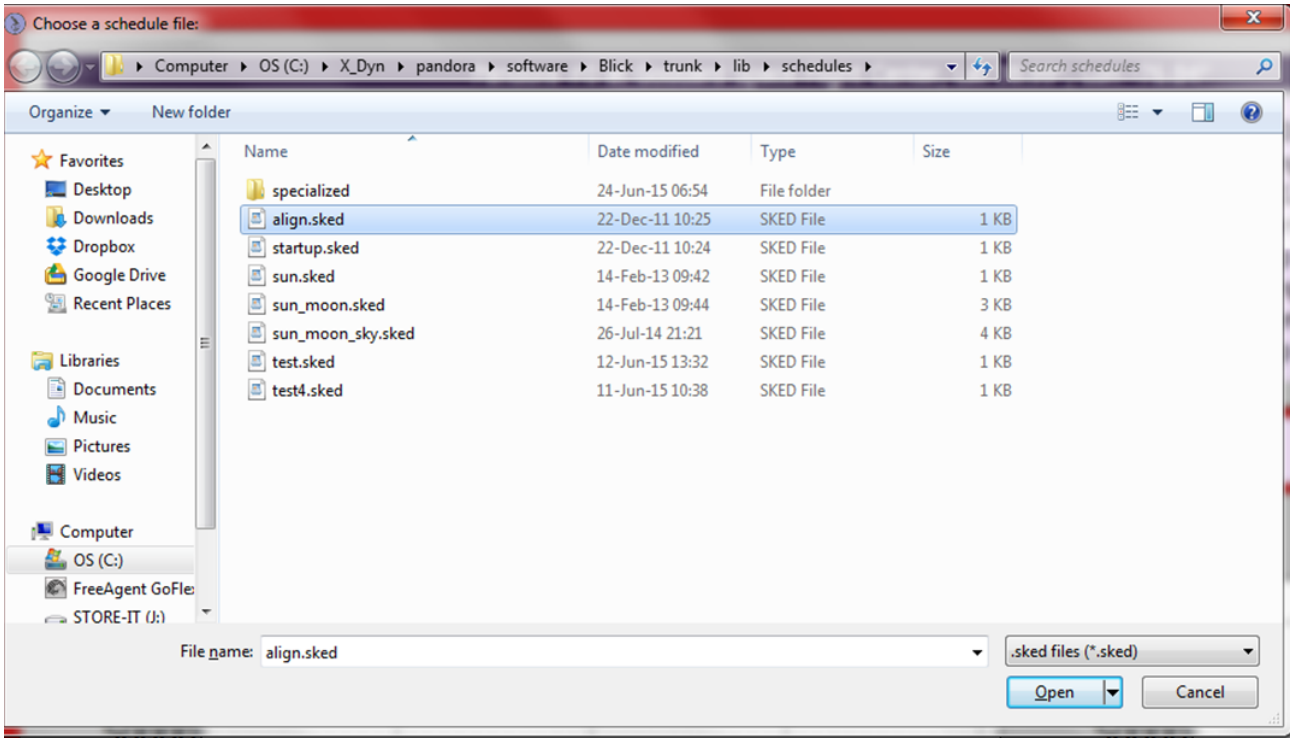


Figure 4: File dialog to select a schedule.

3.2 BlickF - File Handling and Operation Monitoring

The Blick file-transfer and operation-monitoring software is a command line program serving two purposes. The 'File Handling task' is used to automatically push files from a local directory to one or two remote servers (section 3.2.2). The 'Operation Monitoring task' is used to monitor BlickO and restart it if needed (section 3.2.3).

3.2.1 BlickF Start and Stop

When installing BlickO, BlickF will automatically be installed as well. All the necessary files are in directories `/bin/` and `/lib/fslib/`. The BlickF configuration is given in the text-file `/lib/fslib/BlickF_config.txt`. Each of the keywords in this file has to be manually edited by the user (see section 5.6).

To execute BlickF, double-click the executable file `/bin/BlickF.exe` or the BlickF-icon on the desktop. When BlickF is started, a command prompt window is opened (see figure 5). At first BlickF reads the BlickF Configuration File (section 5.6). If this fails, an error message is displayed in the command window. Otherwise, BlickF goes into a periodic loop at a frequency determined by the parameter POLLING_RATE in the configuration file, typically set to 10 s. In this period BlickF will check whether it needs to do a File Handling task and/or a Operation Monitoring task and writes a corresponding line in the command window. At the end of each command line it adds the 'OMessage' and the 'FMessage' (see 3.2.3) in the form `(OF=01)`, where the first number is the OMessage (in this case 0) and the second number the FMessage (in this case 1).

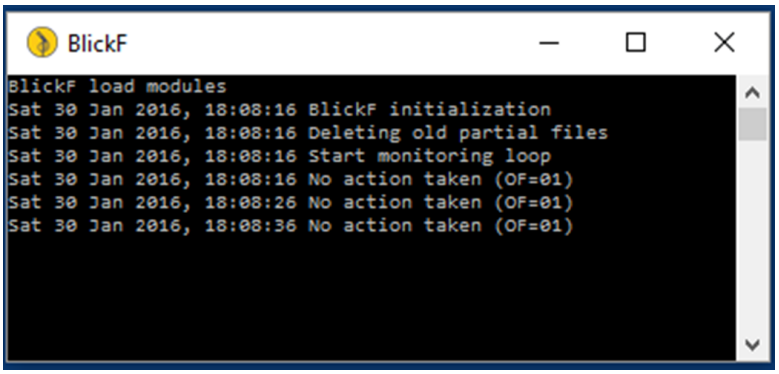


Figure 5: BlickF screenshot.

Both BlickO and BlickF write to and read from the so-called "BlickO-BlickF Messenger File" `/log/Blick_message.txt`, which is needed to perform the Operation Monitoring task (see section 3.2.3).

To exit for BlickF properly, the user shall press 'q' in the command windows at any time and not just close the command prompt window!

3.2.2 BlickF File Handling task

BlickF compares the file names in the local directory (given by parameter DIR_LOCAL in the configuration file, usually `/data/L0/`), with the file names listed in the "already-copied-files-file" (given by parameter FILES_COPIED in the configuration file) and pushes all files that have not already been copied in the remote directory. It will add the names of the newly copied files to the content of the already-copied-files-file.

The first file transfer will start at BlickF startup. Then a new file transfer will be done whenever new data are available.

At the very first use of BlickF, Putty's FTP client will ask the user for confirmation that the host can be trusted. Then a "y" has to be entered at the question "Store key in cache?".

The comparison of the file names in the local directory with those in the already-copied-files-file takes longer the more files are in the local directory. Therefore we recommend to "clean" the local directory at least once per year, e.g. by moving in January all L0 files from the previous year into a separate directory outside of the local directory.

3.2.3 BlickF Operation Monitoring task

This task is controlled by the BlickO-BlickF Messenger file `/log/Blick_message.txt`. This is an ascii file containing exactly 2 characters representing a hexadecimal number, i.e. between 0 and f, and therefore has a size of exactly 2 bytes. The first character is called "OMessage" and is used by BlickO, the second number is called "FMessage" and is used by BlickF. OMessage and FMessage indicate, in which status BlickO and BlickF are. Tables 1 and 2 list the meanings of both O+F messages.

BlickF performs different actions depending on the value of OMessage as decribed in table 3. Note that OMessages 4, 5 and 7 will only ever happen, if parameter 'Do autostart' in the BlickO General Configuration File is set to 1 (see section 5.4). Furthermore the BlickF action for OMessages 5, i.e. restarting the computer, will only happen if parameter 'DO_RESTART' in the BlickF configuration file (section 5.6) is set to 1. Otherwise BlickF will just do a BlickO restart.

Setting parameter 'DO_RESTART' in the BlickF configuration file to 1 is only useful, if BlickF is in the list of startup programs of the computer, i.e. it starts automatically after a restart. The procedure to add BlickF into the startup programs is different for each operating system, also changes from one Windows version to another. We recommend to search on the web for "add startup program XXX", where XXX is the operating system you are using.

Table 1: FMessage description

FMessage	Description
0	BlickF is not running
1	BlickF is running and no BlickO restart has been initiated
2	BlickF is running and has initiated a BlickO restart
3	BlickF has done a computer restart, is now running, and has initiated a BlickO restart
4	BlickF has initiated to kill BlickO

Table 2: OMessage description

OMessage	Description
0	BlickO is not running
1	BlickO is performing autostart and L0 data access is free
2	BlickO is running, but not in schedule mode, and L0 data access is free
3	BlickO is running in schedule mode and L0 data access is free
4	BlickO has closed itself and should be restarted
5	BlickO has closed itself and the whole computer should be restarted and then BlickO should be restarted
6	BlickO is still working, but in internal recovery mode
7	BlickO autostart has failed, although the computer was previously rebooted
12=c	BlickO is running, but not in schedule mode, and L0 data access is blocked
13=d	BlickO is running in schedule mode and L0 data access is blocked

Table 3: BlickF operation monitoring actions

OMessage	BlickF action
0, 2	Nothing
1, 6	At the first occurrence of OMessage 1 or 6, BlickF takes the time. If OMessage stays at this value for more than 5 min, then BlickF tries a computer restart, if that has not been done before. In the case a computer restart was already done, it will send an automated warning email to the network operator.
3	BlickF remembers the time when new files have arrived in the local L0 data directory. If no new partial file(s) arrive(s) within 10 minutes after the arrival due date (determined by parameter "File push time [min]" in the BlickO General Configuration File (section 5.4), then BlickF understands that BlickO is "frozen" and will "kill" BlickO, will set the OMessage to 4, and will then try to reopen BlickO.
4	BlickF restarts BlickO.
5	BlickF sets FMessage to 2, restarts the computer and then restarts BlickO.
7	BlickF will send an automated email to the network operator.
12=c, 13=d	BlickF skips the filepush due to the blocked access to the L0 file.

3.3 BlickP - Data Processing

BlickP is a console application, which processes L0 data up to all higher data levels L1, L2Fit and L2. It needs two configuration files to operate, named `/config/logging.ini` and `/config/BlickP.ini` respectively.

The first file configures the logging system. A working logging system is provided with the Blick Software Suite distribution. The user does in general not need to edit this file. Advanced users, who may want to customize logging, are referred to the Python Standard libraries documentation `https://docs.python.org/2/library/logging.config.html#configuration-file-format`.

The second configuration file specifies the parameters needed for processing. This file must be edited by

the user and is described in section 5.9.

When starting BlickP, the program expects to find both configuration files in the correct directories and starts the data processing. Each processing step is displayed in the command window and also added to a BlickP log-file (see section 5.15).

4 Blick Software Suite Operations Setup

4.1 Routines

The concept of "routines", i.e., sequences of commands to be executed by the Pandora system, is taken from the way Brewer spectrometers are operated [21]. Each routine is identified by two characters, a combination of two letters (e.g. SO) or one letter followed by one number (e.g. W1). The commands for a routine with identifier XY are written in the text file `/lib/routines/XY.rout`. At startup, BlickO reads through all routines in the directory `/lib/routines/` and converts the content of these text files into Python code. This Python code is then executed when the routine is called, i.e. entered in the routine control (GUI-section 9).

4.1.1 BlickO Standard Routine Library

This section describes the BlickO standard routine library, which is stored in directory `/lib/routines/` during installation of BlickO. A more detailed description of each routine can be obtained entering "?" in the routine control (GUI-section 9). Most routines are part of a logical group characterized by the first letter of the routine identifier.

Almucantar routines A*

AO	Almucantar without filter
AU	Almucantar with U340 (U340 is a UV bandpass filter with maximum transmission at 340nm)

Change system settings routines C*

CA	Change maximum pointing azimuth adjustment and decide whether the alignment history should be frozen
CB	Change the beep mode
CE	Change positioning system parameters
CK	Change the camera mode
CL	Change the location
CN	Change tracker zenith and azimuth parking positions
CP	Change the partial file update time
CT	Change the temperature controller parameters for this session
CX	Change the figure drawing parameters

Diagnostic routines D*

DC	Reads and displays the counts of routine SO in the current level 0 file at one pixel
DD	Makes dark count measurements at three different temperatures and different integration times from lowest to highest
DM	Reads and displays the counts of routine MO in the current level 0 file at one pixel
DR	Reads and displays the sensor readings (temperatures, humidities, etc.) in the current level 0 file

Elevation scan routines E*

EK	Detailed sky scan at standard azimuth without filter; the standard azimuth is the one given in the BlickO Instrument Configuration File (section 5.5), entry "Standard azimuth for elevation scans [deg]".
EL	Detailed sky scan at standard azimuth with U340
EO	Quick sky scan (5 zenith angles) at standard azimuth without filter
EU	Quick sky scan (5 zenith angles) at standard azimuth with open U340

Find routines F*

FA	=FS, but also saving the spectral data
FD	=FS, but with diffuser in the optical path
FF	Search routine with all "search options" listed
FI	Find Initialization, moves to sun and opens a dialog, which allows the user to move the tracker manually
FJ	Like FI but using the moon
FM	=FS, but searching moon instead of the sun
FN	=FA, but without doing a reset in the case the difference is to large
FO	=FD, but scanning only around the center of the FOV with longer measurement duration. This is not used to "find" the sun.
FP	=FU, but scanning only around the center of the FOV with longer measurement duration. This is not used to "find" the sun.
FQ	Quick sun search (system-optimized)
FS	Find Sun; long sun search for all spectrometers, saves final figure and averaged data, but not spectral data
FU	=FS, but with U340 plus diffuser combination in the optical path
FV	Quick sun search
FW	=FA, but showing the results in 4 wavelength regions
F1	=FS, but only doing the search for spectrometer 1
F2	=FS, but only doing the search for spectrometer 2

Help routines H*

HE	Displays routine descriptions (same as "?")
HS	Displays a dialog to allow low level serial communication

Camera routines K*

KA	Camera adjustment
KC	Camera calibration
KD	Displays camera images
KK	Opens camera configuration dialog
KM	Camera supported moon search
KP	Saves the last image taken by the camera in JPEG format
KS	Camera supported sun search
KX	Camera calibration using static target

Loading routines L*

LF	Allows the user to display a previously stored figure on the figure panel
LR	Reloads all the measurements routines
LW	Checks light source and temperature stability

Direct Moon routines M*

MD	Direct moon measurements during daytime without filter; three measurement sets, off-moon right side, on-moon, off-moon left side; the off-moon measurements are taken at the lunar zenith angle with the azimuth shifted by the sky-cutoff angle (see table 13)
MO	Direct-Moon without filter
MU	Direct-Moon with U340
MT	Like MD but using U340

Principal plane routines P*

PO	Standard principal solar plane routine at open hole
PU	Standard principal solar plane routine with U340

Reset routines R*

RF	Reset filterwheel(s)
RO	Restart BlickO and possibly also the whole computer
RP	Power reset
RS	Reset spectrometer(s)
RT	Reset tracker

Direct Sun routines S*

SB	Direct-Sun with BP300 (BP300 is a UVB bandpass filter with maximum transmission at 300nm)
SQ	Quick direct-Sun without filter
SO	Direct-Sun without filter
SS	Quick direct-Sun with U340
SU	Direct-Sun with U340

Target, tracker or test routines T*

TD	Moves the tracker to point down (i.e. to the maximum allowed zenith angle), waits for 5 secs, and then moves to the horizon
TG	High load filterhweels test
TO	Target routine using open hole
TP	Parks the tracker or wakes it up from parking
TR	Moves tracker to the horizon in all four directions and to the zenith in between
TT	Test routine checking spectrometer(s), head sensor and tracker
TU	Target routine using U340
T0	Moves the tracker to the zenith

Waiting routines W*

W0	Wait for 2^0=1 minute
W1	Wait for 2^1=2 minutes
W2	Wait for 2^2=4 minutes
...	etc. until
W9	Wait for 2^9=512 minutes

Zenith sky routines Z*

ZB	Zenith-Sky with BP300
ZO	Zenith-Sky without filter
ZU	Zenith-Sky with U340

4.1.2 Routine Syntax

The user can also modify routines or create new routines. In this case the source code of BlickO does not have to be changed. The only action needed is to save the (modified or new) file `/lib/routines/XY.panr` and then restart BlickO or execute routine 'LR' (="Load Routines"). Note that BlickO does not check, whether the newly created routine makes sense or is potentially even damaging the instrument. E.g. if the user tells the instrument to move to the sun and measure without any attenuation filter, then the detector will be extremely over-illuminated, which produces useless data and could even harm the instrument if this is done frequently.

In general we recommend not to edit the existing standard routines, but rather create new routines, i.e. giving them new names. The main reason for this is that when the software is updated, all routines from the standard routine library are updated (overwritten) as well and the user would loose all the changes he made.

The routine files use a proper syntax, which is explained in this section. Errors in the syntax may be immediately detected by BlickO, in which case an error message will be displayed at the program start or after executing routine 'LR'. If the error is not detected at that initial stage, it will in general be detected once the routine is called.

When BlickO translates the Blick syntax to Python commands, it looks for lines that start with a so-called routine command. Only those lines will be analyzed. All other lines can be considered comment lines. All possible routine commands are listed in the left column of table 4.

Some routine commands are 'stand-alone' (those with no entries in column 'Related routine keywords').

The other ones are followed by the string "->" and then a series of routine keywords with associated settings, separated by ";" in the form

```
ROUTINE COMMAND -> KEYWORD1=VALUE1;KEYWORD2=VALUE2;...
```

The right column of table 4 lists all possible keywords for a routine command. Keywords that appear in table 5, but are not listed in the command line, stay at their default setting as listed in column 3 of table 5.

Table 4: Routine commands and related keywords

Routine command	**Related routine keywords**
DESCRIPTION	
GETSCRIPT	
COMMAND	
DURATION	LENGTH, TIMEMODE
SET FILTERWHEELS	FUNCFILT, FW1, FW2
SET POINTING	DELTA, AZI, ZEN, AZIMODE, ZENMODE
SET SPECTROMETER	IT*, NCYCLES*, NREPETITIONS*, DURATION, DARKRATIO
MEASURE	DISPLAY, SAVE, SATCHECK
CHECK INTENSITY	ADJUSTIT*, ADJUSTND, %SATURATION*, DARKESTIMATION*, ITLIMIT*
PROCESSINFO	TYPE, DISTANCE
START LOOP	XIJ
STOP LOOP	

Those routine keywords in table 4 marked with an asterisk can also be "spectrometer specific". In that case they have an "_X" added, where X is the spectrometer number. E.g. for the integration time the keyword can be IT, IT_1 or IT_2. More details about this are given below.

Table 5 gives an overview of all routine keywords, their possible settings and their default settings. Every keyword except for XIJ itself can also be set to the value XIJ, if it is used in a loop (see description of command START LOOP). Settings FUNCFILT, FW1 and FW2 can be set to "Any valid filter name". The valid filter names are listed in table 6. Column 'Func' says whether the filter is considered a so-called 'Functional filter', which means it is not just used for attenuation or polarization (more in section 5.11). A detailed description of each routine command is given in the following sections.

Table 5: Routine keywords and possible settings

Routine keyword	Possible setting	Default setting
LENGTH	USERINPUT, float≥0	0
TIMEMODE	TOTAL, ADDED	ADDED
IT	CURRENT, CHANGE, MIN, MAX, min(IT)≤float≤max(IT), x+float≥0	CURRENT
DURATION	AUTO, float≥0, x+float≥0	AUTO
NCYCLES	AUTO, CURRENT, integer≥1	AUTO
NREPETITIONS	AUTO, CURRENT, integer≥0, x+integer≥0, MAX1	AUTO
DARKRATIO	OPTIMIZED, OPT1, OPT2, 0≤float≤0.5	0
DISPLAY	NO, MEAN, MEAN+STD, CURRENT	MEAN
SAVE	NO, STDERR, STDERRTOLINE	NO
SATCHECK	NO, YES, WARN	YES
ADJUSTIT	FROMCURRENT, FROMMIN	FROMCURRENT
ADJUSTND	NO, FROMCURRENT, FROMMAX, FROMLASTDS, NO-MAX	NO
%SATURATION	-100≤float≤10000, SATPERC	80
DARKESTIMATION	NEGLECT, THEORY	THEORY
ITLIMIT	ITMAX, min(IT)≤float≤max(IT), xITMAX, x+min(IT)≤float≤max(IT)	ITMAX
DELTA	MIDDLE, CONT, CAMERA, float≥0	MIDDLE
AZI	RESET, POWER, CURRENT, STANDARD, DAZI, -360≤float≤360	CURRENT
ZEN	CURRENT, DZEN, PARK, MAX, -180≤float≤180	CURRENT
AZIMODE	ABS, RELSUN, RELMOON, ANGSUN, ANGMOON	ABS
ZENMODE	ABS, RELSUN, RELMOON	ABS
FUNCFILT	Any valid filter name, XXX	XXX
FW1	RESET, CURRENT, MOVE, 1≤integer≤9, any valid filter name	CURRENT
FW2	RESET, CURRENT, MOVE, 1≤integer≤9, any valid filter name	CURRENT
TYPE	ONLYL1, NOL1, SUN, MOON, SKY, TARGET, PROFILE, ALMUCANTAR, LAMP, SPECIAL	ONLYL1
DISTANCE	NO, float≥0	NO
XIJ	→ see section 4.1.13	0

Table 6: Allowed filter names

Filter type	Filter name	Func	Description
Open hole	OPEN	YES	No filter in place
Opaque blank	OPAQUE	NO	Non-transmissive blank
U340 filter	U340	YES	Colored glass filter with maximum transmission at 340 nm
BP300 filter	BP300	YES	Interference filter with maximum transmission at 300 nm
Diffuser	DIFF	YES	Grounded quartz diffuser
U340-Diffuser sandwich	U340+DIFF	YES	Combination of U340 filter and grounded quartz diffuser
BP300-Diffuser sandwich	BP300+DIFF	YES	Combination of BP300 filter and grounded quartz diffuser
Neutral density filter	NDx	NO	Reflective neutral density filter with attenuation x, $0.1 \leq x \leq 5.0$ in steps of 0.1
Polarization filter	POLx	NO	Polymer linear polarizer paced in polarization angle x, $0 \leq x \leq 359$, integer
Generic filter	FILTERx	NO	Generic filter name for test purposes, $1 \leq x \leq 9$, integer

4.1.3 Routine Command DESCRIPTION

The text after "->" will be a line in the routine description, which is listed when the user enters "?" in the routine control (GUI-section 9). The routine file can have multiple lines with routine command DESCRIPTION. Each one will be a separate line in the displayed routine description. Here e.g. is a 3-line description:

```
DESCRIPTION -> Scans at fixed azimuth with open hole in filterwheel 1;
DESCRIPTION -> measures at selected zenith angles for 20 secs
DESCRIPTION -> at each position including dark
```

4.1.4 Routine Command GETSCRIPT

The text after "->" must be a special function in module `src/blick_routinereader.py`. The only existing functions of this type at this time are function "SunSearchScript" and function "DiagnoseScript". The former is used for the "Find routines" FS, FA, etc. and the latter is used for the "Diagnistic routines" DC, DT, etc. E.g. this is the use of routine command GETSCRIPT in the sun search routine FS.

```
GETSCRIPT -> self.SunSearchScript(savfig=[0,-1])
```

4.1.5 Routine Command COMMAND

The text after "->" must be directly a command in Python. The command will be called in function "ExecuteCommands()" inside the main module `/src/blick_osmain.py`. Except for simple calls, this routine command should only be used by a programmer familiar with the Python language. Below is an example for a simple command, which makes the computer beep for a duration of 500 ms at a frequency of 200 Hz.

```
COMMAND -> xfus.xbeep(200,500)
```

4.1.6 Routine Command DURATION

Routine command DURATION gives an estimation of the duration for a routine. It is in most cases not needed, since BlickO automatically calculates the approximate time a routine will take. This duration-estimation of BlickO can be found looking at the schedule-protocol file created when a schedule is started (see section 4.2).

Routine command DURATION should only be used either if the routine needs user input or if the user notices that the duration of the routine is significantly different from what BlickO estimates.

In the first case (user input needed) the keyword LENGTH should be set to USERINPUT and keyword TIMEMODE is not needed. This tells BlickO that at some stage the routine will stop and wait for keyboard input from the user. So the duration of the routine is "user-dependent". Routines with LENGTH=USERINPUT are not allowed in a schedule (section 4.2).

In the second case (the time the routine takes is significantly different from what BlickO estimates) the keyword LENGTH should be set to a number in seconds. BlickO will then take this value to estimate the routine duration, if keyword TIMEMODE=TOTAL, or it will add this number to its own estimation of the duration, if keyword TIMEMODE=ADDED. So e.g. if BlickO estimates the duration of a routine to 60 s, but the user notices it usually takes 80 s, he can use routine command DURATION in one of these two ways:

```
DURATION -> LENGTH=80;TIMEMODE=TOTAL

DURATION -> LENGTH=20;TIMEMODE=ADDED
```

There should only be one routine command DURATION in a routine file. The knowledge of the routine duration is not needed if BlickO is in manual mode or in routine mode. It is only needed for schedule operation (section 4.2).

4.1.7 Routine Command SET FILTERWHEELS

This command positions the filterwheels. Keyword FW1 refers to filterwheel 1, FW2 to filterwheel 2. RESET means the filterwheel is reset. CURRENT means the filterwheel position is not changed. MOVE means the filterwheel position is changed to the position listed in element 0 (filterwheel 1) or 1 (filterwheel 2) of global variable `self.sys_status[5]`. An integer between 1 and 9 moves the filterwheel to this position. Keywords FW1 and FW2 can also be set to filterwheel positions as given in the IOF. E.g. the command line below puts filterwheel 1 in open position.

```
SET FILTERWHEELS -> FW1=OPEN
```

Another option for command SET FILTERWHEELS is keyword FUNCFILT. If FUNCFILT is set to any value other than XXX, it overrules the settings for FW1 and FW2. In this case the software looks for a solution in the filterwheel settings, which best matches the desired filter. E.g. this command

```
SET FILTERWHEELS -> FUNCFILT=U340
```

looks for the U340 filter in both filterwheels. If it finds it in any filterwheel, it will set this filterwheel to the position U340 and the other one to OPEN.

All settings for keyword SET FILTERWHEELS can also be combined by a ",", if they are used for Pandora systems with more than one spectrometer. E.g. this command

```
SET FILTERWHEELS -> FW1=U340,OPEN;FW2=4
```

will set filterwheel 2 to position 4 and filterwheel 1 in such a position, that spectrometer 1 is at U340 and spectrometer 2 is at OPEN. This is of course only possible if this combination exists.

Setting FUNCFILT can and should preferably be used for situations with more than one spectrometer. E.g. the command

```
SET FILTERWHEELS -> FUNCFILT=U340,OPEN
```

will find the best choice of the filterwheels, so that spectrometer 1 measures at U340 and spectrometer 2 at OPEN. Note that in all usages of FUNCFILT the spectrometer with lower index (usually spectrometer 1) has priority. This means e.g. that if the filterwheel settings are such that it is impossible that both spectrometers measure at U340, then this command

```
SET FILTERWHEELS -> FUNCFILT=U340,U340
```

will place the filterwheels so that spectrometer 1 measures at U340 and spectrometer 2 at something else. If the setting of FUNCFILT does not include a ",", then BlickO assumes that the setting should be obtained for all connected spectrometers. This means that the following two command lines are identical:

```
SET FILTERWHEELS -> FUNCFILT=U340,U340

SET FILTERWHEELS -> FUNCFILT=U340
```

4.1.8 Routine Command SET POINTING

This command is used to control the tracker. If keyword AZI=RESET or POWER, then a tracker reset or power reset is initiated and no other keyword is needed. For all other cases the tracker is pointed to azimuth and zenith angle positions as set in keywords AZI and ZEN.

Keywords AZIMODE and ZENMODE indicate whether the settings of AZI and ZEN are absolute or relative numbers. If keyword ZENMODE=ABS, then the setting of ZEN is considered an absolute position in degrees. If keyword ZENMODE=RELSUN, then the setting of ZEN is considered a zenith angle offset relative to the solar zenith angle (SZA) in degrees. E.g. if the (refraction corrected) SZA is 46° and ZENMODE=RELSUN and ZEN=-1.5, then the tracker will point to zenith angle 46°-1.5°=44.5°. If keyword ZENMODE=RELMOON, then the zenith angle offset is relative to the lunar zenith angle.

ABS, RELSUN and RELMOON have the same meaning for keyword AZIMODE. In addition, AZIMODE can also be set to ANGSUN or ANGMOON. In this case the offset is not in azimuth, but in scattering angle, i.e. the azimuth difference is divided by the sine of the solar (or lunar) zenith angle. E.g. if the (refraction corrected) SZA is 30°, the solar azimuth 105°, AZIMODE=RELSUN and AZI=2, then the tracker will point to azimuth 105°+2°=107°. Differently, if AZIMODE=ANGSUN, the tracker will point to azimuth 105°+2°/sin(30°)=109°.

Keyword AZI can also be STANDARD. In this case the azimuth angle given in the BlickO Instrument Configuration File (section 5.5), entry "Standard azimuth for elevation scans [deg]" is used.

Keyword ZEN can also be PARK or MAX. PARK means the tracker points to the "parking position", which is given in the BlickO Instrument Configuration File (section 5.5), entry "Tracker parking zenith angle and azimuth". MAX means the tracker points to the maximum zenith angle in the range of the tracker (defined in in the IOF entry "Maximum tracker pointing zenith angle [deg]"; see section 5.3).

Another option for AZI and ZEN is DAZI and DZEN respectively. In this case the settings for AZI and ZEN are given by the global variables `self.dazi` and `self.dzen` respectively. These variables are initialized with setting 0, but could be modified by the user with routine command COMMAND. E.g. the following sequence would point the tracker to zenith angle 1° higher than the SZA (i.e. pointing closer to the horizon).

```
COMMAND -> self.dzen=1
SET POINTING -> ZEN=DZEN;ZENMODE=RELSUN
```

Keyword DELTA decides when the tracking is applied and if it is a one-time movement or a continuous tracking. If the setting of DELTA is a positive number, then a one-time tracking is done pointing the tracker to the desired position using the calculated solar (or lunar) angles this many seconds from now. E.g. when ZEN=0, ZENMODE=RELSUN and DELTA=30 then the tracking moves to the zenith angle, where the sun will be 30 s from now.

If DELTA=MIDDLE then a one-time tracking is done pointing the tracker to the desired position using the calculated solar (or lunar) angles for the time in the middle of the next spectrometer measurement set. E.g. when ZEN=0, ZENMODE=RELSUN, DELTA=MIDDLE and the duration of the next spectrometer measurements is 20 s, then the tracking moves to the zenith angle, where the sun will be 10 s from now.

DELTA=CONT means the tracking is updated continuously. The update interval is given in global variable `op.tperiods[4]` with default setting 2 s. E.g. the command line below does continuous sun tracking.

```
SET POINTING -> DELTA=CONT;AZI=0;ZEN=0;AZIMODE=RELSUN;ZENMODE=RELSUN
```

DELTA=CAMERA means the camera is in automatic mode and the tracking is solely guided by the camera. In this case all other keywords in SET POINTING have no effect. This situation is usually started calling routine CK and selecting "Automatic" in the dialog. Note that once the tracking is guided by the camera, any subsequent call to SET POINTING has no effect.

4.1.9 Routine Command SET SPECTROMETER

This command is used to prepare the spectrometers for measurements. As mentioned before, several keywords of this command can be set individually for each spectrometer, e.g. IT_1, IT_2 etc. Keyword IT (or IT_1, IT_2, etc.), which stands for "integration time", can be set to...

- CURRENT: the integration time is not changed.
- CHANGE: the integration time for spectrometer j (j=1 or 2) is changed to the value listed in global variable `self.sys_status[7][j-1][0]`.
- MIN: the integration time is set to the allowed minimum as given in the IOF.
- MAX: the integration time is set to the allowed maximum as given in the IOF.
- Any number between the allowed minimum and maximum integration time: the integration time is set to this value (in units of ms).
- "x" plus a number: This sets the integration time to that many times the current integration time (as long as it is not above the allowed maximum). So e.g. if the integration time is 10 ms and keyword IT=x2.5, then the integration time will be set to 25 ms.

Keywords NCYCLES, NREPETITIONS determine the number of cycles and number of repetitions used for the next spectrometer measurement respectively. Their meaning also depends on the value of keyword DURATION, which can either be set to AUTO (default), or a positive number, which fixes the total duration of the

next spectrometer measurement sequence to exactly this value, or an "x" plus a positive number, which sets a maximum total duration of the next spectrometer measurement sequence to this value (more below).

NREPETITIONS can be AUTO (default), CURRENT, a positive integer, zero, MAX1 or an "x" plus an integer. AUTO means the number of repetitions is adjusted based on the settings of DURATION and NCYCLES (more details below). CURRENT means the current number of repetitions is used. NREPETITIONS as an integer sets this number of repetitions. "x" plus an integer means the number of repetitions is set to that many times the current number of repetitions. So e.g. if the current number of repetitions is 2 and keyword NREPETITIONS=x3, then the next number of repetitions will be 6. MAX1 means the number of repetitions are set to 1 at the maximum. I.e. they stay 0 if they are already 0 and become 1 otherwise. Note that the number of repetitions does not affect the dark measurements in case keyword DARKRATIO is not set to 0 (see below). Hence, even if the number of repetitions is >1, at most one dark measurement will be done.

NCYCLES can be AUTO (default), CURRENT or a positive integer. AUTO means the number of cycles is adjusted based on the settings of DURATION and NREPETITIONS (more details below). CURRENT means the current number of cycles is used. NCYCLES as a positive integer sets the this number of cycles.

If DURATION is set to AUTO, the next spectrometer measurement sequence is made using exactly the number of cycles and repetitions as set in NCYCLES and NREPETITIONS. In this case, setting NREPETITIONS=AUTO or NCYCLES=AUTO is equal to setting them NREPETITIONS=1 or NCYCLES=1. E.g. the following line means that both spectrometers will measure at an integration time of 50 ms, spectrometer 1 measures 1 repetition for 100 cycles each and spectrometer 2 measures 3 repetitions at 1 cycle each.

```
SET SPECTROMETER -> IT=50;NCYCLES_1=100;NCYCLES_2=AUTO;
NREPETITIONS_1=AUTO;NREPETITIONS_2=3;DURATION=AUTO
```

If DURATION is not AUTO, then the following sequence applies:

- The number of repetitions is set to the initial value as described above. If NREPETITIONS equals AUTO, it is set to 1.
- The number of cycles is set to the initial value as described above. If NCYCLES equals AUTO, it is adjusted so that the requested total duration is maintained.
- In case NREPETITIONS equals AUTO, but NCYCLES does not equal AUTO, the number of repetitions is adjusted so that the requested total duration is maintained.
- If these values for the number of repetitions and cycles give a total measurement duration that is longer than the requested one, then they are adjusted with the principle that the adjusted number of repetitions is not larger than the requested number of repetitions and the adjusted number of cycles if not smaller than the requested number of cycles, if possible.
- If these values for the number of repetitions and cycles give a total measurement duration that is shorter than the requested one, the number of cycles is increased to match the requested duration, but only if DURATION is a directly number. If DURATION is "x" plus a number, then the number of repetitions and cycles is kept and the routine lasts less the the value in DURATION.

In other words, BlickO tries to adjust the number of repetitions and number of cycles in the best way to match the requested total measurement time. Unless set to AUTO, NREPETITIONS can be considered the maximum number of repetitions to be used and, unless set to AUTO, NCYCLES can be considered the minimum number of cycles to be used.

E.g. the following line means that in principle the user would like to take 5 repetitions and 250 cycles for each spectrometer within one minute. However, for spectrometer 1, measuring at 50 ms this would

last 62.5 s. Therefore for spectrometer 1 the number of repetitions is reduced from 5 to 4. At the same time the number of cycles is set to 300 to match the total duration. For spectrometer 2, 5 repetitions are possible and will be done, and the number of cycles is increased from 250 to 480 to "fill" the measurement time.

```
SET SPECTROMETER -> IT_1=50;IT_2=25;NCYCLES=250;NREPETITIONS=5;DURATION=60
```

If the line above is replaced by the one below, the situation does not change for spectrometer 1, since 4 repetitions is the maximum possible. However, spectrometer 2 will measure 9 repetitions at 267 cycles.

```
SET SPECTROMETER -> IT_1=50;IT_2=25;NCYCLES=250;NREPETITIONS=AUTO;
DURATION=60
```

Keyword DARKRATIO decides what fraction of the total measuring time is used for dark measurements. If it is set to 0, then no dark count is measured. If it is a number between 0 and 0.5, then this fraction of the total measurements time is used for dark measurements. So if e.g. 2000 (bright) measurement cycles are to be taken and DARKRATIO=0.2, then after the last repetition of "bright" measurements the OPAQUE filter is placed in the filterwheels and 500 cycles are measured at the same integration time. In this way from the total time (2500 cycles), 20% are dark measurements. At the end the filterwheels are set back to their initial positions.

DARKRATIO=OPT1 or DARKRATIO=OPTIMIZED mean that the first value of entry "Optimized dark ratio" in the IOF is used (see section 6.2). DARKRATIO=OPT2 means that the last value of entry "Optimized dark ratio" in the IOF is used (i.e. the second value, if it exists, otherwise the first one).

Note that when DARKRATIO is not 0 and there is more than one spectrometer, the dark measurements are synchronized, since the filterwheel change affects both spectrometers. In this case the dark measurements take the time, which is needed for that spectrometer that needs a longer dark measurements duration. Consider this line:

```
SET SPECTROMETER -> IT_1=50;IT_2=25;NCYCLES=250;NREPETITIONS=5;
DURATION=60;DARKRATIO=0.2
```

Here spectrometer 1 measures 4 repetitions (since 5 takes too much time), the number of cycles is set to 282 and at the end 70 dark cycles are measured. In this way 4 times 282 plus 70 equals a total of 1198 cycles, which matches the one minute requested duration as close as possible and the dark ratio is 70 over 282+70, close to 20%. Spectrometer 2 measures 5 repetitions, the number of cycles is set to 451 and at the end 140 dark cycles are measured. This means 5 times 451 plus 140 equals a total of 2395 cycles, which matches the one minute requested duration as close as possible. The dark ratio is 140 over 451+140, which is 24%. Hence the dark time for spectrometer 2 was increased in order to synchronize the filterwheel change with spectrometer 1.

4.1.10 Routine Command MEASURE

This command is used to measure spectra. Keyword DISPLAY decides how the data are drawn on the figure (GUI-section 8). Setting NO means the data are not drawn, MEAN means the average of all measurement cycles is drawn and MEAN+STD means the average plus the standard deviation over all cycles is drawn, if the number of cycles exceeds one (otherwise just the average will be drawn). CURRENT means the value in variable `self.figdrawmode` is used.

Keyword SAVE decides whether the measured data are saved in the level 0 data file. Setting NO means they are not saved, STDERR means the average and the standard error of the measurements is saved and STDERRTOLINE means the average and the root mean square deviation to a fitted straight line through the measurements is saved.

Keyword SATCHECK decides whether the measurements are checked for saturation. Setting NO means the data are not checked for saturation. YES means the data are checked for saturation and the routine is stopped if saturation has been detected. WARN is the same as YES, but a warning message is displayed at the end of the routine, which means no further routine is executed.

The simplest call is MEASURE without setting any keyword.

```
MEASURE
```

In this case the default settings are used, i.e. the average of the measured data is displayed, the data are not saved to the L0 file and the data are checked for saturation.

4.1.11 Routine Command CHECK INTENSITY

This command is used to check the strength of the light input and adjust the filterwheel settings and the integration time accordingly. Also for this command several keywords can be set individually for each spectrometer, e.g. ADJUSTIT_1, ADJUSTIT_2 etc.

Keyword ADJUSTIT decides what initial integration time should be used for the intensity-check measurements. FROMCURRENT means the current integration time is used. FROMMIN means the minimum integration time as given in the IOF is used.

Keyword ADJUSTND decides if and how the neutral density filters in the filterwheels are adjusted (this keyword has no meaning if the Pandora system does not have neutral density filters). NO means the neutral densities are not adjusted. FROMCURRENT means the neutral densities are adjusted, starting with the current neutral density. FROMMAX means the neutral densities are adjusted, starting with the highest neutral density in the system. FROMLASTDS means the neutral densities are adjusted, starting with the neutral density that was used during the last direct sun measurement, where the same filterwheel positions were used. NOMAX means the filterwheels are positioned to have maximum attenuation, but are not adjusted afterwards.

Keyword %SATURATION decides to what percentage of the saturation value the intensity will be adjusted. Negative numbers mean the intensity is adjusted to this percentage of the "nominal saturation limit" (taking first the absolute value of the number, i.e. -80 means 80%). The nominal saturation limit is simply 2^{nbits}-1, with nbits being the number of bits of the instrument's AD converter as given in the IOF (see section 5.3). Positive numbers below 100 mean the intensity is adjusted to this percentage of the "effective saturation limit". The effective saturation limit is the nominal saturation limit times the value of entry "Effective saturation limit [%]" from the IOF. Positive numbers between 1000 and 10000 mean the following: in the case the effective saturation limit exists, then the intensity is adjusted to this number modulo 100 as a percentage of the effective saturation limit. Otherwise (the effective saturation limit does not exist), then the intensity is adjusted to this number div 100 as a percentage of the nominal saturation limit. If keyword %SATURATION is set to SATPERC, then the value in global variable `self.satperc` is used as saturation limit.

Keyword DARKESTIMATION decides how the dark count should be accounted for when determining the best integration time. NEGLECT means the influence of the dark count is ignored. THEORY means the dark behavior, as given in entries "Dark offset [counts]" and "Dark slope [counts/s]" of the IOF, is taken into account.

Keyword ITLIMIT decides what the maximum allowed integration time can be after the intensity check. It can be ITMAX, xITMAX, a number between the allowed minimum and maximum integration time, or "x" plus such a number. ITMAX means the maximum allowed integration time as given in the IOF is used. A number means this setting is used (in units of ms). "x" plus a number or xITMAX means that the routine is skipped in case the optimized integration exceeds this value for at least one spectrometer.

Note that if the number of repetitions for any spectrometer is set to zero, then no intensity check is done for this spectrometer.

As an example, the line below calls for an intensity check starting at minimum integration time, the neutral

density used at the last direct sun measurement, trying to adjust to 80% of the instrument's effective saturation limit and taking the dark behavior into account. The routine will not be executed if the optimized integration time exceeds 2000 ms for all spectrometers.

```
CHECK INTENSITY -> ADJUSTIT=FROMMIN;ADJUSTND=FROMLASTDS;%SATURATION=80;
DARKESTIMATION=THEORY;ITLIMIT=x2000
```

4.1.12 Routine Command PROCESSINFO

This command is needed for the processing software BlickP. It tells BlickP how the data measured by this routine should be analyzed. Keyword TYPE defines the measurement type. The options for TYPE are shown in table 7. Column "Index" is an integer representing a certain TYPE. This index is also saved in a column of the L0 data, called "Data processing type index" (see section 5.7).

Table 7: Processing type

TYPE	Index	Description
ONLYL1	0	BlickP converts the L0 data of this routine to L1 data, but does not produce data levels higher than L1.
NOL1	1	BlickP ignores this routine.
SUN	2	Direct sun data. BlickP produces L1 and L2 data for this routine.
MOON	3	Direct moon data. BlickP produces L1 and L2 data for this routine.
SKY	4	Not further specified sky radiance data. BlickP produces L1 and L2 data for this routine.
TARGET	5	"Target routines", where measurements from a reflecting surface are made. BlickP produces L1 and L2 data for this routine.
PROFILE	6	Routines, which allow retrieving profile information (e.g. sky scans at different viewing zenith angles for fixed azimuth). BlickP produces L1 and L2 data for this routine.
ALMUCANTAR	7	"Almucantar routines", where sky radiance is measured at a fixed zenith angle for different azimuths. BlickP produces L1 and L2 data for this routine.
LAMP	8	Lamp measurements or more generally for any measurement, where the input does not originate from the sun. BlickP produces L1 and L2 data, but does not retrieve a wavelength shift even if requested.
SPECIAL	9	Not further specified "specialized" routine. BlickP produces L1 and L2 data for this routine.

Keyword DISTANCE is only used if keyword TYPE=TARGET. Otherwise it is set to NO. The setting of DISTANCE gives the distance in m of the reflecting object, of which the measurements are made. While command PROCESSINFO with keyword TYPE should only be used once in a routine, with keyword DISTANCE it can be used as many times as needed. E.g. the lines below mean that a target routine takes measurements of an object at a distance of 0.2 m and then of an object at 98 m from the head sensor.

```
PROCESSINFO -> TYPE=TARGET;DISTANCE=0.2
...
```

```
PROCESSINFO -> DISTANCE=98
...
```

4.1.13 Routine Commands START LOOP and STOP LOOP

These routine commands indicate the start and stop of a loop. The number of times the loop is run is defined by keyword XIJ in command START LOOP. It can either be comma-separated list of numbers like

```
START LOOP -> XIJ=0,1,2,3,4
```

or a Python expression inside brackets after the word MAKE like

```
START LOOP -> XIJ=MAKE(range(5))
```

These two examples of command START LOOP have actually the same effect. In both cases all commands from the line with START LOOP until the line with command STOP LOOP are repeated 5 times. The variable XIJ takes the value 0 in the 1st run, 1 in the 2nd run, etc. XIJ can also be used for any keyword of the routine commands inside the loop. Here an example:

```
START LOOP -> XIJ=10,30,100
SET SPECTROMETER -> IT=XIJ;NCYCLES=10;NREPETITIONS=1
MEASURE
STOP LOOP
```

This command sequence takes spectra with 10 cycles, first at integration time 10 ms, then at 30 ms and finally at 100 ms.

Note that MAKE is usually used when the number of loops is depending on the length of a variable. E.g.

```
START LOOP -> XIJ=MAKE(range(len(self.hh)))
```

means that as many loops are done as there are elements in global variable self.hh. Since the BlickO interpreter of the routine syntax translates the content of all routines at program startup and self.hh possibly has a different length at program execution than at startup, BlickO cannot determine how long the routine including MAKE will take. Therefore, if a routine includes MAKE and the routine is used in schedule mode, routine command DURATION must also be used in the same routine with TIMEMODE=TOTAL (see 4.1.6). Otherwise an error message will appear at program startup saying "... Routine ... includes 'MAKE', but does not include keyword 'DURATION' with subkeyword 'TOTAL'. This is not allowed in a schedule. Execution is stopped." Hence when this error message appears one can simply replace the MAKE in the START LOOP section with directly numbers (as in the first example of this section) or, if this is not possible, estimate how long this routine will take and add routine command DURATION with TIMEMODE=TOTAL.

4.2 Schedules

Also the concept of "schedules", i.e. a daily sequence of routines to be executed by the Pandora system, is taken from the way Brewer spectrometers are operated [21]. Schedules are stored in text files `/lib/schedules/XXX.sked`, where XXX is the name of the schedule, which can be of any length. Some standard schedule templates are automatically included during the software installation and are explained at the end of this section. To call a schedule, the "Load schedule" button (GUI-section 9) must be pressed, then a

schedule selected and finally the Start-Stop-button pressed. The first thing BlickO does is to read through the schedule commands and convert them into its own internal format.

4.2.1 Schedule file syntax

The schedule files use a proper syntax, which is explained in this section. Errors in the syntax will in general be detected by BlickO, in which case an error message will be displayed.

Comment lines in the schedule files have to start with "#", otherwise they will be interpreted. Apart from the comment lines, a schedule file consists of one or more "routine sequence blocks", which start with an open brace "{" and end with a closed brace "}". Inside the braces are strings separated by commas. Each string starts with a keyword, followed by an arrow "->" and then a value. The order of the keywords inside the block does not matter. Below is an example of a schedule called "simple", which consists of only one routine sequence block, which repeats routines RF, SO an SU all throughout the day from sunrise to sunset.

```
# Simple schedule:  Direct sun from sunrise to sunset
{
label -> AllDay,
start -> solarzen90am,
end -> solarzen90pm,
priority -> 1,
repetitions -> -1,
commands -> rfsosu
}
```

Note that it is not necessary to include a line break after each keyword-value pair, it is just somewhat more readable in that way. The keywords and their allowed values are listed in table 8.

Table 8: Keywords for a routine sequence block in a schedule file

Keyword	Description
label	This mandatory keyword is a string used to identify the routine sequence block.
start	This mandatory keyword gives the start time for the routine sequence block. The allowed values are given in table 9. A time in format "HH:MM" can be added or subtracted, e.g. "solarday_noon-00:10" means 10 min before local noon.
end	This is the optional end time for the routine sequence. The allowed values are the same as for keyword "start", except for "THEN" and "NOW". In addition it can be set to "start+HH:MM", which means the block ends the time HH:MM after it has started. Value "undefined" (the default setting) means the software calculates the end time automatically using the estimated duration of the routines included in the routine sequence block.
priority	This mandatory keyword is a positive integer used to assign a priority to the routine sequence block. It is used to decide, which block should prevail in case there are conflicting blocks. Higher numbers have higher preference. E.g. if there are two blocks, one with settings "start -> 11:47, priority -> 2," and the other with "start -> solarday_noon, priority -> 1", and on a specific day it happens that the local noon is around 11:47 UTC, then only the second block with priority 2 will be executed.
commands	This mandatory string is a routine sequence just as it could also be written in the routine control (GUI-section 9).
repetitions	This optional positive integer gives the number of times the routine sequence given in the keyword "commands" is executed. It can also be set to -1, in which case an infinite loop is executed that only ends when a next blocks starts. The default value is 1 in case keyword "end" is "undefined", otherwise it is -1.
startwith	If given, this optional keyword holds a string with a routine sequence that will be executed exactly one time before the routine sequence indicated in "commands" starts, independently of the number of repetitions set in keyword "repetitions".
refrout	This optional string sets the "reference routine" and is either the 2-character-identifier of one of the routines listed in keyword "commands" or string "startwith". The time indicated in keyword "start" will be applied to the first occurrence of this reference routine. This can be used for the case it is critical to start a specific routine exactly at a determined moment. If this keyword is not given, then the start time will refer to the first routine in the routine sequence, either from the sequence given in "startwith" or simply the first one in keyword "commands" in case “startwith” is not defined.
reftime	This is the optional reference time of the reference routine defined in keyword "refrout". It can be a "b" (default), an "m" or an "e" meaning the beginning, the middle or the end of the reference routine.
if	This optional keyword can put an additional filter on the execution of a routine sequence block. The allowed values are: - "sun_visible": the routine sequence block will be ignored if between the defined "start" and "end" time period the sun is never visible (SZA is always >90°) - "moon_visible": The routine sequence block will be ignored if between the defined "start" and "end" time period the moon is never visible (LZA is always >90°). - "moonphase_MP": The routine sequence block will only be executed if moon phase "MP" is present either at the "start" or "end" time of the routine sequence block. MP can be one of the following strings: newmoon, waxingcrescent, firstquarter, waxinggibbous, fullmoon, waninggibbous, lastquarter, waningcrescent. - "monthday_DD": The routine sequence block will only be executed on the specified day of the month (0<DD<32). Note that the local solar noon date is used to check this.

Table 9: Allowed timestamps for keywords "start" and "end"

Timestamp	Description
HH:MM	Specific hour and minute of the day in UTC. The minutes can have decimals. E.g. "16:40.5" means UTC 16:40:30.
solarday_start	The starting local midnight of the day. This is the time with the largest SZA before the moment the schedule is started.
solarday_end	The ending local midnight of the day. This is the time with the largest SZA after the moment the schedule is started.
solarday_noon	The local noon of the day. This is the time with the smallest SZA within ± 12 hours around the moment the schedule is started.
solarday_rise	The time of the geometrical local sunrise of the day including refraction correction within ± 12 hours around the moment the schedule is started.
solarday_set	The time of the geometrical local sunset of the day including refraction correction within ± 12 hours around the moment the schedule is started.
lunarday_start	The time with the largest LZA before the moment the schedule is started.
lunarday_end	The time with the largest LZA after the moment the schedule is started.
lunarday_noon	The time with the smallest LZA within ± 12 hours around the moment the schedule is started.
lunarday_rise	The time of the geometrical local moonrise of the day within ± 12 hours around the moment the schedule is started.
lunarday_set	The time of the geometrical local moonset of the day within ± 12 hours around the moment the schedule is started.
solarzenXXam	The time corresponding to SZA XX before local solar noon (0≤XX≤100).
solarzenXXpm	The time corresponding to SZA XX after local solar noon (0≤XX≤180).
lunarzenXXam	The time corresponding to LZA XX before local lunar noon (0≤XX≤180).
lunarzenXXpm	The time corresponding to LZA XX after local lunar noon (0≤XX≤180).
solarelevXX%am	Moment before local solar noon, where the solar elevation is XX% of the maximum solar elevation of the day (0≤XX≤100). XX=0 means sunsrise.
solarelevXX%pm	Moment after local solar noon, where the solar elevation is XX% of the maximum solar elevation of the day (0≤XX≤100). XX=0 means sunset.
lunarelevXX%am	Moment before local solar noon, where the lunar elevation is XX% of the lunar elevation at solar noon (0≤XX≤100).
lunarelevXX%pm	Moment after local solar noon, where the lunar elevation is XX% of the lunar elevation at solar noon (0≤XX≤100).
THEN	This is the time, where the latest of the previous routine sequence blocks ends. This value is not allowed for the first block. Note that if none of the previous blocks has a proper start or end time, it will be set to "solarday_start". When this value is used, it is important to write the schedule in a chronological order, at least for the blocks before the one using "THEN".
NOW	This is the current time + 10 seconds. It is mainly used to test the schedule functionalities, or to run a specific routine sequence every time the schedule is started.

Note that if a (solar or lunar) zenith angle does not occur at this day and latitude, then this block of the schedule will be skipped.

If BlickO can successfully read through the schedule file, it will first create a "protocol file" of name `/data/protocolfiles/YYYYMMDDTHHMMSSZ_XXX.prot`, where YYYYMMDDTHHMMSSZ is the time the protocol file was created and XXX is the name of the schedule. This is a text file with the "translated" schedule for the day and the location. E.g. the schedule "simple" from above creates the following protocol file for 7 April 2021 for the location Goddard Space Flight Center, USA (it is truncated in the middle):

```
Predicted Pandora #0 measurements based on schedule 'simple'
Goddard Space Flight Center, USA, Lat 38.99°, Long -76.84°, 90m a.s.l.
File created on Wed 7 Apr 2021, 01:31:04 UT.
Astro events for the current solar day:
Start -> 20210406T050935Z
Sunrise -> 20210406T104534Z
Noon -> 20210406T170950Z
Sunset -> 20210406T233427Z
End -> 20210407T050919Z
------------------------------------------------------------

Final routine sequence 1 (schedule file routine sequence 1)
Routine sequence definition:  'label=AllDay, start=solarzen90am,
end=solarzen90pm, repetitions=-1, priority=1, refrout=rf, reftime=b,
commands=rfsosu'
Summary:
Start time of routine sequence 1:  20210406T104533Z
End time of routine sequence 1:  20210406T233427Z
Routines:
RF 10:45:33-10:45:45 (SolarZEN 89.92-89.88) Tue 6 Apr 2021
SO 10:45:45-10:46:37 (SolarZEN 89.88-89.72) Tue 6 Apr 2021
SU 10:46:37-10:47:49 (SolarZEN 89.72-89.49) Tue 6 Apr 2021
RF 10:47:49-10:48:01 (SolarZEN 89.49-89.46) Tue 6 Apr 2021
SO 10:48:01-10:48:53 (SolarZEN 89.46-89.32) Tue 6 Apr 2021
SU 10:48:53-10:50:05 (SolarZEN 89.32-89.13) Tue 6 Apr 2021
...
SU 23:30:29-23:31:41 (SolarZEN 89.25-89.44) Tue 6 Apr 2021
RF 23:31:41-23:31:53 (SolarZEN 89.44-89.47) Tue 6 Apr 2021
SO 23:31:53-23:32:45 (SolarZEN 89.47-89.63) Tue 6 Apr 2021
SU 23:32:45-23:33:57 (SolarZEN 89.63-89.86) Tue 6 Apr 2021
RF 23:33:57-23:34:09 (SolarZEN 89.86-89.89) Tue 6 Apr 2021
SO 23:34:09-23:35:01 (SolarZEN 89.89-90.06) Tue 6 Apr 2021
-> last routine probably not executed due to time restriction

------------------------------------------------------------
Estimated number of occurrences for each routine
RF 340
SO 339
SU 339
------------------------------------------------------------
```

After the protocol file has been created, BlickO starts the schedule for the day. At the end of the day it translates the schedule file again for the next day, creates a new protocol file with the next day's information and starts the schedule for the next day. This continues until the user presses "Stop".

Whenever there is a break for more than 20 min in the schedule (e.g. during the night), the tracker will go in parking position as given in the BlickO Instrument Configuration File (section 5.5), entry "Tracker parking zenith angle and azimuth". Note that the parking position is interrupted periodically to avoid accumulation of ice according to the BlickO Instrument Configuration File entry "Tracker warming interval [min]" (section 5.5).

4.2.2 Overlapping routine sequences

Different routine sequences in a schedule may overlap in time. Blick is able to detect such an overlap and splits the routine sequences to ensure that the routine sequence with higher priority (based in the keyword "priority") will be executed at the desired time, while the sequence with lower priority will be interrupted, or starting later, or finishing earlier, or even not being executed at all, which is illustrated in figure 6.

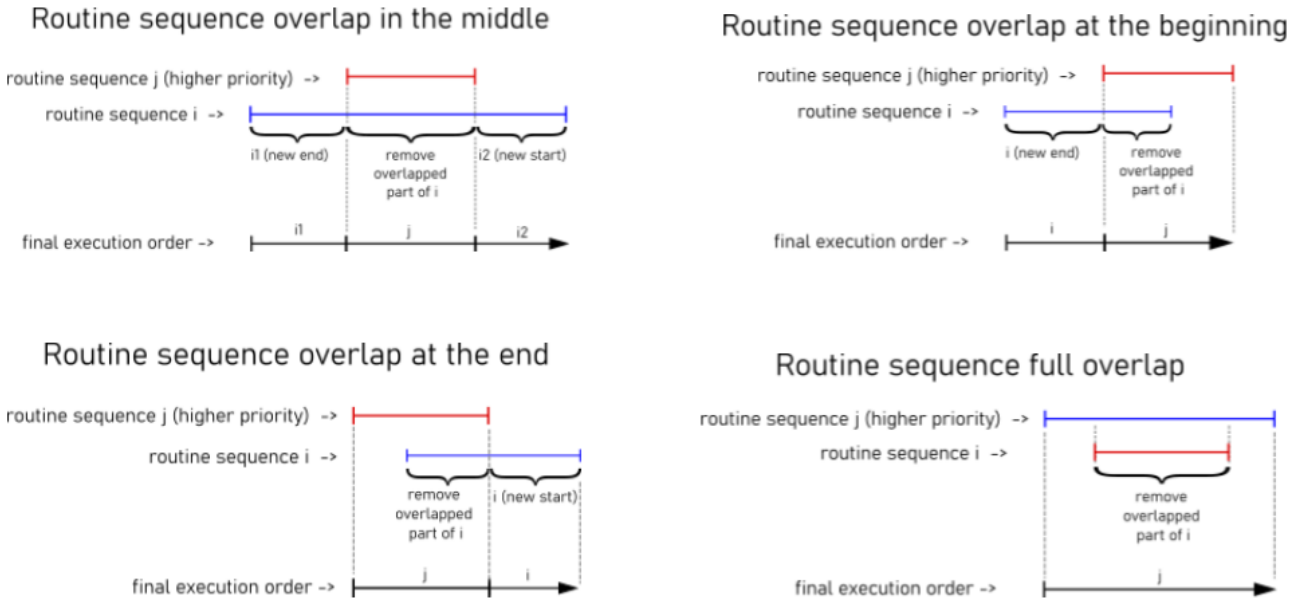


Figure 6: Different situations, where a routine sequence i with lower priority (blue) is modified, so that the routine sequence j with higher priority (red) is fully executed. The lower priority routine sequence can be interrupted in the middle (top left panel), cropped at the end (top right panel), cropped at the beginning (bottom left panel) or not being executed at all (bottom right panel).

4.2.3 Standard schedules

The "standard schedules" listed in table 10 are automatically included during the software installation. Schedules "startup" and "align" can be used without any modification. All other schedules are actually templates, which the user may modify to adapt the specific scientific goal and the topography at the measurement site. More details about each schedule template can be found in the files themselves.

A typical procedure after instrument installation is to start with schedule "startup" for about 30 min (during conditions with visible sun), then "align" for about one day (preferably mostly with visible sun, see also section 6.1), and then a customized version of the given schedule templates (see table 10). The schedule templates

are optimized for UV Pandoras (usually Pandora-1S systems), with prefix "uv" versus UV-Vis Pandoras (usually Pandora-2S systems), with prefix "uvvis". "hsm" stands for "high speed mode", where the direct sun observations are taken at a higher data rate. This provides better time resolution, but also increases the size of the raw data significantly and should therefore only be used for systems with good internet connection.

Table 10: BlickO standard schedule

Schedule name	**Description**
startup	Schedule used check tracking performance
align	Schedule used for instrument alignment
uv_sun, uvvis_sun, uv_sun_hsm, uvvis_sun_hsm	Schedule with direct sun observations
uv_sun_moon, uvvis_sun_moon, uv_sun_moon_hsm, uvvis_sun_moon_hsm	Schedule with direct sun and moon observations
uv_sun_moon_sky, uvvis_sun_moon_sky_hsm, uv_sun_moon_sky, uvvis_sun_moon_sky_hsm	Schedule with direct sun, direct moon and sky observations

5 Input Output Data Specifications

This section describes all files that are used as input or created as output by the Blick Software Suite. Table 11 gives an overview of all files. Column 'IO' says whether this file is an input (I) or output (O) or both (IO). Column 'SW' says, which specific software is using this file. 'O' stands for BlickO, 'F' for BlickF and 'P' for BlickP. Column 'Type' says which format the file is written in. This can be ASCII or HDF. Column 'Sect' lists the section of the manual, where this file type is described.

Most input and output data include meta data information in the header. The meta data are described in section 5.1.

Table 11: Input Output Files Overview

File	IO	SW	Type	Sect	Content
Locations File	I	O	HDF	5.2	List of locations
Instrument Operation File	I	O,P	ASCII	5.3	Hardware information for a Pandora unit
BlickO-BlickF Messenger File	IO	O,F	ASCII	3.2.3	Hexadecimal number to exchange messages between BlickO and BlickF
BlickO General Configuration File	IO	O	ASCII	5.4	General BlickO configuration information
BlickO Instrument Configuration File	IO	O	ASCII	5.5	BlickO configuration information specific for one Pandora unit
BlickF Configuration File	I	F	ASCII	5.6	BlickF configuration information
L0 File	O	O	ASCII	5.7	L0 data
BlickO Status File	IO	O,F	ASCII	5.8	Information about the current instrument status
BlickP Configuration File	I	P	ASCII	5.9	BlickP configuration information
L1 File	O	P	ASCII	5.12	L1 data
Processing Setups File	I	P	HDF	5.10	File with configuration options for data processing
Instrument Calibration File	I	P	ASCII	5.11	Calibration results for a Pandora unit
L2 Files	O	P	ASCII	5.14	L2 data
Log Files	O	O,F,P	ASCII	5.15	Logger lines
Alignment Files	IO	O	ASCII	5.16	Sun/Moon search results

5.1 Meta Data

Table 12 lists all the meta data used in the Blick Software Suite. Not all meta data are used in each file type. Column 'Used by' indicates, which files include the respective meta data information. The acronyms used for this column are:

IOF	Instrument operation file
ICF	Instrument calibration file
L0	Level 0 file (raw signals)
L1	Level 1 file (corrected signals)
L2Fit	Level 2 spectral fitting results file
L2	Level 2 files with column amounts, concentrations, profiles, etc.
L2*	Both L2Fit and L2
All	All of the above files
Align	Alignment file

Table 12: Meta Data Overview

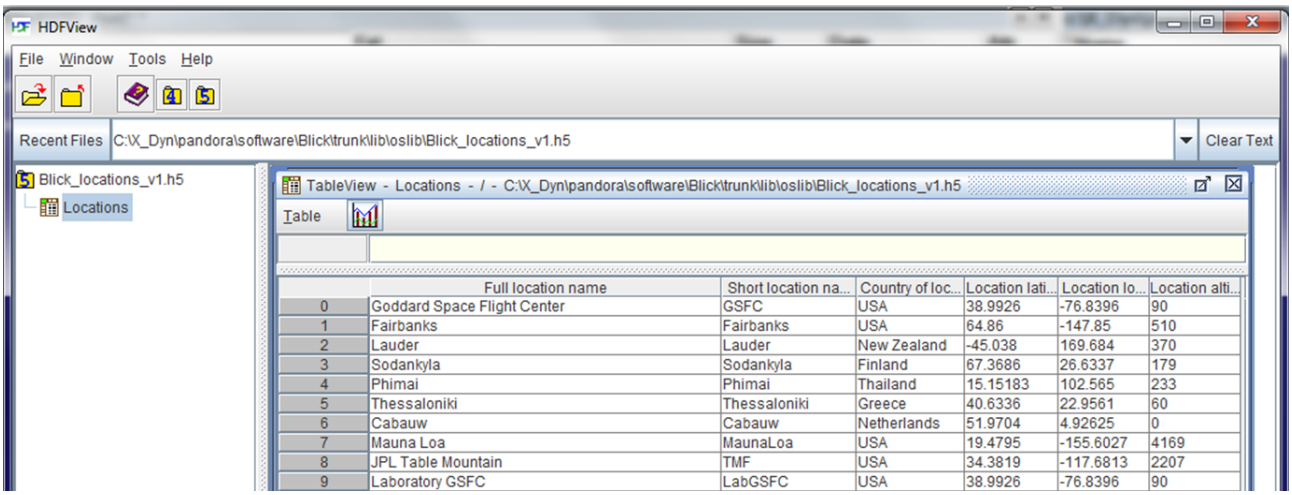
Name	Used by	Description
File name	All	Name of file
File generation date	All	File generation date as ISO 8601 string
Data description	All	Description of file type, e.g "Instrument operation file"
Data file version	All but L0	typically a combination of characters and numbers, e.g. "c2p1s4"
Data originator name	IOF, ICF	Name of person that created the file
Data product status	L2	Status of the data product (see section 5.10.4)
Local principal investigator	All but ICF	Name of responsible person at the network location
Network principal investigator	L1, L2*	Name of the responsible person for the Pandonia Global Network (PGN)
Instrument type	All	"Pandora"
Instrument number	All	integer>0, e.g. 0 for Pandora 0
Spectrometer number	All but IOF	1 for spectrometer 1 and 2 for spectrometer 2
Operation software version used	L0	BlickO version used
Processing software version used	L1, L2*	BlickP version used
Instrument operation file used	All but IOF, L2	Name of IOF used to run the instrument or to create the ICF
Calibration session number	ICF	integer>0 indicating which calibration session was used to produce the ICF
Instrument operation file created	ICF	Name of IOF, which was created in the calibration session

Name	Used by	Description
Calibration data validity starting date	ICF	Same as in ICF name
Instrument calibration file used	L1, L2Fit	Name of the ICF used to process data
Level 0 file used	L1	Name of L0 file on which the L1 file is based on
Level 1 file used	L2Fit	Name of L1 file on which the L2Fit file is based on
Full location name	All but IOF, ICF	See section 5.2
Short location name	All but IOF, ICF	See section 5.2
Country of location	All but IOF, ICF	See section 5.2
Location latitude [deg]	All but IOF, ICF	See section 5.2
Location longitude [deg]	All but IOF, ICF	See section 5.2
Location altitude [m]	All but IOF, ICF	See section 5.2
Local noon date	L0, L1, L2Fit	Date of local noon at the selected location
Data start time	L2	Time of first data entry in file
Data end time	L2	Time of last data entry in file
Notes on s-code (L1 configuration)	L1, L2*	Lists data corrections, which are requested by the s-code, but not possible for this instrument
Data caveats	All but IOF, L0	Caveats such as "Based on preliminary calibration"
First and last pixel inside fitting window	L2Fit	Starts counting at 1 (not 0); note that this says "Depends on filterwheel settings" in case relative number were used for WL-starts or WL-ends (see table 25)
Nominal wavelengths [nm]	L1	Given for all regular pixels
Nominal wavelengths inside fitting window [nm]	L2Fit	Given for all pixels inside the fitting window; note that this says "Depends on filterwheel settings" in case relative number were used for WL-starts or WL-ends (see table 25)

5.2 Locations File

5.2.1 Format

The locations file is a HDF file called `/lib/oslib/Blick_locations.h5`. It is provided in the software distribution and can also be downloaded under `https://www.pandonia-global-network.org/home/documents/software/`. The file includes one table called "Locations". Every row of the table contains the information of one instrument location (see figure 7).



	Full location name	Short location na...	Country of loc...	Location lati...	Location lo...	Location alti...
0	Goddard Space Flight Center	GSFC	USA	38.9926	-76.8396	90
1	Fairbanks	Fairbanks	USA	64.86	-147.85	510
2	Lauder	Lauder	New Zealand	-45.038	169.684	370
3	Sodankyla	Sodankyla	Finland	67.3686	26.6337	179
4	Phimai	Phimai	Thailand	15.15183	102.565	233
5	Thessaloniki	Thessaloniki	Greece	40.6336	22.9561	60
6	Cabauw	Cabauw	Netherlands	51.9704	4.92625	0
7	Mauna Loa	MaunaLoa	USA	19.4795	-155.6027	4169
8	JPL Table Mountain	TMF	USA	34.3819	-117.6813	2207
9	Laboratory GSFC	LabGSFC	USA	38.9926	-76.8396	90

Figure 7: Screen short of location file opened with HDF viewer

For each location the following information is given:

1. Location number
2. Full location name
3. Short location name (used in file output, only alphanumeric!)
4. Country of location
5. Location latitude in degrees [-90°, 90°] (Minus=South of equator, Plus=North of equator)
6. Location longitude in degrees [-180°, 180°] (Minus=West of Greenwich, Plus=East of Greenwich)
7. Location altitude above sea level in meter

5.2.2 When is a new Locations File Entry needed?

The general rule for this is that a new Locations File Entry should be created, when the new location is in a different physical environment than any existing location. In most cases this is not in question, e.g. when there is some spatial distance to any existing location. But what if the instrument is in close proximity to an existing location? Then the station investigators have to decide. E.g. if an instrument is moved for about 10 m and the environment is basically the same as it was before, one could continue using the previous Location File Entry. However when this short move causes the environment to be different (e.g. the view in one direction is now blocked), then a new entry should be created.

A special case are moving platforms such as cars, ships, etc. For these cases we do not recommend to create a new Locations File Entry e.g. every day after the platform has moved. Instead one should use the same entry and change the coordinates once per day if needed. Instruments on such platforms should in principle be equipped with a GPS anyway, which reports the correct position for each measurement.

5.2.3 Adding/Updating a Locations File Entry

In principle one can edit the locations file locally. However it is strongly recommended to do it in the way as described in this section to avoid duplicated use of names or coordinates etc. An email should be written to `admin@pandonia-global-network.org` with subject "New PGN Location Request". This email should include the following information:

- The full location information (all 7 entries) keeping in mind the rules listed in the next section 5.2.4.
- Name, address and contact information (email and phone number) of the PGN station manager and operator (which can be the same or different persons).
- Email address to which PGN correspondence should be sent.

You will receive an email as soon as the request has been resolved by LuftBlick. Then you can download the updated locations file from `http://pandonia.net/docs/` and copy it in directory `/lib/oslib/`.

5.2.4 Rules for Constructing a Locations File Entry

These rules/guidelines need to be followed when choosing a location name:

Short location name

- Use only capital letters, small letters, numbers and hyphens. Hence e.g. spaces, underscores, dots etc. are not allowed.
- Maximum of 20 characters.
- In order to give the station good visibility, one should use a short name, which is best recognized to a broader international audience. This is most often simply the name of the town or area. E.g. use "Helsinki" instead of "FMI".
- Use CamelCase, e.g. "Rome" instead of "ROME".
- If more than one instrument is in the vicinity of a specific location, then start with the name of the town and then add an additional identifier to distinguish them. E.g. for the three stations in and near the city of Rome we use "Rome-ISAC", "Rome-SAP" and "Rome-IIA".
- If state or country names are used, they should be added to the name of the town and must follow the ISO 3166-1 alpha 2 standard. E.g. "FourCornersNM" for the station in the US-state of New Mexico.
- A moving station shall carry the location name of its platform (ship, plane, car), its base or the greater geographic area, whatever fits best, but NOT different station names for each new acquisition setup.

Full location name

The full location name is limited to 80 characters, can be free text, must relate to the short name and should enhance the short name's description. The level of given details should provide uniqueness of the description. Example: GSFC -> Goddard Space Flight Center or GSFC -> Goddard Space Flight Center, Greenbelt. Do not use GSFC -> Greenbelt. The latter might be used for a separate location.

Country of location

Use the name as it appears in `http://www.un.org/en/members/`. Examples: Use 'United States of America' and 'Republic of Korea'. Do not use 'USA' and 'South Korea'.

Latitude, Longitude and Altitude

Use GPS coordinates of actual image location to four digits after the comma. For altitude, use digital elevation model/map or merged barometric and GPS altitude if available.

5.3 Instrument Operation File

The IOF is in directory `/data/operationfiles` and is called `PandoraX_OF_vVdYYYYMMDD.txt`, where X is the instrument number, V the version number and YYYYMMDD the operation data validity starting date. It is an ASCII-text file containing hardware information for a Pandora unit and is needed to run the instrument with BlickO as well as processing data with BlickP. The validity starting date is changed, when there are changes in the optical hardware, e.g. a new filter wheel setup. The version number typically changes at non-hardware modifications, e.g. new settings for the temperature parameters. Note that there is no operation data validity ending date in the file name. The validity simply ends with the starting date of the next IOF.

Each line of the IOF gives either metadata or an instrument property and its setting, separated by the string "->". Some of the instrument properties are mandatory, some are optional. E.g. if no filterwheel properties are given (they are optional), then BlickO will still start, but assumes that this specific Pandora unit does not have a head sensor. Table 13 lists all possible IOF entries and their allowed settings, which are not already listed in the meta data table 12.

Rows 1 to 8 are mandatory entries, all other ones are optional. Rows 1 to 16 refer to the spectrometer. Rows 17 to 24 refer to the head sensor. Rows 25 to 32 refer to the field of view (FOV). Rows 33 to 35 refer to the tracker. Rows 36 and 37 refer to the shadowband. Rows 38 to 42 refer to the positioning system. Rows 43 to 51 refer to the temperature controller. Row 52 refers to additional existing sensors (temperature, humidity, etc.). Rows 53 to 66 refer to the camera.

Rows 22 and 23 are actually several entries (maximum 9 per filterwheel). Valid filterwheel settings for either filterwheel are given in table 6.

The entries for the spectrometer (rows 1-16), temperature controller (rows 43-51) and FOV (rows 25-32) can also be followed by a " 2" or a " 3" (e.g. "Spectrometer read out type 2"), which means the Pandora unit has not just one, but 2 or 3 spectrometers (or temperature controllers). Note that for all values that can be lists, a space is used as separator.

Entry "Dispersion polynomial" (row 13) lists the coefficients of the dispersion polynomial starting with the highest order. To obtain the nominal air-wavelength centers of the Pandora unit, the coefficients have to be applied on the "scaled pixels". The scaled pixels pixs are given by equation 1:

$$\text{pixs} = 3.46 \cdot \left(\frac{\text{pix}}{\text{npix}} - 0.5 \right) \tag{1}$$

npix is the number of pixels (first element of entry 3 of the IOF) and pix are the regular pixel numbers starting with 1 for the first pixel (i.e. 1, 2, 3, ..., npix).

Table 13: Entries of IOF

#	Entry	Description / Allowed settings
1	Spectrometer read out type	"Ava1", "Hama1", "OcOpt1" or "JETI1"
2	Spectrometer unit ID	ID-string unique for spectrometer
3	Number of pixels	one or two elements list of integers>0, the mandatory first element gives the total number of pixels, the optional second element number gives the number of pixels read in a separate function call (usually blind pixels)
4	A/D converter number of bits	integer>0
5	Raw data discriminator factor	float>0, the detector counts are divided by this number by the manufacturer-provided data read function
6	Minimum integration time [ms]	float>0, this is at or slightly above the minimum time given by the spectrometer manufacturer
7	Maximum integration time [ms]	float>0, usually set to 4 s
8	Integration time resolution [ms]	float>0
9	Dark offset [counts]	float, average dark offset over all pixels at standard temperature
10	Dark slope [counts/s]	float, average dark slope over all pixels at standard temperature
11	Optimized dark ratio	One or two floats with 0<float≤0.5, optimized split between dark and bright measurements based on detector properties (equation 59); the first number is for the case no dark map is given (equation 60), the optional second number is for the case a dark map is given (equation 62)
12	Limiting pixels of reference FOV	2-elements-list of integers, is >0 and <number of pixels
13	Dispersion polynomial	list of floats
14	Shutter function	0 (1) for a spectrometer without (with) electronic shutter
15	Spectrometer board temperature sensor type	1 (2) for a spectrometer with analog (digital) temperature sensor
16	Effective saturation limit [%]	0<float≤100
17	Head sensor-tracker connection type	"RS232"
18	Head sensor-tracker connection baudrate	integer>0
19	Head sensor-tracker ID	ID-string
20	Head sensor type	"SciGlobHSN1", "SciGlobHSN2"
21	Head sensor port number	integer between 0 and 256; 0 means the port is not known and BlickO scans through all ports
22	Filterwheel 1, position 1 to 9	Valid filterwheel setting
23	Filterwheel 2, position 1 to 9	Valid filterwheel setting
24	Filter position offsets	list of integers >0

25	FWHM, ... for reference sky FOV	3 floats>0
26	FWHM, ... for reference sun FOV	3 floats>0
27	FOV shape angular grid [deg]; first, last and step	3 floats>0
28	Shape of zenith scan sky FOV	list of floats
29	Shape of azimuth scan sky FOV	list of floats
30	Shape of zenith scan sun FOV	list of floats
31	Shape of azimuth scan sun FOV	list of floats
32	Sky FOV cutoff angle	float>0, any strong light source like the sun should not have an influence on the data if it is at least this distance away from the pointing position
33	Tracker type	"Directed Perceptions", "LuftBlickTR1"
34	Tracker resolution [degrees per step]	float>0
35	Tracker motion limits [deg]	4 floats with min-max zenith angle and min-max azimuth motion range
36	Shadowband resolution [degrees per step]	float>0
37	Shadowband offset-to-radius ratio	0<float<0.9
38	Positioning system type	"", "Novatel", "GlobalSat"
39	Positioning system connection type	"RS232"
40	Positioning system baud rate	integer>0
41	Positioning system port number	integer between 0 and 256; 0 means the port is not known and BlickO scans through all ports
42	Positioning system reference angles [deg]	9 floats
43	Temperature controller connection type	"RS232"
44	Temperature controller connection baudrate	integer>0
45	Temperature controller ID	ID-string
46	Temperature controller type	"SciGlobTC1", "TETech1", "TETech2"
47	Temperature controller port number	integer between 0 and 256; 0 means the port is not known and BlickO scans through all ports
48	Temperature controller set temperature [degC]	-10≤float≤35
50	Temperature controller proportional bandwidth [degC]	0.5≤float≤100
51	Temperature controller integral gain	0≤float≤10
52	Auxiliary sensor indices	space separated indices as in table 14

53	Camera read module	"DirectX", "OpenCV"
54	Camera ID	ID-string
55	Camera resolution [pixels]	two integers>0
56	Camera gain (sun and moon)	two floats
57	Camera exposure time (sun and moon)	two floats
58	Camera tracking update interval [ms]	float>0
59	Camera effective center [pixels]	two floats>0
60	Camera effective solar radius [pixels]	float>0
61	Camera pixels per degree	float>0
62	Camera rms tolerances (sun and moon)	two floats>0
63	Camera optical FOV full angle [deg]	float
64	Camera rotation angle [deg]	float
65	Camera angular tolerance [deg]	float>0
66	Camera frame rate [1/s]	float>0

Table 14: Auxiliary sensor indices

Index	**Name**	**Placement**
11 or 111	Temperature at detector of spec. 1	Directly at the detector
211	Temperature at detector of spec. 2	Directly at the detector
12 or 112	Temperature at electronics board of spec. 1	On the electronics board
212	Temperature at electronics board of spec. 2	On the electronics board
13 or 113	Spectrometer 1 control temperature	At the cooling element of the 1st temperature controller
213	Spectrometer 2 control temperature	At the cooling element of the 2nd temperature controller
14 or 114	Auxiliary spectrometer 1 temperature	Usually on the spectrometer 1 bench
214	Auxiliary spectrometer 2 temperature	Usually on the spectrometer 1 bench
18	Azimuth motor temperature	Inside the azimuth motor
19	Azimuth driver temperature	Attached to the azimuth motor driver
20	Zenith motor temperature	Inside the zenith motor
21	Zenith driver temperature	Attached to the zenith motor driver
53	Humidity in head sensor	On the electronics board in the head sensor
71	Pressure in head sensor	On the electronics board in the head sensor

5.4 BlickO General Configuration Files

The BlickO General Configuration File is in directory `/config` and is called `BlickO_config.txt`. It is an ASCII-text file with four lines described in table 15. While parameters 1, 2, 4 and 6 should in

general not be changed by the user, parameters 3 'Do autostart' and 5 'File push time [min]' have to be set by the user. Only if the user does not want to use the autostart feature at all, 'Do autostart' should be set to 0 (see section 3.2.3). The exact meaning of parameter 'File push time [min]' is explained in section 5.7.

Table 15: Entries of BlickO General Configuration File

#	**Parameter**	**Description**
1	Last operation file name	The name of the operation file used in the last execution of BlickO (see section 5.3)
2	Last status file name	The name of the status file used in the last execution of BlickO (see section 5.8)
3	Do autostart	0=don't use autostart, 1=use autostart if applicable
4	Latest schedule file name	The name of the schedule file used in the last execution of BlickO (see section 4.2)
5	Partial file update time [min]	-1=no partial files are made by BlickO, >0 is partial file creation interval in minutes
6	Last operation file checksum	The checksum of the operation file used in the last execution of BlickO

5.5 BlickO Instrument Configuration File

The BlickO Instrument Configuration File is in directory `/config` and is called `PandoraX_config.txt`, where X is the instrument number. It is an ASCII-text file listing some parameters of the current or previous use of BlickO. At the end of each BlickO-session, the BlickO Instrument Configuration File is updated. The parameters of the BlickO Instrument Configuration File are described in table 16. All parameters can be edited by the user or in some cases by a C*-routine during BlickO execution. This is indicated in the last column of the table. A C*-routine is a "Change system settings routine" (see section 4.1).

Table 16: Entries of BlickO Instrument Configuration File

Parameter	Description	C*
Selected location (short name)	The short name of the selected location from the locations file (see section 5.2)	CL
Instrument usage mode	0=simulation mode, 1=real mode with the instrument not in use, 2=real mode with the instrument in use (for more details see section 3.1)	
Last window coordinates [pixels]	Four integer numbers with the screen coordinates of the BlickO-window. These numbers change whenever the BlickO-window is resized.	
Beep mode	0=do not beep at error, 1= beep once at error, 2= beep continuously at error	CB
Data output mode	Currently not used	
X-axis parameter	0=pixels, 1=wavelength	CX
Show author information	0=do not show author information, 1=show author information (this is only 1 for the very first use of BlickO)	
Custom cursor	If this entry is given, it must be the name of a cursor (i.e. a file with extension "cur") in directory `/lib/oslib/`. In that case the given cursor is used by BlickO instead of the standard cursors, which are a white arrow and an hourglass. The given cursor `rd_cur.cur` is often useful, when the computer screen has to be watched in the field.	
Camera data mode	0=do not save camera data, 1=save camera images and data, 2=save camera data only, 3=save camera images only	
Freeze alignment history	0=alignment history is not frozen, 1=alignment history is frozen	CA
Figure draw mode	0=one figure panel is drawn; 1=one figure panel for each spectrometer, panels arranged horizontally, separate axis for each panel; 2=one figure panel for each spectrometer, panels arranged vertically, separate axis for each panel; 3=one figure panel for each spectrometer, panels arranged in rectangle, separate axis for each panel 4=one figure panel for each spectrometer, panels arranged horizontally, same axis for all panels; 5=one figure panel for each spectrometer, panels arranged vertically, same axis for all panels; 6=one figure panel for each spectrometer, panels arranged in rectangle, same axis for all panels	CX

Parameter	Description	C*
Show grid lines	0=default figure has no grid lines, 1=default figure has grid lines	CX
Make logarithmic figures	0=y-data are in linear representation, 1=y-data are in logarithmic representation	CX
IP authenticating server	Name of server to be used for IP address authentication, if empty then PGN-server is used	
Tracker parking zenith angle and azimuth	Two integer numbers with parking zenith angle and azimuth respectively	CN
Tracker warming interval [min]	Time interval in minutes to move the tracker to the zenith and back to the parking position, while it is parked. This is important to avoid freezing of the instrument or cables during long parking periods.	
Maximum pointing adjustment [deg]	This number sets a compromise between 'exact tracking' and 'limited tracker movement'. It only manifests for pointing near the zenith, where sometimes the best tracking solution requires a long azimuth movement of the tracker. If this number is e.g. set to 20°, then if the best pointing position needs an azimuth motion above 20°, another option with less azimuth motion is picked, although the pointing is not that exact (see also section 6.1). If always the best pointing should be picked, this number can simply be set to a large value (e.g. 500°)	
Positioning system tracking update interval [ms]	This number defines the repetition rate of the tracking using the positioning system	CE
Positioning system logging interval [s]	This number defines the interval, in which the positioning system is asked for a new position	CE
Standard azimuth for elevation scans [deg]	This is the azimuth direction used, when keyword AZI in command "SET POINTING" is set to "STANDARD" (see section 4.1.8). Its default value is 0° (North).	
Maximum unobstructed pointing zenith angle at standard azimuth [deg]	This number is connected to the previous one giving the largest pointing zenith angle with unobstructed view at the standard azimuth. Its value is used when the global variable `self.dzen` (see section 4.1.8) is set to "MAX" or "MAX-1" etc, as done in the elevation scan routines, like EO, EU etc. Its default value is 89°.	
Required motion limit clearance for tracker reset [deg]	The tracker is moved at least this amount away from the tracker motion limits before a tracker reset is done; the default value is 20deg	
Maximum allowed azimuth correction [deg]	The software will not allow an azimuth correction above this number; the default value is 70deg	
Maximum allowed zenith angle correction [deg]	The software will not allow an azimuth correction above this number; the default value is 3deg	
Current session connected hardware parts	List of strings that indicates, which hardware parts of the instrument are connected in the current BlickO session. This shall not be edited by the user as it is automatically modified by BlickO in order to apply a correct autostart when needed.	

5.6 BlickF Configuration File

The BlickF Configuration File is in directory `/config` and is called `BlickF_config.txt`. It is an ASCII-text file setting the parameters needed for the file handling.

Each line of the BlickF Configuration File gives a configuration parameter and its setting, separated by the string "->" (table 17). Note that the local directory DIR_LOCAL is relative to the directory of the program execution, which is `/bin/` in the case the program is run as an executable and `/src/` in the case the program is run by clicking on the Python sourcecode file. Therefore use `./`, `../` etc. to address directories at the same or higher level, e.g. `../data/L0/` to use the raw data directory. The remote directories are relative to the remote directory after the login to the remote server. The files LOG_FILE and FILES_COPIED are assumed to be in directory `/log/fslog/`. All entries are strings unless the description says otherwise.

All parameters starting with 'AUX' are optional (i.e. if they do not exist, BlickF will still work).

Table 17: Entries of BlickF Configuration File

Name	Description	Default value
PUSH_METHOD	File push method; -1=no pushing, 0=Python sftp for all operating systems, 1=Python sftp for Windows, otherwise scp, 2=putty for Windows, otherwise Python sftp, 3=putty for Windows, otherwise scp	3
SERVER_REMOTE	Fully qualified host and domain name	lb3.pandonia.net
PORT_REMOTE	Remote port for file push connection; leave this blank for default value	
USER_REMOTE	Remote user name; if left empty a default user will be used	
PASSWD_REMOTE	Remote password for user USER_REMOTE; if left empty a default password will be used	
DIR_REMOTE	Remote directory, where the data will be uploaded, if left empty no data upload will be done	./incoming/

Name	Description	Default value
AUX_PUSH_METHOD	Like PUSH_METHOD, but for auxiliary server	
AUX_SERVER_REMOTE	Like SERVER_METHOD, but for auxiliary server	lb1.pandonia.net
AUX_PORT_REMOTE	Like PORT_METHOD, but for auxiliary server	
AUX_USER_REMOTE	Remote user name for the auxiliary file push	
AUX_PASSWD_REMOTE	Remote password for user AUX_USER_REMOTE	
AUX_DIR_REMOTE	Like DIR_REMOTE, but for auxiliary server	
DIR_LOCAL	Local directory, from which data will be copied to remote location	../data/L0/
PUSH_TIMES	Time interval during which file push is allowed, leave empty for no restrictions. Format e.g. "07:00-08:00, 10:00-10:10", times in UTC	
LOG_FILE	BlickF actions log file name; lists actions done and errors occurred	BlickF_log.txt
FILES_COPIED	Lists all files already copied; if empty or removed BlickF will sync all available files	BlickF_alreadycopied.txt
MAX_FILES_COPY	Number of files which should be copied in one session; if left empty, all files will be copied, integer>0	10
ZIP	Zip files before copy (0=no, 1=yes); if set to 0 all new files will be transmitted the way they are; if set to 1 all new files will be zipped before transmitting them (unless they are already zip-files)	0
MESSAGE_FILE	BlickO messenger file name	./log/Blick_message.txt
POLLING_RATE	BlickF monitoring rate in seconds, float>0	10
DO_RESTART	Allow instrument host computer restart (0=no, 1=yes)	0
EMAIL_ADDRESS	Email address(es) of operator(s) to be informed when there are issues (comma separated, empty means no email is sent)	pgn_operators@luftblick.at

5.7 L0 File

BlickO writes the L0 data first in directory `/data/tmp` and then pushes them in directory `/data/L0`. There are 'full L0 files' and 'partial L0 files', which are described in the next sections.

5.7.1 Full L0 File

The full L0 file is a daily ASCII-text files with a header, which includes meta data (see section 5.1), a description of the data columns and the L0 data. It is called `PandoraXsY_LLL_YYYYMMDD_L0.txt`. X is the instrument number, Y the spectrometer number, LLL the Short Location Name (see section 5.2) and YYYYMMDD is the UT-date for the time of the local noon. A new line is written to the file each time a spectrometer measurement is saved or a comment is added. For a spectrometer with 2048 pixels one data line in the L0 file occupies approximately 17 kB. This file is moved in the L0-directory after local midnight, when the L0 file of the new day is started. If sun, sky and moon measurements are done, this file can easily contain several thousands of data lines and therefore occupy 100 MB and more.

Table 18 lists the maximum possible data columns in the L0 file. The real number of columns varies from instrument to instrument. E.g. if an instrument does not have a filterwheel 2, then there is no column "Position of filterwheel #2". The meaning of each column is described in the header after the meta data. Temperature data can be followed by the spectrometer number, e.g. "Temperature at electronics board 2" refers to spectrometer 2 (see table 18).

Below the header, there are only two types of L0 lines. "Data lines", which have exactly the number of columns listed in the header, and "Comment lines", which have only 5 columns. The first 4 columns are as for data lines and the 5th column is a comment starting with "#". These comments can be info- or error-logs (see section 5.15), results from sun search routines, etc. An example of a L0 file header is shown in figure 8.

Table 18: Columns in L0 file

Column name	Remark
Two letter code of measurement routine (** for manual operation)	See section 4.1
UT date and time for beginning of measurement, yyyymmddThhmmssZ (ISO 8601)	
Routine count (1 for the first routine of the day, 2 for the second, etc.)	
Repetition count (1 for the first set in the routine, 2 for the second, etc.)	
Total duration of measurement set in seconds (=# if the line is a comment line)	
Latitude at the beginning of the measurement [deg], negative=South of equator, positive=North of equator, -999=no latitude retrieved	
Longitude at the beginning of the measurement [deg], negative=West of Greenwich, positive=East of Greenwich, -999=no longitude retrieved	
Altitude a.s.l. at the beginning of the measurement [m], -999=no altitude retrieved	
West-East inclination angle at the beginning of the measurement [deg], -999=angle not retrieved	
North-South inclination angle at the beginning of the measurement [deg], -999=angle not retrieved	
Rotation angle at the beginning of the measurement [deg], -999=angle not retrieved	

Column name	Remark
Integration time [ms]	
Number of cycles	
Saturation index: positive integer is the number of saturated cycles included in the data, negative integer is the number of cycles skipped due to saturation	
Position of filterwheel #1, 0=filterwheel not used, 1-9 are valid positions	
Position of filterwheel #2, 0=filterwheel not used, 1-9 are valid positions	
Pointing zenith angle in degree, absolute or relative (see next column), 999=tracker not used	
Zenith pointing mode: zenith angle is... 0=absolute, 1=relative to sun, 2=relative to moon	
Pointing azimuth in degree, increases clockwise, absolute (0=north) or relative (see next column), 999=tracker not used	
Azimuth pointing mode: like zenith angle mode but also fixed scattering angles relative to sun (3) or moon (4)	
Mean over camera offsets [deg], -9=camera not in automatic mode	
Maximum of camera offsets [deg], -9=camera not in automatic mode	
Data processing type index, -9=manual operation	See table 7
Target distance [m], -1=not pointed on target	See section 4.1.12
Temperature at detector X [°C], 999=no temperature signal	X=1, 2 or empty
Temperature at electronics board X [°C], 999=no temperature signal	X=1, 2 or empty
Spectrometer control temperature X [°C], 999=no temperature signal	X=1, 2 or empty
Auxiliary spectrometer temperature X [°C], 999=no temperature signal	X=1, 2 or empty
Temperature in head sensor [°C], 999=no temperature signal	
Azimuth motor temperature [°C], 999=no temperature signal	
Azimuth driver temperature [°C], 999=no temperature signal	
Zenith motor temperature [°C], 999=no temperature signal	
Zenith driver temperature [°C], 999=no temperature signal	
Humidity in head sensor [%], -9=no humidity signal	Relative humidity
Pressure in head sensor [hPa], -9=no pressure signal	
Scale factor for data (to obtain unscaled data and uncertainty divide then by this number)	
Uncertainty indicator: uncertainty is... 0=not given, 1=standard deviation, 2=rms to a fitted straight line	See section 6.3.3
Mean over all cycles of raw counts for each pixel	
Uncertainty of raw counts for each pixel divided by the square root of the number of cycles	See section 6.3.3

```
File name: Pandora0s1_IBK_20170117_L0.txt
File generation date: 20170117T101522Z
Data description: Level 0 file (raw signals)
Local principal investigator: Martin Tiefengraber
Instrument type: Pandora
Instrument number: 0
Spectrometer number: 1
Operation software version used: BlickO v1.2.8
Instrument operation file used: Pandora0_OF_v1d20160916.txt
Full location name: Medical University Innsbruck
Short location name: IBK
Country of location: Austria
Location latitude [deg]: 47.2643
Location longitude [deg]: 11.3852
Location altitude [m]: 616
Local noon date: 20170117
-------------------------------------------------------------------------------
Column 1: Two letter code of measurement routine (** for manual operation)
Column 2: UT date and time for beginning of measurement, yyyymmddThhmmssZ (ISO 8601)
Column 3: Routine count (1 for the first routine of the day, 2 for the second, etc.)
Column 4: Repetition count (1 for the first set in the routine, 2 for the second, etc.)
Column 5: Total duration of measurement set in seconds (=# if the line is a comment line)
Column 6: Latitude at the beginning of the measurement [deg], negative=South of equator, positi
Column 7: Longitude at the beginning of the measurement [deg], negative=West of Greenwich, posi
Column 8: Altitude a.s.l. at the beginning of the measurement [m], -999=no altitude retrieved
Column 9: West-East inclination angle at the beginning of the measurement [deg], -999=angle not
Column 10: North-South inclination angle at the beginning of the measurement [deg], -999=angle
Column 11: Rotation angle at the beginning of the measurement [deg], -999=angle not retrieved
Column 12: Integration time [ms]
Column 13: Number of cycles
Column 14: Saturation index: positive integer is the number of saturated cycles included in the
Column 15: Position of filterwheel #1, 0=filterwheel not used, 1-9 are valid positions
Column 16: Position of filterwheel #2, 0=filterwheel not used, 1-9 are valid positions
Column 17: Pointing zenith angle in degree, absolute or relative (see next column), 999=tracker
Column 18: Zenith pointing mode: zenith angle is... 0=absolute, 1=relative to sun, 2=relative t
Column 19: Pointing azimuth in degree, increases clockwise, absolute (0=north) or relative (see
Column 20: Azimuth pointing mode: like zenith angle mode but also fixed scattering angles relat
Column 21: Mean over camera offsets [deg], -9=camera not in automatic mode
Column 22: Maximum of camera offsets [deg], -9=camera not in automatic mode
Column 23: Data processing type index, -9=manual operation
Column 24: Target distance [m], -1=not pointed on target
Column 25: Temperature at detector 1 [°C], 999=no temperature signal
Column 26: Temperature at electronics board 1 [°C], 999=no temperature signal
Column 27: Spectrometer control temperature 1 [°C], 999=no temperature signal
Column 28: Auxiliary spectrometer temperature 1 [°C], 999=no temperature signal
Column 29: Temperature at electronics board 2 [°C], 999=no temperature signal
Column 30: Spectrometer control temperature 2 [°C], 999=no temperature signal
Column 31: Auxiliary spectrometer temperature 2 [°C], 999=no temperature signal
Column 32: Scale factor for data (to obtain unscaled data and uncertainty divide then by this r
Column 33: Uncertainty indicator: uncertainty is... 0=not given, 1=standard deviation, 2=rms to
Columns 34-2085: Mean over all cycles of raw counts for each pixel
Columns 2086-4137: Uncertainty of raw counts for each pixel divided by the square root of the r
-------------------------------------------------------------------------------
```

Figure 8: Header for L0 file from Pandora 0, spectrometer 1

5.7.2 Partial L0 File

If the parameter "File push time [min]" in the BlickO General Configuration File (section 5.4) is set to -1, then no partial files are created. Otherwise, i.e. if the file push time is a positive number, partial files are created and

pushed by BlickO in the L0-directory at the interval set by the file push time. The partial L0 files are called `PandoraXsY_LLL_YYYYMMDD_L0_partZ.txt`, where Z is an increasing number starting at 0 for the first partial L0 file of the day. Once pushed in the L0-directory, each partial L0 file has a "Status line" added at the end, which gives information about the current instrument status (see section 5.8). Not counting this status line, the combination of all partial L0 files equals the full L0 file (section 5.7.1). This means that only the first partial L0 file (Z=0) has a header. If the L0 data are pushed in the L0 directory every 10 min, then the partial files contains typically 20 to 50 measurements, i.e. occupies 340 to 850 kB. This means both the copy process and a possible transmission to a server can be done in a relatively short time. Partial files are only pushed if the instrument is in "schedule mode" (see section 3.1.6) and no routine is currently running. Therefore partial L0 files always have complete routines, i.e. the measurements of one routine cannot be in different partial files. Therefore the effective file push time is in general somewhat larger then the nominal file push time set in the BlickO General Configuration File. Note that when the instrument is in schedule mode, but not taking data (e.g. during night), partial files are still created and pushed. They do not include data lines, only the status line. However this is done at a maximum rate of 1 min, even if the file push time was below 1 min.

5.8 BlickO Status File / Status Line

A status line is added to each partial L0 file, once the partial file is pushed from the temporary directory in the L0 directory. Hence even if no data were measured in the time period of a partial L0 file, then the file includes at least the status line. The status line is used to give information about the current instrument status. The line is a sequence of strings in square brackets. Inside each square bracket there is a status line keyword and a corresponding value (table 19). This is an example of the beginning of a status line:

```
[STATUSLINE 20141218T102443Z] [MODE MANUAL] [LOCATION GSFC] [WARN 0] ...
```

Table 19: Entries of Status Line

Status keyword	Description
CURRFILEDATE	Current date as used in the L0 file; 8-character string "YYYYMMDD"
PARTIALNUMBER	Number of this partial file; integer≥0
CURRTIME	Current time; 16-characters string ISO8601 format "YYYYMMDDTHHMMSSZ"
OMESSAGE	Current OMessage as in table 2
MODE	Current measurement mode; "MANUAL" for manual operation, "ROUTSEQU(xxx)" if routine sequence "xxx" is running or "SCHEDULE(xxx)" if schedule "xxx" is running)
LOCATION	Current short location name (see section 5.2.1); string
SOLARPOS	Solar angles at the time when status line was sent; zenith angle and azimuth as floats separated by a semicolon
LUNARPOS	Lunar angles at the time when status line was sent; zenith angle and azimuth as floats separated by a semicolon
HOURS2SUNRISE	Hours to (since) sunrise (positive numbers during night, negative numbers during day), e.g. 8.5 means it will last 8 hours and 30 min to sunrise; float
NWARN	Number of warnings so far; integer≥0
NTRACKRESET	Number of tracker resets needed so far; integer≥0
LASTROUT	Name of last measurement routine that was started; 2-character string with routine name, or "" if no routine was started yet, or "wait" if schedule is waiting to be resumed (e.g. during night)
TIMELASTROUT	Time when last routine was started; 16-characters string ISO8601 format "YYYYMMDDTHHMMSSZ" or "NONE", if no routine was started yet
NFINDSUN	Number of sun-searches so; four semicolon-separated integers≥0 with number of long sun searches, quick sun searches, camera sun searches and moon searches respectively
NFINDSUNOK	Number of successful sun-searches so far; four semicolon-separated integers≥0 with number of successful long sun searches, quick sun searches, camera sun searches and moon searches respectively
TIMELASTFINDSUN	Time when last sun-search had started; four semicolon-separated ISO8601-strings with time of last long sun search, quick sun search, camera sun search and moon search respectively; "NONE" if no sun search has started yet
TIMELASTFINDSUNOK	Time when last successful sun-search had finished; four semicolon-separated ISO8601-strings with time of last successful long sun search, quick sun search, camera sun search and moon search respectively; "NONE" if no successful sun search yet
RMSLASTFINDSUNOK	rms from last successful long sun-search; two or four semicolon-separated floats with azimuth rms for spectrometer 1, zenith rms for spectrometer 1, azimuth rms for spectrometer 2 and zenith rms for spectrometer 2; -1 if no sun search was made yet or if the respective spectrometer was not included in the sun search
DELTALASTFINDSUNOK	offset from last successful long sun-search; two or four semicolon-separated floats with azimuth offset for spectrometer 1, zenith offset for spectrometer 1, azimuth offset for spectrometer 2 and zenith offset for spectrometer 2; all numbers in degrees; -1 if no sun search was made yet or if the respective spectrometer was not included in the sun search

Status keyword	Description
FWHMLASTFINDSUNOK	FWHM from last successful long sun-search; two or four semicolon-separated floats with azimuth FWHM for spectrometer 1, zenith FWHM for spectrometer 1, azimuth FWHM for spectrometer 2 and zenith FWHM for spectrometer 2; all numbers in degrees; -1 if no sun search was made yet or if the respective spectrometer was not included in the sun search
TIMELASTDS	Times when last direct sun and direct moon measurement was finished; two semicolon-separated ISO8601-strings; "NONE" means no direct measurement has started yet
SZALASTDS	SZA during last direct sun and direct moon measurement; two semicolon-separated floats; -1 means no direct measurement has started yet
FILTLASTDS	Filter used by spectrometer 1 during last direct sun and direct moon measurement; two semicolon-separated strings with filter position, e.g. "6-ND4,8-U340+DIFF"; an empty string means no direct measurement has started yet
ITLASTDS	Integration time [ms] used by spectrometer 1 during last direct sun and direct moon measurement; two semicolon-separated floats; -1 means no direct measurement has started yet
FIRSTTEMP	First effective temperature of the day [°C]; float, -99 means no temperature could be read yet
LASTTEMP	Last measured effective temperature [°C]; float, -99 means last temperature could not be read
TIMELASTTEMP	Time of last attempt for a temperature reading; ISO8601-string
SETTEMP	Set temperature of the temperature controller for spectrometer 1 [°C]; float
L0SIZE	Total size of full L0 file for spectrometer 1 so far [MB]; float
IPINT	Internal IP address; string with IP-address or "ERR1", if the IP-address could not be read for the first time, or "ERR" if the IP-address could not be read more than once
IPEXT	External IP address; string with IP-address or "ERR1", if the IP-address could not be read for the first time, or "ERR" if the IP-address could not be read more than once
LASTIP	Time of last attempt to read the IP address; ISO8601-string
LASTPOWER	Last retrieved power status; "ACPOWER" if the system is running on AC-power) or "BATTxx" if the system is running on battery power, where "xx" is the percentage of battery power left, or "ERR1", if the power status could not be read for the first time, or "ERR", if the power status could not be read more than once
TIMELASTPOWER	Time of last attempt to read the power status; ISO8601-string
WINERR	Result of last checking of window error log file; string with the windows error message or "", if there is no error log file (i.e. all is OK), or "ERR1", if the windows error log file could not be accessed for the first time, or "ERR", if the windows error log file could not be accessed more than once
TIMEWINERR	Time of last checking of the window error log file; ISO8601-string
PUSHTIME	File push period [min]; float, which is identical to parameter "Partial file update time [min]" of the BlickO General Configuration File (see section 5.4)

5.9 BlickP Configuration File

The BlickP configuration file is an ASCII file called `/config/BlickP.ini`. This file specifies the parameters needed for the data processing, i.e. which instrument, what time periods, what data levels, etc. It is written as a standard python INI-file (see `https://docs.python.org/2/library/configparser.html#module-ConfigParse`) and includes two sections, "paths" and "retrieval", which will be described in the following sections. A template configuration file is automatically placed in the config-directory during software installation.

5.9.1 Section [paths]

This section specifies, where the different files needed for the processing or produced during the processing are located. Below is the path-section for the configuration file, which comes with the software installation. If the user stays with the standard directory structure of the Blick Software Suite, he never needs to edit this section.

```
[paths]
l0_directory = /data/L0
l1_directory = /data/L1
l2fit_directory = /data/L2Fit
l2_directory = /data/L2
operation_directory = /data/operationfiles
calibration_directory = /data/calibrationfiles
processing_setups = /lib/pslib/Blick_ProcessingSetups.h5
```

- l0_directory is the path, where the L0 data (section 5.7) should be located.
- l1_directory, l2fit_directory and l2_directory are the paths, where the processed L1, L2Fit and L2 data (sections 5.12 and 5.14) will be stored.
- operation_directory and calibration_directory are the paths, where the instrument operation files and instrument calibration files (sections 5.3 and 5.11) should be located.
- processing_setups is the name of the processing setups file (section 5.10).

5.9.2 Section [retrieval]

The retrieval section defines which instruments are processed, what time periods, what data levels, etc. There is a total of seven settings in this section, of which not all are mandatory. The settings are explained in table 20. Examples are given in the next section 5.9.3.

Table 20: Settings of section [retrieval]

Setting	Description
instruments	This mandatory entry is a space separated list of instrument specifiers (here we assume there are N specifiers). Each instrument specifier has the form XsY/L, where XsY is the instrument number X including the spectrometer number Y and L is the short location name (section 5.2).
rcodes	Space separated list of N (!) specifiers, i.e. the same number as 'instruments'. Each specifier itself can be a semicolon separated string with rcodes (see section 5.10.4) or the word 'NA' if no rcodes should be processed for the respective instrument specifier. By default existing L1, L2Fit and L2 data are used. If the user wants to reprocess existing data, each rcode can be followed by a 'reprocessing specifier' after a colon (see table 21). Note that if this entire setting is missing, then no rcodes are processed.
fcodes	This is the same structure as rcodes, but refers to additional fcodes (see section 5.10.3) to be processed, even if they are not needed by the rcodes.
scodes	This is the same structure as rcodes, but refers to additional scodes (see section 5.10.2) to be processed, even if they are not needed by the rcodes or fcodes. Note that at least one of the settings rcodes, fcodes or scodes must be given for data processing to happen.
start_date	This mandatory entry is a space separated list of N dates in the format YYYY/MM/DD, which define the start of the processing for the respective instrument specifier. Missing L0 files to be processed issue a warning, but the processing continues anyway.
end_date	Space separated list of N dates in the format YYYY/MM/DD, which define the end of the processing for the respective instrument specifier. Instead of a date it can also be the word 'today', which means data are processed until the current day for this instrument specifier. Note that if this entire setting is missing, the end date is set to the current day for all instrument specifiers.
fixed_calfiles	Space separated list of N full filenames (including path), which give the ICFs to be used for the respective instrument specifier. If this entire setting is missing, then the ICFs are determined automatically by using that ICF, which has the newest validity date (see section 5.11) before the date the measurements were taken. If there are more ICFs with the same validity date, then the ICF with the highest version number is used.

Table 21: Valid reprocessing identifiers.

Name	Description
	If no identifier is set, BlickP uses existing L1, L2Fit and L2 data and does not recalculate those. In the case of L2 data this means it looks at the data series in the existing file and only adds the data lines, which are new.
`from_l2fit`	If this identifier is set, BlickP uses existing L1 and L2Fit data and does not recalculate them. It does however completely rewrite the L2 file. This identifier can be used for rcodes only.
`from_l1`	If this identifier is set, BlickP uses existing L1 data and does not recalculate them. It does however completely rewrite the L2Fit and L2 files. This identifier can be used for rcodes and fcodes.
`from_l0`	If this identifier is set, BlickP does not use any existing data files and rewrites all L1, L2Fit and L2 files, even if they already exist. This identifier can be used for rcodes, fcodes and scodes.

5.9.3 Section [retrieval] examples

The example below processes data from Pandora 110s1 at IBK, from 9 May 2016 until today. It processes rcodes out0 and nvs0 keeping all existing data, i.e. does not rewrite any existing file.

```
[retrieval]
instruments = 110s1/IBK
rcodes      = out0;nvs0
start_date = 2016/05/09
```

The second example below processes data for three instruments, for 110s1 at IBK from 9 May 2016 until 9 June 2016, for 110s2 at IBK from 1 May 2016 until the current day and for 32s1 at GSFC from 15 April 2016 until the current day.

For Pandora 110s1 at IBK and Pandora 32s1 at GSFC it processes rcodes out0 and nvs0, keeping all existing data. For 110s1 at IBK it also processes scode mca0, keeping all existing data. For 110s2 at IBK it processes rcode nvs0, keeps all existing L1 data, but reprocesses and rewrites L2Fit and L2 data.

Note that in this example the entire line 'fcodes ...' could be omitted without changing the processing.

```
[retrieval]
instruments = 110s1/IBK    110s2/IBK     32s1/GSFC
rcodes      = out0;nvs0   nvs0:from_l1   out0;nvs0
fcodes      =    NA           NA           NA
scodes      =   mca0          NA           NA
start_date  = 2016/05/09   2016/05/01   2016/04/15
end_date    = 2016/06/09      today        today
```

5.10 Processing Setups File

The processing setups file is a HDF file called `/lib/pslib/Blick_ProcessingSetups.h5`. It can be downloaded under `https://www.pandonia-global-network.org/home/documents/software/`. The file includes seven tables called "Trace Gases", "s-codes", "qs-codes", "f-codes", "qf-codes", "r-codes" and "qr-codes". The tables "q*-codes" include data quality (DQ) parameters corresponding to the "*-codes". Each code consists of 4 characters, e.g. '1234'. The idea is to add codes over time (i.e. lines to the tables), but never remove any, so that a specific code has always the same parameters associated with it. Since the s-codes, f-codes and r-codes also appear in the filenames, characters like '_', '/', '.', '\' etc. are not allowed. For simplicity we recommend staying with only letters (small or capital, which is not distinguished by the software!) and numbers for all the codes. There is a certain (not mandatory) syntax we are using for the codes, which is described in the respective sections.

5.10.1 Table "Trace Gases"

Table "Trace Gases" lists the short name, chemical symbol, full name, standard column amount and information about a typical profile of each trace gas included in the Blick Software Suite. The "standard amount" is just a rough estimation of the order of magnitude for each gas abundance in the atmosphere and is used to calculate typical optical depths (OD, see section 6.5.3). For all gases the SI unit for column density is used, which is mole per square meter, mol/m^2. The only exception is the oxygen dimer, which is given in units of mol^2/m^5. For some gases in table 22 a non-SI unit is also given in parenthesis for historic reasons, e.g. DU for ozone, cm for water vapor or molec/cm^2 for bromine oxide.

From the profile information the effective height h_{EFFj} and effective temperature T_{EFFj} for extinction process j (or trace gas j) can be calculated. Typical values for h_{EFFj} and T_{EFFj} are also listed in table 22, but these values are not used at any place in the Blick Software Suite. If a new trace gas is added to the Blick Software Suite, then this table has to be extended in order to use it.

The effective height h_{EFFj} is given by:

$$h_{EFFj} = \frac{\int_{SURF}^{ToA} n_j(h) \cdot h \cdot dh}{\int_{SURF}^{ToA} n_j(h) \cdot dh} \tag{2}$$

The integral runs from the surface SURF to the top of the atmosphere ToA along the vertical path h. $n_j(h)$ is the particle density of the extinction process j at height h. The effective temperature is given by:

$$T_{EFFj} = \frac{\int_{SURF}^{ToA} n_j(h) \cdot T_{AIR}(h) \cdot dh}{\int_{SURF}^{ToA} n_j(h) \cdot dh} \tag{3}$$

$T_{AIR}(h)$ is the air temperature at height h.

Table 22: Table "Trace Gases" in the fitting setups file

Short name	**Symbol**	**Full name**	**Standard amount [mol/m^2]**	**h_{EFF} [km]**	**T_{EFF} [K]**
BIACET	CH3C(O)C(O)CH3	Biacetyl	9.9632e-6 (=6e14 molec/cm^2)	4.3	256.9
BrO	BrO	Bromine oxide	6.6422e-7 (=4e13 molec/cm^2)	22.4	221.0
CH4	CH_4	Methane	0.6692 (=1500 DU)	7.3	249.9
ClO	ClO	Chloride oxide	1.6605e-6 (=1e14 molec/cm^2)	22.4	221.0
CO2	CO_2	Carbon dioxide	135.87 (=380 ppm of 1 std atmosphere)	7.3	249.9
GLY	CHOCHO	Glyoxal	9.9632e-6 (=6e14 molec/cm^2)	4.3	256.9
HCHO	HCHO	Formaldehyde	2.2307e-4 (=0.5 DU)	4.3	256.9
HONO	HONO	Nitrous acid	4.4615e-5 (=0.1 DU)	4.3	256.9
H2O	H_2O	Water vapor	555.08 (=1 cm precipitable water)	1.8	273.1
ICE	H_2O	Ice	555.08 (=1 cm)	8.0	245.0
IO	IO	Iodine monoxide	3.3211e-8 (=2e12 molec/cm^2)	22.4	221.0
I2	I_2	Molecular iodine	1.6605e-5 (=1e15 molec/cm^2)	3.4	262.9
MGLY	CH3COCOH	Methylglyoxal	9.9632e-6 (=6e14 molec/cm^2)	4.3	256.9
NO2	NO_2	Nitrogen dioxide	2.2307e-4 (=0.5 DU)	7.2	254.5
NO3	NO_3	Nitrate	3.3211e-6 (=2e14 molec/cm^2)	3.4	262.9
OBrO	OBrO	Bromine dioxide	1.6605e-7 (=1e13 molec/cm^2)	22.4	221.0
OClO	OClO	Chloride dioxide	1.6605e-7 (=1e13 molec/cm^2)	22.4	221.0
OH	OH	Hydroxyl radical	8.3027e-7 (=5e13 molec/cm^2)	22.4	221.0
OIO	OIO	Iodine dioxide	1.6605e-6 (=1e14 molec/cm^2)	3.4	262.9
O2	O_2	Oxygen	7.4895e4 (=20.95 % of 1 std atmosphere)	7.3	249.9
O2O2	O_2O_2	Oxygen dimer	3.4995e5 mol^2/m^5 (amount in 1 std atmosphere)	4.2	262.0
O3	O_3	Ozone	0.13384 (=300 DU)	20.4	225.0
PYRAC	CH3C(O)C(O)OH	Pyruvic Acid	1.7846e-05 (=0.04 DU)	4.3	256.9
SO2	SO_2	Sulfur dioxide	2.2307e-4 (=0.5 DU)	4.0	259.2
WAT	H_2O	Liquid water	555.08 (=1 cm)	3.0	283.0

5.10.2 Tables "s-codes" and "qs-codes"

Each line of table "s-codes" is a so-called "L1 configuration", which is used by the Blick Software Suite to produce L1 data (see sections 3.3 and 6.4). Each L1 configuration consists of a series of parameters, which make up one row of the L1 configuration table (see table 23). The first parameter of a L1 configuration is a unique 4-characters-string (the s-code), which is part of all L1 file names (see section 5.12). If any L1 configuration parameters changes, a new line is added to the table and a new s-code is given.

For the standard s-codes we use this syntax:

- First digit: this refers to the dark correction method. Letter 'i' stands for the immediate dark method with blind pixels subtracted, letter 'j' for the immediate dark method without blind pixels subtracted, letter 'm' for the dark map method with blind pixels subtracted and letter 'n' for the dark map method without blind pixels subtracted (see sections 6.2 and 6.4.2).
- Second digit: this refers to the stray light correction method. 'n' means no stray light correction, 's' simple stray light correction, 'm' the (uncorrected) matrix method and 'c' the corrected matrix method (see section 6.4.8).
- Third digit: this refers to application of the sensitivity correction. Letter 'r' means no sensitivity is applied, i.e. the L1 data units are counts per second. Letter 'a' means that the sensitivity is applied, i.e. the L1 data are (ir)radiances in the case the instrument has been absolutely calibrated (see section 6.4.9).
- Forth digit: This has no special meaning and often just has a number between 0 and 9.

Entry "qs-code" indicates, which set of parameters is used to determine the data quality flag (DQF) for the L1 data. The meaning of the DQF is described in section 6.3.2. The qs-codes are listed in table 24. The first entry of a quality setup is a unique 4-characters-string (the qs-code). If any quality entry changes, a new quality setup line is added and a new qs-code is given.

Except for the first two and last two entries of the qs-code, all entries are so-called "Level 1 data quality limits" for a specific quality indicator (e.g. the retrieved wavelength shift). If the value of the indicator exceeds the limit, the data quality is reduced. All quality limits are given as comma separated strings, with each string being either 'YES', 'NO' or a number. The first string is the limit to change from data quality 0 (DQ0) to data quality 1 (DQ1) and the second string to change from DQ1 to data quality 2 (DQ2). The syntax for the standard qs-codes is simply the combination of 'st' plus a number between 00 and 99.

Table 23: Columns of table "s-codes" in the Processing Setups File. In column format "S*" stands for a string with * characters. The last column shows in parenthesis as an example the value of this parameter for s-code 'mca0'.

Column name	**Format**	**Description** *[Value for s-code mca0]*
s-code	S4	s-code *[mca0]*
s-name	S100	s-code descriptive name *[All corrections applied]*
Subtract blind	S3	Are blind pixels subtracted from bright and dark counts? YES/NO *[YES]*
Dark method	S8	Dark correction method, 'NO'=no dark correction applied, 'MEAS'=measured dark count is subtracted, 'MAP'=a dark estimation based on the measurements and the dark map is subtracted, 'MAPSIGMA'=like method 'MAP', but for pixels, where measured and mapped dark count differ more than 10 sigmas, the measured one is used *[MAPSIGMA]*
Non-lin corr	S3	Non-linearity correction applied? YES/NO *[YES]*
Latency corr	S3	Latency correction applied? YES/NO *[YES]*
Flat-field corr	S3	Flat field correction? YES/NO *[YES]*
Make count rates	S3	Conversion to count rates? YES/NO *[YES]*
Temp corr	S3	Temperature correction applied? YES/NO *[YES]*
Stray corr method	S6	Stray light correction method (see section 6.4.8), 'NO'=no stray light correction, 'SIMPLE'=simple method, 'MM'=Uncorrected matrix method, 'CORRMM'=Corrected matrix method *[CORRMM]*
Sensitivity corr	S3	Instrument sensitivity included? YES/NO *[YES]*
Wavelength corr	S3	Wavelength correction? YES/NO *[YES]*
qs-code	S4	qs-code used to determine the level 1 data quality (see table 24) *[st00]*
Creation date	S11	Date when this s-code was added *[20-Jan-2017]*
Author info	S50	Information about author of s-code *[Alexander Cede]*

Table 24: Columns of table "qs-codes" in the processing setups file. The last column shows in parenthesis as an example the value of this parameter for qs-code 'st00'.

Column name	**Format**	**Description** *[Value for quality setup st00]*
qs-code	S4	qs-code *[st00]*
qs-name	S100	qs-code descriptive name *[Standard L1 correction quality limits]*
Saturation allowed	S11	Are saturated pixels allowed and do all cycles have to be measured? YES/NO/ALLCY; YES means saturation is allowed and the quality is not reduced, even if it happened; NO means saturation is not allowed, but not necessarily all cycles have to be measured; ALLCY means all requested cycles have to be measured; i.e. YES means L0-column "Saturation index" can have any value, NO means it must be $\leq$0 and ALLCY means it must equal 0 *[ALLCY,ALLCY]*
dc cycles needed	S21	Number of measured dark cycles needed; e.g. 2 means the quality is reduced if less than 2 dark cycles were measured *[1,1]*
Eff temp diff limits	S21	Effective temperature difference limits in °; e.g. 5 means the quality is reduced if the effective temperature differs more than 5° from the reference temperature *[5,10]*
nsig dc difference	S21	Limits for number of sigmas in dark count difference; e.g. 5 means the quality is reduced if the dark count minus 5 sigmas is larger than the bright count plus 5 sigmas for at least one pixel *[5,100]*
Dark BG fitting needed	S7	Is successful dark background fitting needed? YES/NO; YES means the quality is reduced if the dark background fitting was not successful; this is only 'active' if the dark correction method 'MAP' was requested AND if the ICF contains the dark map parameters *[YES,NO]*
Dark map difference limits	S21	Limits for percentage of pixels, which differ from the dark map by more than 10 sigmas; this is only 'active' if the ICF contains the dark map parameters *[2,10]*
Stray light level limits	S21	Limits for estimated average residual stray light level in percent; e.g. 2 means the quality is reduced if the estimated residuals stray light level is above 2 %; this is only 'active' if the matrix stray light correction method was done *[2,10]*
WLchange retrieval needed	S7	Is successful wavelength change retrieval needed? YES/NO; YES means the quality is reduced if the wavelength change retrieval was not successful *[YES,NO]*
WLshift limits	S21	Wavelength shift limits in nm; e.g. 0.5 means the quality is reduced if the retrieved wavelength shift differs more than 0.5 nm from the nominal wavelength *[0.5,1.0]*
Pred WLshift limits	S21	Limits for wavelength shift difference from predicted shift in nm; e.g. 0.7 means the quality is reduced if the retrieved wavelength shift differs more than 0.5 nm from the expected shift based on the temperature *[0.7,1.2]*
Creation date	S11	Date when this qs-code was added *[20-Jan-2017]*
Author info	S50	Information about author of qs-code *[Alexander Cede]*

5.10.3 Tables "f-codes" and "qf-codes"

Each line of table "f-codes" is a so-called "fitting setup", that is used by the Blick Software Suite to produce L2Fit data (see sections 5.13 and 6.5). Each fitting setup consists of a series of parameters, which make up one row of the f-codes table (see table 25). The first parameter of a fitting setup is a unique 4-characters-string (the "f-code"), which is part of all L2Fit file names. If any fitting parameter changes, a new fitting setup line is added and a new f-code is given.

For the standard f-codes we use this syntax:

- First digit: this is the first letter of the name of the primary gas in the fitting.
- Second digit: this letter refers to the approximate wavelength region of the fitting windows and can be 'u' for ultraviolet, 'v' for visible and 'n' for near infrared.
- Third digit: this letter refers to the reference used in the spectral fitting (see table 26). 't' stands for the theoretical extraterrestrial reference ("ExtRef" in table 26), 's' for the synthetic reference ("SyntRef"), 'n' or 'f' for the spectrum of the same routine at the nearest or farest target distance ("MeasNear", "MeasFar"), 'l' or 'h' for the spectrum of the same routine at the lowest or highest pointing zenith angle ("MeasLow", "MeasHigh") and 'e' for an external reference spectrum (e.g. from another routine, "Ref_XXX").
- Forth digit: this has no special meaning and often just has a number between 0 and 9.

Some of the f-code parameters can also be taken from another f-code, a so-called "heritage f-code". In general this means that spectral fitting with the heritage f-code is done first and the output of that is used. Heritage f-codes are indicated in table 25 as *f-code. In particular this means:

- npol, noffs, nwlc: if any of these parameters is set to a heritage f-code instead of an integer, then the respective polynomial is obtained from the heritage f-code first, then subtracted from the (logarithm of) the measurements and the spectral fitting is done without this polynomial. E.g. npol=3 means a 3rd order smoothing polynomial is included in the fitting, while npol='nvs0' means f-code nvs0 is done first, the smoothing polynomial obtained from nvs0 is used and the final spectral fitting is done setting npol=-1, i.e. no smoothing polynomial is included anymore. Note that npol, noffs, and nwlc can also be set to -9, in which case the values from the respective ICF-entry "Wavelength change retrieval parameters for FUNCFILT" is taken.
- Ring: if this is set to a heritage f-code, then the Ring spectrum obtained from the heritage f-code is subtracted from the (logarithm of) the measurements and the final spectral fitting is done setting Ring='NO'.
- Fitted gases: here there is the possibility that any gas is followed by a heritage f-code in round parenthesis. If this is the case, then the slant column of this trace gas is calculated from the heritage f-code, the optical depth is subtracted from the (logarithm of) the measurements and the final spectral fitting is done without fitting the respective trace gas. This also means that all other parameters related to this trace gas (Gas sources, Gas OD meths, Gas temps and Fitted temps) are not used anymore. E.g. if parameter Fitted gases is set to 'O3,NO2(nvs0)', then first the NO2 amount is obtained from f-code nvs0, then the NO2 optical depth is subtracted from the (logarithm of) the measurements and the final spectral fitting is done setting Fitted gases to 'O3'.

If the respective parameter in the heritage f-code is itself referring to another f-code, then obviously this "further" f-code is used. Note that the "final" heritage f-codes are not allowed to use f-codes for other parameters themselves, otherwise the processing will return an error.

Entry "qf-code" indicates which set of parameters is used to determine the DQ for the L2Fit data (table 28). The principle is the same as for the qs-codes. The syntax for the standard qf-codes is usually the same as for the f-code, for which it is primarily used.

Table 25: Columns of table "f-codes" in the processing setups file. The last column shows in parenthesis as an example the value of this parameter for f-code 'nvs2'.

Column name	**Format**	**Description** *[Value for fitting setup out0]*
f-code	S4	f-code *[nvs2]*
f-name	S300	f-code descriptive name *[Direct sun tropospheric NO2 code]*
Process types	S50	Comma separated string of process types, for which retrieval is applied (see table 7); it can also be "ALL", in which case the retrieval is applied to any process type *[SUN]*
Filter types	S50	Comma separated string of functional filters, for which retrieval is applied; it can also be "ALL", in which case the retrieval is applied to any filter type *[OPEN]*
Reference	S100	Reference spectrum used; for options see table 26 *[SyntOPEN]*
WL-starts	S50	Comma separated string with starting wavelengths of the fitting window [nm]. Positive numbers are absolute wavelengths. Negative numbers are differences to the minimum wavelength, for which the sensitivity is characterized. To get the absolute wavelength, this number needs to be subtracted from the minimum wavelength. E.g. if the sensitivity is characterized from 298 to 385 nm, then WL-starts=-10 means the fitting windows starts at 298 nm - (-10 nm) = 308 nm. When converted in absolute wavelengths, they must be monotonically increasing. *[462.2]*
WL-ends	S50	Comma separated string with ending wavelengths of the fitting window [nm]. Positive numbers are absolute wavelengths. Negative numbers are differences to the maximum wavelength, for which the sensitivity is characterized. To get the absolute wavelength, this number needs to be added to the maximum wavelength. E.g. if the sensitivity is characterized from 298 to 385 nm, then WL-ends=-5 means the fitting windows ends at 385 nm + (-5 nm) = 380 nm. When converted in absolute wavelengths, the ending wavelengths must be monotonically increasing, have the same length as the starting wavelengths, and each element must be larger than the corresponding element of the starting wavelengths. The final fitting window is then composed of all the partial fitting windows determined by the wavelength starts and ends. *[490.1]*

Column name	**Format**	**Description** *[Value for fitting setup 1]*
npol	S4	Order of fitting polynomial or -1 for no polynomial or -9 for respective value from ICF-entry "Wavelength change retrieval parameters for FUNCFILT" or *f-code (see section 6.5) *[4]*
noffs	S4	Order of offset polynomial or -1 for no polynomial or -9 for respective value from ICF-entry "Wavelength change retrieval parameters for FUNCFILT" or *f-code (see section 6.5) *[0]*
nwlc	S4	Order of wavelength change polynomial or -1 for no polynomial or -9 for respective value from ICF-entry "Wavelength change retrieval parameters for FUNCFILT" or *f-code (see section 6.5) *[0]*
nresc	S4	Order of resolution change polynomial (see section 6.5) *[-1]*
Fitted gases	S100	Comma separated string with short names of gases to be fitted (see table 27) *[O3,NO2,O2O2,H2O,OIO]*
Gas sources	S500	Comma separated string with cross section source for each gas in column "Fitted Gases" (see table 27). Since only one source per gas is listed in a given ICF, the processing can only be done, if the selected ICF matches the gas sources listed in this entry. *[HarmonicsShift3pm_H2012,Vandaele,ThalmanNewnhamQPol,H2012,Spietz]*
Gas OD meths	S50	Comma separated string with optical depth fitting method used (between 0 and 3) for each gas in column "Fitted Gases" (see section 6.5.3). The processing will only be done, if the selected fitting method is is given in the corresponding ICF. *[3,1,1,3,1]*
Gas temps	S50	Comma separated string with effective temperatures for each gas in column "Fitted Gases", which should be used in the fitting. This is either the string "FIT", or a value in Kelvin, or a string representing a profile type from a climatology. "FIT" means the gas temperature is fitted, while all other settings mean it is fixed to a certain value. The options for the climatologies are described in section 6.8.2. The string can be followed by an uncertainty estimation in round parenthesis. Again this estimation can be a value in Kelvin or a string representing a profile type. E.g. "225.0(O3)" would mean the effective temperature is 225K and its uncertainty is taken from the ozone climatology. If the uncertainty estimation is not given and a string representing a profile type is set for the effective temperature, then the uncertainty estimation is taken from the same climatology too, i.e. "O3" has the same effect as "O3(O3)". If the uncertainty estimation is not given and a value in Kelvin is set for the effective temperature, then 50 K is taken as an uncertainty estimation, i.e. "225.0" has the same effect as "225.0(50.0)". If the cross sections of a specific gas are only given for one temperature in the ICF, this entry has no effect for this gas. *[O3,BL,O2O2,BL,BL]*
Ring	S4	Is the Ring spectrum fitted (see section 6.5)? YES/NO/AUTO/*f-code. AUTO means the Ring is fitted for sky observations only. *[NO]*
Mol scatt	S4	Optical depth fitting method used for molecular scattering optical depth to be subtracted before the spectral fitting (see section 6.5)? NO means molecular scattering is not subtracted, 0, 1, 2 or 3 are the fitting methods *[1]*
Linear fit	S3	Is linear fitting forced (see section 6.5)? YES/NO *[NO]*

Column name	**Format**	**Description** *[Value for fitting setup 1]*
Uncertainty	S5	Which uncertainty is used for the spectral fitting (see section 6.5)? NO means no uncertainty is included. INSTR means the independent instrumental uncertainty is used. MEAS means the measured standard error is used as if it was an independent uncertainty. *[INSTR]*
s-code	S4	s-code for the L1 data that are used in the spectral fitting *[mca1]*
Diffuse correction	S14	How are measurements on sun or moon corrected for the diffuser radiance entering the instrument's FOV? NO=no diffuse correction is applied and spectral fitting is done on all measurements. CALC=the diffuse fraction is calculated and subtracted from the data and spectral fitting is done on all measurements (this option is not implemented yet in the current version). OFFMEAS and OFFMEAS_WLCORR are for routines, where measurements slightly off the target (sun or moon) were made in addition to the measurements on target. OFFMEAS=subtract the 'off-target' data from the 'on-target' data without wavelength correction. Spectral fitting is only done on the corrected on-target measurement. OFFMEAS_WLCORR=the off-target spectra are wavelength corrected towards the on-target spectrum before the subtraction and spectral fitting is only done on the corrected on-target measurement. If there are more than one off-target measurement, the data will be interpolated in time to the on-target measurement before subtraction *[OFFMEAS_WLCORR]*
Time interpolation	S10	This is for routines, where spectra are measured symmetrically around a central measurement, to which the others are interpolated. NO=no time interpolation is done and spectral fitting is done on all measurements. YES=spectra with the same pointing angles are interpolated in time towards the central measurement without wavelength correction. YES_WLCORR=spectra with the same pointing angles are wavelength corrected and interpolated in time towards the central measurement. Unless NO is selected, the number of measurements in the routine must be odd, with exactly two measurements for each set of pointing angles, one before and one after the central measurement. *[NO]*
Pixels to use	S6	Are all regular pixels used in the fitting or are hot/warm pixels not included? ALL=all regular pixels, NOHOT=all regular pixels except for hot pixels, NOWARM=all regular pixels except for warm and hot pixels. Note that even if NOHOT or NOWARM is selected, the fitting residuals are given for all regular pixels inside the fitting window limits with pixels not used in the fitting set to -9e99. *[ALL]*
qf-code	S4	qf-code used to determine the L2Fit data quality (see table 28) *[nvs1]*
Creation date	S11	Date when this f-code was added *[10-Nov-2020]*
Author info	S50	Information about author of f-code *[Martin Tiefengraber]*

Table 26: Options for "Reference"

Reference	**Description**
ExtRef or ExtFUNCFILT	References starting with "Ext" refer to an extraterrestrial spectrum from another source (i.e. not measured by the Pandora unit), convoluted with the Pandora filter function and sensitivity for functional filter FUNCFILT; in the case of ExtRef the functional filter is determined from the measurements, i.e. if the data were taken using the U340 filter, then ExtRef equals ExtU340; BlickP uses for this purpose a high resolution extraterrestrial spectrum from 270 nm to 1000 nm merged from different sources in a similar way as described in *Bernhard et al.* [6]; the sources are: #1: *Kurucz* [23] spectrum normalized to *Thuillier et al.* [48], #2: SUSIM/Atlas 3 spectrum [52], #3: *Gueymard* [17] spectrum; the merged spectrum is #2 for $\lambda \leq$299.8 nm; #1 corrected with smoothed #2 (triangular 0.7 nm FWHM slit) for 299.8 nm<$\lambda \leq$338.5 nm; #1 corrected with smoothed #2 (triangular 4 nm FWHM slit) for 338.5 nm<$\lambda \leq$419.9 nm; #1 corrected with smoothed #3 (triangular 20 nm FWHM slit) for 419.9 nm<$\lambda \leq$946.5 nm; and #1 for λ>946.5 nm; the SW will select that extraterrestrial reference, which corresponds to the functional filter being measured
SyntRef or SyntFUNCFILT	A synthetic spectrum, which is usually the average over several spectra measured by the Pandora unit and corrected for the estimated total OD included in it; in case of SyntRef, just as for ExtRef, the SW will select that synthetic reference, which corresponds to the functional filter being measured
MeasLow or MeasHigh	A single measured spectrum of the same routine at the lowest or highest pointing zenith angle
MeasNear or MeasFar	A single measured spectrum of the same routine at the nearest or farest target distance
Ref_XXX	A reference from an external file, where XXX is the filename (e.g. "C:/refspec1.txt"). Unless the extension of this file is 'ddf', it should be an ascii file with only numbers inside and 2, 3 or 4 data columns. The first column are the wavelengths in nm, the second column the reference spectrum, the optional third column the instrumental and input uncertainty of the reference spectrum and the optional forth column the instrumental uncertainty of the reference spectrum.

Table 27: Options for "Gas Sources"; column "Gas" corresponds to column "Short Name" of table 22

Gas	Name	Description
BIACET	Horowitz	*Horowitz et al.* [19]
BrO	Wilmouth	*Wilmouth et al.* [56]
BrO	Fleischmann	*Fleischmann et al.* [15]
CH4	H2007	HITRAN 2008 *Rothman et al.* [37]
CH4	H2012	HITRAN 2012 *Rothman et al.* [38]
ClO	Sander	*Sander and Friedl* [41]
CO2	HITRAN	HITRAN 2004 *Rothman et al.* [36]
CO2	H2007	HITRAN 2008 *Rothman et al.* [37]
CO2	H2012	HITRAN 2012 *Rothman et al.* [38]
GLY	Volkhamer	*Volkamer et al.* [53]
GLY	Horowitz	*Horowitz et al.* [19]
HCHO	MellMoort2000	*Meller and Moortgat* [26]
HONO	Bongartz	*Bongartz et al.* [11]
HONO	Stutz	*Stutz et al.* [46]
H2O	HITRAN	HITRAN 2004 *Rothman et al.* [36]
H2O	H2012	HITRAN 2012 *Rothman et al.* [38]
ICE	Warren	*Warren* [55]
IO	Spietz	*Spietz et al.* [45]
I2	Saiz-Lopez	*Saiz-Lopez et al.* [39]
MGLY	Meller	*Meller et al.* [25]
NO2	Vandaele	*Vandaele et al.* [49]
NO3	Sander	*Sander* [40]
OBrO	Fleischmann	*Fle* [2]
OBrO	Knight	*Knight et al.* [22]
OClO	Wahner	*Wahner et al.* [54]
OH	H2012	HITRAN 2012 *Rothman et al.* [38]
OIO	Spietz	*Spietz* [44]
O2	H2012	HITRAN 2012 *Rothman et al.* [38]
O2O2	HermansNewnham	*Hermans et al.* [18] for $\lambda \leq$454.42 nm combined with *Newnham and Ballard* [28] for λ>454.42 nm
O2O2	ThalmanNewnhamQPol	*Thalman and Volkamer* [47] for $\lambda \leq$596 nm combined with *Newnham and Ballard* [28] for λ>596 nm

Gas	Name	Description
O3	BassPaurGOME	*Bass and Paur* [4] for $\lambda \leq$332.69 nm combined with *Burrows et al.* [14] for λ>332.69 nm
O3	Harmonics_H2012	*Serdyuchenko et al.* [43] for $\lambda \leq$1100 nm combined with HITRAN 2012 *Rothman et al.* [38] for λ>1100 nm
O3	HarmonicsShift3pm_H2012	*Serdyuchenko et al.* [43] shifted by +3 pm for $\lambda \leq$1100 nm combined with HITRAN 2012 *Rothman et al.* [38] for λ>1100 nm
O3	Daumont4TGOME	*Malicet et al.* [24] without using 273 K for $\lambda \leq$522 nm plus *Burrows et al.* [14] for λ>522 nm, both taken from `http://igaco-o3.fmi.fi/ACSO/cross_sections.html`
PYRAC	Horowitz	*Horowitz et al.* [19]
SO2	Vandaele	*Vandaele et al.* [50]
SO2	Vandaele2009	*Vandaele et al.* [51]
SO2	Bogumil	*Bogumil et al.* [10]
WAT	QBPP	Combination of *Quickenden and Irvin* [35] for λ<280 nm, *Buiteveld et al.* [13] for λ<402 nm, *Pope and Fry* [33] for λ<730 nm and *Palmer and Williams* [30] for λ>730 nm
WAT	QBPPcP	QBPP corrected with *Peters et al.* [31] between 402 nm and 507 nm

Table 28: Columns of table "qf-codes" in the processing setups file. The last column shows in parenthesis as an example the value of this parameter for qf-code 'nvs1'.

Column name	Format	Description *[Value for quality setup nvs1]*
qf-cumber	S4	qf-code *[nvs1]*
qf-Name	S100	qf-code descriptive name *[V1 direct sun NO2 setup using synthetic reference quality limits]*
Fitting result	S5	Limits for fitting result index (see table 38) *[2,10]*
WL shift limits	S21	Wavelength shift limits in nm; e.g. 0.2 means the quality is reduced if the retrieved wavelength shift differs more than 0.2 nm from the nominal wavelength; differently from the quality parameter in the qs-code, this refers to the total wavelength shift as retrieved by the spectral fitting, not as retrieved in the L0 to L1 data conversion *[0.05,0.1]*
wrms limits	S21	Limits for the normalized rms of fitting residuals weighted with independent uncertainty *[1e-3,3e-3]*
Creation date	S11	Date when this qf-code was added *[04-Nov-2019]*
Author info	S50	Information about author of qf-code *[Manuel Gebetsberger]*

5.10.4 Tables "r-codes" and "qr-codes"

Each line of table "r-codes" is a so-called "retrieval setup", that is used by the Blick Software Suite to produce L2 data (see section 5.14). Each retrieval setup consists of a series of parameters, which make up one row of the r-codes table (table 29). The first parameter of a fitting setup is a unique 4-characters-string (the "r-code"), which is part of all L2 file names other than L2Fit. If any retrieval parameter changes, a new retrieval setup line is added and a new r-code is given. The syntax for the standard qr-codes is usually the same as for the primary f-code used in the r-code.

Entry "qr-codes" indicates, which set of parameters is used to determine the DQ for the L2 data for each output gas. The principle is the same as for the qs-codes and qf-codes. The parameters are listed in table 31. The syntax for the standard qr-codes is usually the same as for the r-code which it is primarily used for.

Table 29: Columns of table "r-codes" in the processing setups file. The last column shows in parenthesis as an example the value of this parameter for r-code 'nvs2'.

Column name	**Format**	**Description** *[Value for retrieval setup nvs2]*
r-code	S4	r-code *[nvs2]*
r-Name	S100	r-code descriptive name *[V2 direct total NO2 retrieval]*
L2 type	S7	Level 2 data type : Direct or Profile *[Direct]*
Algorithm type	S50	Algorithm type used: 'Direct-Version1', 'AirRatioSky-Version1' *[Direct-Version1]*
Output gases	S50	Comma separated string of gases to be written in output file *[NO2]*
Effective heights	S50	Comma separated string with effective heights for each gas in column "Output Gases", which are used to calculate the direct AMF (see equation 129). The sub-string is either a value in km or a string representing a profile type from a climatology. The current options for the climatology are the same ones as for entry "Gas temps" of the f-codes and described in section 6.8.2. The string can be followed by an uncertainty estimation in round parenthesis. This estimation can be a value in km or a string representing a profile type. E.g. "O3(2.4)" would mean the effective height is taken from the ozone climatology and its uncertainty is 2.4 km. If the uncertainty estimation is not given and a string representing a profile type is set for the effective height, then the uncertainty estimation is taken from the same climatology too, i.e. "O3" has the same effect as "O3(O3)". If the uncertainty estimation is not given and a value in km is set for the effective height, the program uses half of the effective height as uncertainty, i.e. "7.2" has the same effect as "7.2(3.6)". Sub-strings can also be combined using "+" for the Algorithm type "Direct-Version1", e.g. "BL+STRAT". In this case different effective height-estimations are used to get the AMF (see section 6.6) *[BL+NO2s]*
Noise levels	S50	Comma separated string with "maximum desired noise levels" for each output gas in percent; this is only used for Algorithm type "Direct-Version1" (see section 6.6.5) *[100]*
Product status	S50	Comma separated string of product status for each output gas (see table 30); same length as "Output gases" *[official]*
qr-codes	S50	Comma separated string of qr-codes used for each output gas (see table 31); same length as "Output gases" *[nvs1]*
f-codes	S50	Comma separated string of f-codes used in the retrieval; note that Algorithm type "Direct-Version1" only allows to use one or two f-codes (see section 6.6), while Algorithm type "AirRatioSky-Version1" also allows to use more f-codes (see section 6.7) *[nvs2,nvs3]*
Creation date	S11	Date when this r-code was added *[20-Nov-2020]*
Author info	S50	Information about author of r-code *[Alexander Cede]*

Table 30: Options for entry "Product status" in the processing setups file. Note that the Product status applies to all data for the corresponding output gas, i.e. column amounts, effective temperatures, etc.

Status	**Description**
official	Data are currently the official product of the PGN.
disused	Data are a former official product of the PGN, but are not the official product anymore.
unvalidated	Data are not yet officially validated.
develop	Data are in research stage and only produced for testing purposes.
unusable	Data should not be used, since they are typically only for an additional output gas in the spectral fitting, for which the wavelength range is not optimized.

Table 31: Columns of table "qr-codes" in the processing setups file. The last column shows in parenthesis as an example the value of this parameter for qr-code 'out0'.

Column name	**Format**	**Description** *[Value for quality setup nvs1]*
qr-code	S4	qr-code *[nvs1]*
qr-Name	S100	qr-code descriptive name *[V1 direct sun NO2 setup quality limits]*
Error limits	S11	Retrieval error limits *[0,0]*
AMF limits	S21	AMF limits; negative value means this parameter is not used *[7,14]*
AtmVar limits	S21	Atmospheric variation limits [%] *[20,40]*
Creation date	S11	Date when this qr-code was added *[04-Nov-2019]*
Author info	S50	Information about author of qr-code *[Manuel Gebetsberger]*

5.10.5 Adding new Entries to the Processing Setups File

If the user wants to add new s-, f-, q*- or r-codes to the tables in the Processing Setups File, e.g. for test purposes, he can just do this on his own machine and process the L2 data locally. In order to add new codes to the official PGN Processing Setups File, an email has to be written to `admin@pandonia-global-network.org` with subject "New PGN Processing Setup Request". This email should include the following information:

- The full set of parameters needed for the new setup.
- Name and contact information (email and phone number) of the person or group that created the fitting setup.
- A short description of why the new processing setup should be used.

You will receive an email as soon as the request has been resolved by LuftBlick. Then you can download the updated processing setups file from `http://pandonia.net/docs/` and copy it in directory `/lib/pslib/`.

5.11 Instrument Calibration File

The ICF is in directory `/data/calibrationfiles` and is called `PandoraXsY_CF_vVdYYYYMMDD.txt`, where X is the instrument number, Y is the spectrometer number, V the version number and YYYYMMDD the calibration data validity starting date. The version is used for the case that new calibration parameters have been obtained and should be applied to data from the past. In that case one can leave the same calibration data validity starting date and increase the version number, so that the processing software uses the new calibration file, when data are reprocessed. It is an ASCII-text file containing the calibration results for a Pandora unit obtained from laboratory and field calibrations. Note that as for the IOF, there is no calibration data validity ending date in the file name. The validity simply ends with the starting date of the next ICF.

Together with the IOF, this file is needed to run BlickP (see section 3.3). Each line of the ICF gives either metadata or a calibration result and its setting, separated by the string '->'. Note that when BlickP is reading the ICF for the first time, it builds a binary version of the ICF named `PandoraXsY_CF_vVdYYYYMMDD.ddf` and saves it in the same directory. This procedure can last several minutes. In any subsequent call to BlickP, the calibration data will then be directly read from the binary file in order to speed up the data processing.

Not every calibration result listed below will necessarily be given in the ICF. A missing entry can mean that:

- This calibration result has no entries. E.g. if the instrument has no dead pixels, the calibration entry "Dead pixels" will not be present.
- This calibration result simply does not apply to the unit. E.g. if the instrument has no U340 filter, there will be no entry "Synthetic reference spectrum for U340".
- This calibration result has not been determined.

Several calibration results are coefficients of polynomials. The coefficients are always listed in descending order (i.e. the last number is the constant term). The polynomials are usually evaluated on "scaled" values for numerical reasons. The scaling method is given in equation 4.

$$xs = 3.46 \cdot \left(\frac{x - x_{MIN}}{x_{MAX} - x_{MIN}} - 0.5 \right) \tag{4}$$

x is an unscaled data-point, xs is a scaled data-point and x_{MIN} and x_{MAX} are estimates of the minimum and the maximum of the distribution of the unscaled data. So the xs are distributed approximately between -1.73 and +1.73. The values for x_{MIN} and x_{MAX} used to obtain the scaled data are listed in the detailed description of each calibration result below. E.g. the scaled pixels (equation 1) use x_{MIN}=0 and x_{MAX}=npix.

Several calibration results give the rms of measured data around a fitted line. The rms is defined in equation 5.

$$rms = \sqrt{\frac{\sum_{i=1}^{n} (x_i - x_{FITi})^2}{n - n_{FIT}}} \tag{5}$$

The x_i are the measured data (i=1 to n), the x_{FITi} are the fitted data and n_{FIT} is the number of fitting parameters used (e.g. n_{FIT}=3 for a fitted 2nd order polynomial).

Details for every line of the ICF, which is not already given in the meta data table 12, are listed below with the name of the calibration result in bold, larger letters. Sometimes more than one calibration result is

explained in one single paragraph.

Indices of dead pixels; Indices of warm pixels; Indices of hot pixels; Indices of blind pixels; Indices of oversampled pixels

Dead pixels always return the same value, most often this is zero. Blind pixels are behind covered areas of the sensor and are therefore not exposed to incoming light. Hence they measure only dark signal (no stray light either). Oversampled pixels are read more than once. They basically only measure the dark offset (no dark slope either). All pixels that are not dead, blind or oversampled are called regular pixels. Warm (hot) pixels have dark gain (increase of the dark count with integration time), which is 5 (10) standard deviations outside the distribution of all regular pixels. The pixel numbers start at 1 (not 0), so 1 is the 1st pixel, 2 the 2nd pixel, etc.

Dark variance power fit coefficients

The dark variance VD is estimated in equation 6.

$$\mathrm{VD} = \mathrm{V}_0 + \mathrm{V}_1 \cdot \mathrm{IT}^{V_2} \tag{6}$$

IT is the integration time [s] and V_0, V_1 and V_2 are coefficients, which are listed in this entry in the order V_0, V_1 and V_2.

Dark background fitting settings

This are two integers determining how the dark count background should be extracted from the measured dark count (see 6.2.4). The first number is the order of the polynomial used for the fitting. The second number is the index of the pixel, at which the 'hockey stick' extension of the dark background is reduced to approximately zero.

Dark fine structure slope, parameter A [1e-4*counts/ms]

This is the fitting parameter A of the dark fine structure slope (called $\mathrm{A}_{\mathrm{SL}i}$ in equation 72) for each regular pixel in units of 1e-4 counts/ms.

Dark fine structure slope, parameter B [1e-4/K]

This is the fitting parameter B of the dark fine structure slope (called $\mathrm{B}_{\mathrm{SL}i}$ in equation 72) for each regular pixel in units of 1e-4 per K.

Dark fine structure intercept, parameter A [1e-4*counts]

This is the fitting parameter A of the dark fine structure intercept (called $\mathrm{A}_{\mathrm{IC}i}$ in equation 72) for each regular pixel in units of 1e-4 counts.

Dark fine structure intercept, parameter B [1e-4/K]

This is the fitting parameter B of the dark fine structure intercept (called $\mathrm{B}_{\mathrm{IC}i}$ in equation 72) for each regular pixel in units of 1e-4 per K.

Dark map reference temperature [degC]

This is that value of the radiometric effective temperature, which is used in the dark fine structure map.

Linearity parameters

These are the parameters for the "linearity correction function". Dividing the measured counts by this function gives the counts, which would have been obtained if the instrument had a linear response. The first three numbers are amplitude, decay constant and power term of an exponential function. The remaining parameters

are coefficients of a polynomial. The function is evaluated at the dark corrected counts divided by the nominal saturation count 2^{nbits}-1; nbits=number of bits.

Gain [counts per electron]

The detector counts per one electron "accumulated" in the pixel (see also section 6.2).

Latency parameters

Those two numbers are the latency decay and latency gain constants (see also section 6.4.4).

Integration time correction [ms]

This is a correction in ms added to the nominal integration time to obtain the best estimation of the "true" integration time. E.g. 0.1 means that if the instrument is set to measure 4 ms, it actually integrates for 4.1 ms.

Pixel response non uniformity [ppm]

For each pixel the difference of the pixel's response relative to the "average" response of the pixels around it. E.g. a value of 11000 means the value at this pixel is 1.1% higher than the average over the surrounding pixels.

Radiometric reference temperature [degC]

This is that value of the radiometric effective temperature to which the radiometric temperature correction is referenced to.

Temperature correction polynomial

This polynomial is evaluated at the scaled pixels (equation 1). The obtained values are the instrument's radiometric temperature sensitivity in %/K. Equation 7 shows how to obtain the temperature corrected counts C_{CORR}.

$$C_{CORR} = C \cdot \frac{100}{100 + (T_{RE} - T_{RR}) \cdot k} \tag{7}$$

C are the counts before correction, T_{RE} is the radiometric effective temperature (measured and stored in the data files), T_{RR} is the radiometric reference temperature and k is the radiometric temperature sensitivity (i.e. the evaluated polynomial).

Signal shift to radiometric effective temperature [min]

This number is an estimation for the time difference between the change in the signal and the change in the radiometric effective temperature. E.g. 0.5 means the signal "reacts" to temperature changes with a delay of 30 s.

Radiometric effective temperature sensor index

This is that index from the "Auxiliary sensor indices" (see table 14), which is considered most representative for the instrument's radiometric temperature sensitivity. If this ICF-line is not given, the first index of "Auxiliary sensor indices" is used.

Slit function fitting method

The fitting method used for the slit function, more precisely the core slit function, i.e. the slit function without stray light (see also description of entry "Stray light function fitting method"). The options for the slit function fitting method are given in table 32. Note that the Blick Software Suite differentiates between the "slit function" (or slit scatter function) and the "filter function". The former is the signal as it appears when the detector is illuminated by a single wavelength, the latter is the function describing how the instrument filters incoming

light as if it was a filter instrument. The filter function is determined by flipping the slit function around the center wavelength.

Parameters A_0, the air-wavelength of the pixel-center, and A_1, the height of the slit function at the center, which is always a nominal 1, are common to each fitting method and therefore not listed in table 32. Formulas for some of the slit functions are given in equations 8 to 12, where λ is the wavelength and $S(\lambda)$ is the slit function. Typical fitting methods used are "Symmetric modified Lorentzian" and "Symmetric modified Gaussian".

Table 32: Slit function fitting methods

Name	**Parameters**
Symmetric triangle	A_2: half of base width [nm]
Asymmetric triangle	A_2: from center to left edge at base [nm] A_3: from center to right edge at base [nm]
Symmetric trapezoid	A_2: half of base width [nm] A_3: half of top width [nm]
Trapezoid asymmetric on bottom	A_2: half of base width left [nm] A_3: half of base width right [nm] A_4: half of top width [nm]
Symmetric double-trapezoid	A_2: half of base width [nm] A_3: half of top width [nm] A_4: height of flexion point A_5: half of middle width [nm]
Double-trapezoid both sides free	A_2: half of base width left [nm] A_3: half of base width right [nm] A_4: half of top width [nm] A_5: height of left flexion point A_6: height of right flexion point A_7: half of left middle width [nm] A_8: half of right middle width [nm]
Double-trapezoid left side free	A_2: half of base width left [nm] A_3: half of base width right [nm] A_4: half of top width [nm] A_5: height of left flexion point A_6: half of left middle width [nm]
Double-trapezoid right side free	A_2: half of base width left [nm] A_3: half of base width right [nm] A_4: half of top width [nm] A_5: height of right flexion point A_6: half of right middle width [nm]
Symmetric modified Lorentzian (Equation 8 with A_6=1)	A_2: half width [nm] A_3: steepness

Name	Parameters
Asymmetric modified Lorentzian (Equation 9)	A_2: half width [nm] A_3: steepness A_4: asymmetry
Symmetric modified Gaussian (Equation 10 with A_6=1)	A_2: half width [nm] A_3: steepness
Symmetric modified double Lorentzian (Equation 8)	A_2: half width of mode 1 [nm] A_3: steepness of mode 1 A_4: half width of mode 2 [nm] A_5: steepness of mode 2 A_6: fractional strength of mode 1
Symmetric modified double Gaussian (Equation 10)	A_2: half width of mode 1 [nm] A_3: steepness of mode 1 A_4: half width of mode 2 [nm] A_5: steepness of mode 2 A_6: fractional strength of mode 1
Symmetric modified Lorentz-Gauss combo (Equation 11)	A_2: half width of Lorentz mode [nm] A_3: steepness of Lorentz mode A_4: half width of Gauss mode [nm] A_5: steepness of Gauss mode A_6: fractional strength of Lorentz mode
Truncated symmetric modified Gaussian (Equation 12)	A_2: reduced half width [nm] A_3: steepness A_4: cut-off position
Symmetric trapezoid with inclined top-part	A_2: half of base width [nm] A_3: half of top width [nm] A_4: angle of top part [degrees]
Asymmetric modified Gaussian (Equation 10 with A_6=1 for $\lambda \leq A_0$ and equation 10 with A_6=0 for $\lambda > A_0$)	A_2: half width left [nm] A_3: steepness left A_4: half width right [nm] A_5: steepness right [nm]

$$S(\lambda) = A_1 \cdot \left\{ A_6 \cdot \left[1 + \left| \frac{\lambda - A_0}{A_2} \right|^{A_3} \right]^{-1} + (1 - A_6) \cdot \left[1 + \left| \frac{\lambda - A_0}{A_4} \right|^{A_5} \right]^{-1} \right\} \quad (8)$$

$$S(\lambda) = A_1 \cdot \frac{1 + A_4 \cdot \frac{\lambda - A_0}{A_2}}{1 + \left|\frac{\lambda - A_0}{A_2}\right|^{A_3}} \tag{9}$$

$$S(\lambda) = A_1 \cdot \left\{ A_6 \cdot exp\left[-\left|\frac{\lambda - A_0}{A_2}\right|^{A_3} \right] + (1 - A_6) \cdot exp\left[-\left|\frac{\lambda - A_0}{A_4}\right|^{A_5} \right] \right\} \tag{10}$$

$$S(\lambda) = A_1 \cdot \left\{ A_6 \cdot \left[1 + \left|\frac{\lambda - A_0}{A_2}\right|^{A_3} \right]^{-1} + (1 - A_6) \cdot exp\left[-\left|\frac{\lambda - A_0}{A_4}\right|^{A_5} \right] \right\} \tag{11}$$

$$S(\lambda) = A_1 + A_4 \cdot \left[exp\left(-\left|\frac{\lambda - A_0}{A_2}\right|^{A_3} \right) - 1 \right] \tag{12}$$

Dispersion polynomial

This polynomial is evaluated at the scaled pixels. The evaluated data are the air-wavelengths (i.e. parameter A_0 in equations 8 to 12) for the center of each pixel. This ICF-line is identical to the one with the same name in entry the IOF (see table 13).

Dispersion rms [nm]

This is the rms of the dispersion based on the laboratory calibration (something like a "best case rms").

Resolution polynomial

This polynomial is evaluated at the air-wavelengths for the center of each pixel in μm. The evaluated data are the FWHM of the slit function for each pixel.

Resolution rms [nm]

This is the rms of the resolution based on the laboratory calibration.

Slit function parameter Ax polynomial

This polynomial is evaluated at the air-wavelengths for the center of each pixel in μm. The evaluated data are the slit function parameter A_x (x=2, 3, ...) for each pixel (see table 32).

Slit function parameter Ax rms

This is the rms of slit function parameter A_x based on the laboratory calibration.

Wavelength effective temperature sensor index

This is that index from the "Auxiliary sensor indices" (see table 14), which is considered most representative for the instrument's wavelength temperature sensitivity. If this ICF-line is not given, the first index of "Auxiliary sensor indices" is used.

Wavelength reference temperature [degC]

This is the value of the wavelength effective temperature, for which the wavelength parameters (dispersion, slit function) were determined.

Dispersion temperature dependence

This is a polynomial to be evaluated at the scaled pixels. The evaluated data are the wavelength temperature

sensitivity at each pixel k_i [nm/K]. For a given pixel, one can estimate the "best" center-wavelength λ_i using equation 13.

$$\lambda_i = \lambda_{NOMi} - k_i \cdot (T_{WE} - T_{WR}) \tag{13}$$

λ_{NOMi} is the nominal center-wavelength for pixel i (from the dispersion), T_{WE} is the wavelength effective temperature, T_{WR} is the wavelength reference temperature and k_i is the wavelength temperature sensitivity for pixel i.

Resolution temperature dependence

This is analogous to "Dispersion temperature dependence", but refers to the resolution (FWHM of slit function). Equation 13 applies when replacing λ with the resolution.

Stray light function fitting method

The fitting method used for the stray light function. In the Blick Software Suite, the stray light is 'attached' to the core slit function (see also entry "Slit function fitting method"). The options for the stray light function fitting method are given in table 33. Parameter B_0, the air-wavelength of the pixel-center is common to each stray light function fitting method and therefore not listed in table 33. The stray light function replaces the (core) slit function for wavelengths with a distance greater than $\Delta\lambda$ from the central wavelength. $\Delta\lambda$ is determined by parameter B_2 and B_5. Note that all B-parameters are positive numbers and are based on equation 14.

$$S(\lambda, |\lambda - B_0| > \Delta\lambda) = (B_2 - B_3) \cdot \left| \frac{\lambda - B_0}{\Delta\lambda} \right|^{B_1} + B_3 + B_4 \cdot exp\,(B_5 \cdot |\lambda - B_0|) \tag{14}$$

Table 33: Stray light function fitting methods

Name	**Parameters**
Symmetric power decay (B_4=0)	B_1: power parameter B_2: merge level B_3: far field stray light level
Asymmetric power decay (B_4=0, B_4, B_5 and B_6 instead of B_1, B_2 and B_3 for λ>B_0)	B_1: power parameter left side B_2: merge level left side B_3: far field stray light level left side B_4: power parameter right side B_5: merge level right side B_6: far field stray light level right side
Symmetric power decay with far field change	B_1: power parameter B_2: merge level B_3: far field stray light level B_4: far field change amplitude B_5: far field change rate
Symmetric power decay with far field change left side (B_4=0 for λ>B_0)	B_1: power parameter B_2: merge level B_3: far field stray light level B_4: far field change amplitude left side B_5: far field change rate left side
Symmetric power decay with far field change right side (B_4=0 for $\lambda \leq B_0$)	B_1: power parameter B_2: merge level B_3: far field stray light level B_4: far field change amplitude right side B_5: far field change rate right side
Symmetric power decay with far field change both sides (B_6 and B_7 instead of B_4 and B_5 for λ>B_0)	B_1: power parameter B_2: merge level B_3: far field stray light level B_4: far field change amplitude left side B_5: far field change rate left side B_6: far field change amplitude right side B_7: far field change rate right side

Name	Parameters
Asymmetric power decay with far field change left side (B_4=0 for λ>B_0, B_4, B_5 and B_6 instead of B_1, B_2 and B_3 for λ>B_0, B_7 and B_8 instead of B_4 and B_5 for $\lambda \leq B_0$)	B_1: power parameter left side B_2: merge level left side B_3: far field stray light level left side B_4: power parameter right side B_5: merge level right side B_6: far field stray light level right side B_7: far field change amplitude left side B_8: far field change rate left side
Asymmetric power decay with far field change right side (B_4=0 for $\lambda \leq B_0$, B_4, B_5 and B_6 instead of B_1, B_2 and B_3 for λ>B_0, B_7 and B_8 instead of B_4 and B_5 for λ>B_0)	B_1: power parameter left side B_2: merge level left side B_3: far field stray light level left side B_4: power parameter right side B_5: merge level right side B_6: far field stray light level right side B_7: far field change amplitude right side B_8: far field change rate right side
Asymmetric power decay with far field change both sides (B_4, B_5 and B_6 instead of B_1, B_2 and B_3 for λ>B_0, B_7 and B_8 instead of B_4 and B_5 for $\lambda \leq B_0$ B_9 and B_{10} instead of B_4 and B_5 for λ>B_0)	B_1: power parameter left side B_2: merge level left side B_3: far field stray light level left side B_4: power parameter right side B_5: merge level right side B_6: far field stray light level right side B_7: far field change amplitude left side B_8: far field change rate left side B_9: far field change amplitude right side B_{10}: far field change rate right side

Slit function parameter Bx polynomial

This polynomial is evaluated at the air-wavelengths for the center of each pixel in μm. The evaluated data are the slit function parameter B_x (x=1, 2, ...) for each pixel (see table 33).

Slit function parameter Bx rms

This is the rms of slit function parameter B_x based on the laboratory calibration.

Special stray light regions fitting methods

This is a comma-separated string with the fitting methods used for the special regions. Each method is followed by " (dyn)" or " (stat)" for a dynamic or static feature respectively. The name of the method is as in table 32,

but can also be "Baseline" or "Mean".

Special stray light region Y parameter Dx polynomial

This polynomial is evaluated at the air-wavelengths for the center of each pixel in μm. The evaluated data are the special stray light parameter D_x (x=0, 1, 2, ...) from region Y for each pixel.

Special stray light region Y parameter Dx rms

This is the rms of special stray light parameter D_x (x=0, 1, 2, ...) from region Y based on the laboratory calibration.

Inband outband transition method

The transition method used to split the slit function into an inband and outband function (see section 6.4.8). The options for the transition method are given in table table 34. Parameter C_0, the air-wavelength of the pixel-center is common to each transition function and therefore not listed in table 34.

Table 34: Inband outband transition methods

Name	Parameters
Symmetric linear wavelength transition The inband equals S(λ) for $\Delta\lambda$<C_1, 0 for $\Delta\lambda$>(C_1+C_2) and is linear in wavelength between these points.	C_1: center distance [nm] C_2: transition length [nm]
Asymmetric linear wavelength transition 1 The inband equals S(λ) for λ-C_0>-C_1 and for λ-C_0<C_3, 0 for λ-C_0<-C_1-C_2 and for λ-C_0>C_3+C_2 and is linear in wavelength between these points.	C_1: center distance left [nm] C_2: transition length [nm] C_3: center distance right [nm]
Asymmetric linear wavelength transition 2 The inband equals S(λ) for $\Delta\lambda$<C_1, 0 for λ-C_0<-C_1-C_2 and for λ-C_0>C_1+C_3 and is linear in wavelength between these points.	C_1: center distance [nm] C_2: transition length left [nm] C_3: transition length right [nm]
Asymmetric linear wavelength transition both The inband equals S(λ) for λ-C_0>-C_1 and for λ-C_0<C_3, 0 for λ-C_0<-C_1-C_2 and for λ-C_0>C_3+C_4 and is linear in wavelength between these points.	C_1: center distance left [nm] C_2: transition length left [nm] C_3: center distance right [nm] C_4: transition length right [nm]

Slit function parameter Cx polynomial

This polynomial is evaluated at the air-wavelengths for the center of each pixel in μm. The evaluated data are the slit function parameter C_x (x=1, 2, ...) for each pixel (see table 34).

Slit function parameter Cx rms

This is the rms of slit function parameter C_x based on the laboratory calibration.

Simple stray light correction parameters for FUNCFILT

This entry gives three numbers, which are the starting wavelength, ending wavelength and polynomial order used to apply the so-called "simple stray light correction" on the data for stray light correction methods SIMPLE of CORRMM (see section 6.4.8) for "functional filter" FUNCFILT. A functional filter is basically any filter listed in entries 19 or 20 of the IOF (see table 13), which is not a neutral density filter (e.g. U340,

BP300). Note that OPEN is also considered a functional filter. E.g. if the values are "280.0 290.0 0", then a 0-order polynomial is fitted into the data between 280 and 290 nm and subtracted from the spectra.

Stray light matrix creation parameters

This entry has 5 integers, which determine how the stray light correction matrix is built. The first element is 0, if the inversion is built over the slit function, and 1, if it is built over the filter function. The second element is 0, if the inversion is built without weight, and 1, if it is built with weight. The third element is 0, if the inband is not normalized, and 1, if it is normalized. The forth and fifth elements are the first and last index of the extended pixels, for which the slit function includes the dynamic special regions.

Theoretical extended transmission wavelength grid

This is the wavelength grid in pm, for which the extended total transmission is given in the next entry.

Theoretical extended transmission for FUNCFILT

This is the normalized extended total transmission for functional filter FUNCFILT in permille.

Sensitivity types

This entry has as many integer numbers as there are filter-combinations in the system. For instruments with one filterwheel there are nine numbers 'belonging' to positions 1 to 9 respectively. For instruments with two filterwheels there are 81 numbers. The first number refers to filterwheel 2 in position 1 and filterwheel 1 in position 1, the second to filterwheel 2 in position 1 and filterwheel 1 in position 2, etc. The meaning of the sensitivity type is the following:

- 0 means that the sensitivity is a nominal 1 for each pixel.
- The last two digits indicate, which of the sensitivities given in entries "Sensitivity x" or "Sensitivity polynomial x" is valid for this filter-combination.
- Positive values indicate that the sensitivity is given directly for each pixel inside the valid wavelength range, while negative values indicate that the sensitivity is given as a polynomial.
- Absolute values below 100 mean that the unit of the L1 data after applying the sensitivity is counts/s, while absolute values above 100 mean that the unit of the L1 data after applying the sensitivity is W/m^2/nm.

E.g. if the 15th entry in the "Sensitivity types" is -108, this means that when the light input passes through filterwheel 1 position 6 and filterwheel 2 position 2, then the correponding instrument sensitivity is given as a polynomial in wavelength, where the coefficients are listed in entry "Sensitivity polynomial 8", and the L1-units after applying the sensitivity are W/m^2/nm.

Wavelength minima for sensitivities [nm]; Wavelength maxima for sensitivities [nm]; Wavelength steps for sensitivities [nm]

These entries list the minimum wavelengths, maximum wavelengths and wavelength steps for which the sensitivities listed in entries "Sensitivity x" or "Sensitivity polynomial x" are given. L1 data outside these limits will be given values of "0".

Scale factors for sensitivities

This entry lists the scale factors for the data given in entries "Sensitivity x". To obtain the unscaled sensitivity, the values have to be divided by this number. The scale factors are not used for entries "Sensitivity polynomial x".

Sensitivity polynomial x

These are the coefficients of the sensitivity polynomial. The polynomial is evaluated at scaled wavelengths (x_{MIN}=entry "Wavelength minima for sensitivities", x_{MAX}=entry "Wavelength maxima for sensitivities").

Sensitivity x

This is the scaled spectral sensitivity as an integer for wavelengths from "Wavelength minima for sensitivities" to "Wavelength maxima for sensitivities" in steps of "Wavelength steps for sensitivities". If the absolute value of the corresponding "Sensitivity type" is above 100, then it is given in units of counts/s per W/m^2/nm, otherwise it is dimensionless.

Spectral data sources

These space separated strings list the conditions and literature sources for the convoluted values. The 1st string gives the atmospheric pressure used in the convolution of the cross sections, e.g. "p=1013.25hPa". The 2nd string gives the extraterrestrial spectrum used, e.g. "F0:XThoullier" (see table 26). The next strings give the cross section source and the reference temperature used, e.g. "O3:Daumont(225.0K)" (see table 27). The last string gives the extraterrestrial spectrum used to calculate the Ring cross sections, e.g. "RING:XThoullier" (see table 26).

Spectra scale [to W/m2/nm]

This is the scale factor for the "Reference spectrum for FUNCFILT" and "Standard spectrum for FUNCFILT". To obtain the unscaled spectra in W/m^2/nm, they have to be divided by this number.

Ring spectrum scale

This is the scale factor for the "Ring spectrum for FUNCFILT". To obtain the unscaled Ring spectrum, it has to be divided by this number. The so-called Ring effect arises in the atmosphere due to inelastic scattering processes, mainly Rotational Raman Scattering by molecular O_2 and N_2 [16]. Roughly speaking, it manifests itself by a broadening of the solar and atmospheric spectral features present in measured spectra.

Temperature scale [K]

This is the temperature scale factor (see section 6.5.3).

Optical depth scale

This is the scale factor for OD-fitting parameters A, B and C (see section 6.5.3). To obtain the unscaled value of the parameter, it has to be divided by this number. E.g. to obtain the convoluted OD for the standard column amount of a linear absorber (B=C=0) at its reference temperature, just use OD-fitting parameter A divided by the scale factor.

Spectra wavelength grid; first, last and step [nm] for FUNCFILT

This is the air-wavelength grid used for the "Reference spectrum for FUNCFILT", "Standard spectrum for FUNCFILT" and "Ring spectrum for FUNCFILT".

Reference spectrum for FUNCFILT

This is the scaled convoluted extraterrestrial spectrum for "functional filter" FUNCFILT using the data source, wavelength grid and scale as given in the ICF-entries above (see also table 26).

Standard spectrum for FUNCFILT

This is the scaled convoluted "standard" spectrum for FUNCFILT using the data source, wavelength grid and scale as given in the ICF entries above. Here the standard spectrum is a direct sun spectrum for SZA=70° and

the standard amount of the absorbers given in table 22.

Ring spectrum for FUNCFILT

This is the scaled convoluted Ring spectrum for FUNCFILT using the data source, wavelength grid and scale as given in the ICF entries above. The convoluted Ring spectrum is calculated using equation 89, just using the high resolution Ring spectrum instead of $F_0(\lambda)$. The possible sources for the high resolution Ring spectrum are listed in table 27 (name starts with "RING").

Optical depth wavelength grid; first, last and step [nm] for FUNCFILT

This is the air-wavelength grid used for the OD-fitting parameters A, B and C (see section 6.5.3) for FUNCFILT.

GAS: OD-parameter Ax (or Bx, Cx), constant (or linear, quadratic) term for FUNCFILT

This is the constant (or linear, quadratic) term in temperature of the scaled convoluted OD-fitting parameter Ax (or Bx, Cx) (see section 6.5.3) for absorber with name GAS (see table 27) using the data source, wavelength grid and scale as given in the ICF-entries above for FUNCFILT. x refers to the OD-method and can be between 0 and 3 for parameter A, 2 or 3 for parameter B and is always 3 for parameter C. Note that for wavelengths below 280 nm these entries are set to zero.

Molecular scattering: OD-parameter Ax (or Bx, Cx) for FUNCFILT

This is the scaled convoluted OD-fitting parameter Ax (or Bx, Cx) for molecular (Rayleigh and Raman) scattering using the wavelength grid and scale as given in the ICF-entries above (see section 6.5.5) for FUNCFILT.

Reference wavelength for wavelength change retrieval [nm]

This is the reference wavelength λ_{REF} used in the wavelength change polynomial. The wavelength change polynomial is retrieved by comparing the measured spectrum to ICF-entry "Standard spectrum". The wavelength change $\Delta\lambda_i$ for pixel i is given by equation 15:

$$\Delta\lambda_i = \sum_{k=0}^{n_{WLC}} c_k \cdot (\lambda_{iNOM} - \lambda_{REF})^k \tag{15}$$

λ_{iNOM} is the nominal center-wavelength for pixel i (as it comes from the dispersion polynomial) and the c_k are the coefficients of the wavelength change polynomial. c_0 is also called (wavelength) shift and c_1 is also called (wavelength) squeeze. The best estimation of the "true" wavelengths for the measurement before the spectral fitting is given by equation 16. For more details on the wavelength change see section 6.4.10.

$$\lambda_{iBEST} = \lambda_{iNOM} + \Delta\lambda_i \tag{16}$$

Wavelength change retrieval parameters for FUNCFILT

This entry lists parameters needed to retrieve the wavelength change polynomial (see equation 15) for a measurement using FUNCFILT. The parameters are:

1. Starting wavelength of the wavelength change fitting window.
2. Ending wavelength of the wavelength change fitting window.

3. Order of the smoothing polynomial used in the spectral fitting to determine the wavelength change, integer (this is n_{SMO} from section 6.5.5).
4. Order of the wavelength change polynomial used in the spectral fitting to determine the wavelength change, integer (this is n_{WLC} from section 6.5.5 and also in equation 15).
5. Order of the offset polynomial used in the spectral fitting to determine the wavelength change, integer (this is n_{OFFS} from section 6.5.5).
6. Space separated list of gases to be included in the wavelength change fitting.

Synthetic reference spectrum for FUNCFILT wavelength grid; first, last and step [nm]

This is the air-wavelength grid used for the "Synthetic reference spectrum for FUNCFILT". If it is not given, then the wavelengths are not on a regular grid are and given explicitly in entry "Wavelengths for synthetic reference spectrum for FUNCFILT"

Wavelengths for synthetic reference spectrum for FUNCFILT [nm]

Air-wavelength centers in nm for the "Synthetic reference spectrum for FUNCFILT".

Scale factor of synthetic reference spectrum for FUNCFILT

This is the scale factor for the "Synthetic reference spectrum for FUNCFILT". To obtain the unscaled spectrum, it has to be divided by this number.

Synthetic reference spectrum for FUNCFILT

This is the scaled synthetic spectrum for functional filter FUNCFILT. The synthetic spectrum is usually a combination of several measured spectra. Depending on the calibration status of the instrument, this spectrum might be in units of corrected count rates or W/m^2/nm.

Independent instrumental uncertainty of synthetic reference spectrum for FUNCFILT

This is the independent uncertainty of "Synthetic reference spectrum for FUNCFILT" in the same units.

Slant columns in synthetic reference spectrum for FUNCFILT

These space separated strings give the estimations of the slant column amount of a specific trace gas included in the synthetic reference spectrum. Each string starts with the short name of the trace gas as given in table 22, followed by a colon. After this there are three comma separated strings.

1. The slant column of the gas in its standard units (see section 5.10.1), followed by its uncertainty in parenthesis.
2. The effective temperature of the gas optical depth included in the synthetic reference spectrum, followed by its uncertainty in parenthesis, followed by the letter "K".
3. The letters "OD" followed by the optical depth fitting method used to estimated the gas absorption included in the synthetic reference spectrum (see section 6.5).

E.g. the string "O3:2.2421e-01(8.969e-04),258.1(2.3)K,OD3" means that absorption from an estimated 0.2242±0.0009 mol/m^2 of ozone at an effective temperature of 258.1±2.3 K is included in the synthetic reference spectrum and was determined using optical depth fitting method 3. If the gas is not calibrated, then the string says GAS:0(-9),0(-9)K,OD0.

After all the trace gas entries, there are two more strings:

- The word "SCA", followed by a colon and the molecular scattering air mass factor, then a comma followed by the ratio of the surface pressure relative to the standard pressure, e.g. "SCA:1.3495,0.9918".
- The word "AER", followed by a colon and the coefficients of a second order polynomial (constant term first) for the logarithm of the spectral slant aerosol optical depth (AOD)included in the reference as a function of the logarithm of the wavelength in micrometer, e.g. "AER:-4.5927e+00,-4.0296e+00,-1.5547e+00".

Time period and location used for synthetic reference spectrum for FUNCFILT

This line gives the time period and location for the data used to build the synthetic reference spectrum for functional filter FUNCFILT. It is purely informative and not used by BlickP.

Standard total optical depth for FUNCFILT

This is the sum over all individual optical depths for FUNCFILT at standard conditions.

Relative reference spectrum change with resolution for FUNCFILT

This is the change of the logarithm (or relative change) of ICF-entry "Reference spectrum for FUNCFILT" for a 1% increase in the instrument's resolution, scaled by ICF-entry "Optical depth scale".

Standard total optical depth change with resolution for FUNCFILT

This is the change of the ICF-entry "Standard total optical depth for FUNCFILT" for a 1% increase in the instrument's resolution, scaled by ICF-entry "Optical depth scale".

5.12 L1 File

BlickP converts the L0 data into L1 data by applying all instrumental corrections to the raw data (see section 6.4). L1 files are daily ASCII-text files with a header, which includes meta data (see section 5.1), a description of the data columns and the L1 data. Note that only "Data lines" from the L0 file are converted into L1 data. "Comment lines" with information, warnings or errors are ignored (see 5.7). Also, L0 data with a "Data processing type index" of -9 (manual operation) or 1 (processing type "NOL1", see section 4.1.12) are ignored by BlickP.

L1 files are called `PandoraXsY_LLL_YYYYMMDD_L1_sSSSScCdDpP.txt`. X, Y, LLL, YYYYMMDD are as for the L0 file (section 5.7). The segment "sSSSScCdDpP" is the so-called "Data file version". SSSS is the "s-code" or "L1 configuration", that was used for the processing (see section 5.10.2). C is the version number of the ICF used for the processing. It corresponds to the number after "v" in the ICF name (see section 5.11). D is the 8-character validity date of the ICF used for the processing. It corresponds to the number after "d" in the ICF name (see section 5.11). P is the main version number and first subversion number of BlickP used for the processing, combined with a dash instead of a dot. E.g. for BlickP version 1.2.5, P equals 1-2. Obviously if L1 data are processed with different data file versions, different L1 data files are produced, i.e. more than one L1 file can exist for a given L0 file. L1 files occupy around three quarters of the space of the corresponding L0 file. The data lines are approximately cut in half, since the dark measurements have been included in the data correction, but each data line is longer than for L0 since the independent instrumental uncertainty is listed in addition to the so-called "atmospheric variability". For the meaning of the independent uncertainty and atmospheric variability we refer to section 6.3.4.

Table 35 lists the maximum possible data columns in the L1 file. As for the L0 file, the real number of columns varies from instrument to instrument. E.g. if an instrument does not have a filterwheel 2, then there is no column "Effective position of filterwheel #2". The meaning of each column is described in the header after

the meta data. Temperature data can be followed by the spectrometer number, e.g. "Temperature at electronics board 2" refers to spectrometer 2 (see table 35).

In table 35 and also in the descriptions of higher level data, the expression "bright count" is frequently used. With bright count we simply refer to the counts from measurements, where light is entering the instrument, i.e. which do not use the opaque filter to block the input. On the contrary, data taken without light entering the instrument give a so-called "Dark count".

For entry "L1 data quality flag", there are also data quality 10 (DQ10), data quality 11 (DQ11) and data quality 12 (DQ12) in addition to DQ0, DQ1 and DQ2. The difference is that for DQ0, DQ1 and DQ2 quality assurance (QA) has been applied, while for DQ10, DQ11 and DQ12 it has not. In all other aspects, DQ10 equals DQ0, DQ11 equals DQ1 and DQ12 equals DQ2. Currently QA consists of checking the trace gas columns for obvious periods of malfunctioning or a possible calibration change of the instrument. In general one can say that when a new ICF is made, all data before the validity starting date of the new ICF are quality assured and the DQF will be set to 0, 1 or 2. Differently, all new data will have DQF 10, 11 or 12. E.g. DQ10 means that all data quality indicators suggest high data quality, just as for DQ0, but no QA has been applied yet.

Note that the filterwheel positions are now called ’effective’ positions. In the L0 data (table 18) they are the ’nominal’ filterwheel positions as set during the measurements. The ’effective’ filterwheel position says through which position the light for the specific spectrometer was going. For spectrometer 1 the nominal and effective filterwheel positions are the same. For the other spectrometers the effective position is shifted relative to the nominal position by the corresponding number given listed in IOF entry ’Filter position offsets’ (table 13). E.g. if ’Filter position offsets’ equals 3 and the nominal filterwheel position is 4, then the effective filterwheel position for spectrometer 2 is 7.

Table 35: Columns in L1 file

Column name	Remark
Two letter code of measurement routine	See section 4.1
UT date and time for beginning of measurement, yyyymmddThhmmssZ (ISO 8601)	
Fractional days since 1-Jan-2000 UT midnight for beginning of measurement	
Routine count (1 for the first routine of the day, 2 for the second, etc.)	Corresponds to the L0 routine count
Repetition count (1 for the first set in the routine, 2 for the second, etc.)	Does not necessarily correspond to the L0 repetition count
Total duration of measurement set in seconds	This is without the dark count!
Latitude at beginning of measurement [deg], negative=South of equator, positive=North of equator, -999=no latitude retrieved	
Longitude at beginning of measurement [deg], negative=West of Greenwich, positive=East of Greenwich, -999=no longitude retrieved	
Altitude a.s.l. at beginning of measurement [m], -999=no altitude retrieved	
West-East inclination angle at beginning of measurement [deg], -999=angle not retrieved	
North-South inclination angle at beginning of measurement [deg], -999=angle not retrieved	
Rotation angle at beginning of measurement [deg], -999=angle not retrieved	
Data processing type index	See table 7
Integration time [ms]	
Number of bright count cycles	0 if only dark count was measured
Number of dark count cycles	0 if no dark count was measured
Saturation index: positive integer is the number of saturated cycles included in the data, negative integer is the number of cycles skipped due to saturation	
Effective position of filterwheel #1, 0=filterwheel not used, 1-9 are valid positions	
Effective position of filterwheel #2, 0=filterwheel not used, 1-9 are valid positions	
Pointing zenith angle in degree, absolute or relative (see next column), 999=tracker not used	
Zenith pointing mode: zenith angle is... 0=absolute, 1=relative to sun, 2=relative to moon	
Pointing azimuth in degree, increases clockwise, absolute (0=north) or relative (see next column), 999=tracker not used	
Azimuth pointing mode: like zenith angle mode but also fixed scattering angles relative to sun (3) or moon (4)	
Mean over camera offsets [deg], -9=camera not in automatic mode	
Maximum of camera offsets [deg], -9=camera not in automatic mode	
Target distance [m], -1=not pointed on target	See section 4.1.12

Column name	Remark
Sum over 2^i with i being a L0 to L1 conversion step, 0=dark correction, 1=non-linearity correction, 2=latency correction, 3=flat field correction, 4=conversion to count rates, 5=temperature correction, 6=stray light correction, 7=wavelength change determination, 8=sensitivity correction, 9=wavelength correction	See section 6.4
Dark correction method: -9=no dark correction done, since it was not requested, -2=no dark correction done, since there were no bright measurements, -1=no dark correction done, since there was no matching dark measurement, 0=dark correction done with measured dark count only, since input darkmeth was MEAS or no dark map parameters available, 1=dark correction done using dark fine structure map and measured dark count, >1=dark correction done with measured dark count only, since dark background fitting gave an error	
L1 data quality flag: 0=assured high quality, 1=assured medium quality, 2=assured low quality, 10=not-assured high quality, 11=not-assured medium quality, 12=not-assured low quality	
Sum over 2^i using those i, for which the corresponding L1 data quality parameter exceeds the DQ1 limit, 0=Saturated data, 1=Too few dark counts measurements, 2=No temperature given or effective temperature too different from the reference temperature, 3=Dark count too high, 4=Unsuccessful dark background fitting, 5=Absolute value of estimated average residual stray light level too high, 6=Although attempted, no wavelength change could be retrieved, 7=Retrieved wavelength shift too large, 8=Retrieved wavelength shift differs too much from the shift predicted by the effective temperature	See table 24
Sum over 2^i using those i, for which the corresponding L1 data quality parameter exceeds the DQ2 limit (same parameters as for DQ1)	See table 24
Wavelength effective temperature [°], 999=no effective temperature given	
Number of pixels, where dark count is higher than bright count, -9=no bright counts or dark counts measured	
Number of pixels, where DQ1 sigma ranges of dark count and bright count do not overlap, -9=no bright count or dark count standard error measured	
Number of pixels, where DQ2 sigma ranges of dark count and bright count do not overlap, -9=no bright count or dark count standard error measured	
Index of (not dead, blind, warm or saturated) pixel with highest corrected counts	
Standard error of blind and oversampled pixels in the bright counts, -9 if there is no bright count standard error	See also section 6.2
Mean over blind and oversampled pixels in the dark counts, -9 if there is no dark count	See also section 6.2
Standard error of blind and oversampled pixels in the dark counts, -9 if there is no dark count standard error	See also section 6.2

Column name	Remark
Mean over blind and oversampled pixels in the bright counts, -9 if there is no bright count	See also section 6.2
Number of function evaluations used for dark background fitting, -9 if no background fitting was done	See also section 6.4
rms of unweighted fitting residuals for dark background fitting, -9 if no background fitting was done	See also section 6.4
Normalized rms of weighted fitting residuals for dark background fitting, -9 if no background fitting was done	See also section 6.4
Mean difference dark map to measured dark count, -9 if no background fitting was done	See also section 6.4
rms of difference dark map to measured dark count, -9 if no background fitting was done	See also section 6.4
Mean absolute difference dark map to measured dark count expressed in number of standard deviations, -9 if no background fitting was done	See also section 6.4
Number of regular pixels, where the dark map differs from the measured dark by more than 10 sigmas, -9 if no background fitting was done	See also section 6.4
Number of warm pixels, where the dark map differs from the measured dark by more than 10 sigmas, -9 if no background fitting was done	See also section 6.4
Number of hot pixels, where the dark map differs from the measured dark by more than 10 sigmas, -9 if no background fitting was done	See also section 6.4
Index of regular pixel, where the dark map differed most from the measured dark count, -9 if no background fitting was done	See also section 6.4
Number of sigmas the dark map differs from the measured dark for the pixel with the largest difference, -9 if no background fitting was done	See also section 6.4
Retrieved value for dark background fitting parameter X, -9 if no background fitting was done	X=1 until the value of ICF entry "Dark background fitting settings" plus three
Uncertainty of retrieved value for dark background fitting parameter X, -9 if no background fitting was done or no independent instrumental uncertainty was given	X=1 until the value of ICF entry "Dark background fitting settings" plus two
Stray light correction method: 0=no stray light correction, 1=simple method, 2=uncorrected matrix method, 3=corrected matrix method	See also section 6.4.8
Estimated average residual stray light level [%] (for methods 1 and 3 this is before the subtraction of the signal at no-input pixel)	See also section 6.4.8
Estimated stray light in the signal before correction at X nm [%], -9=no stray light correction, -1=signal after stray light correction negative, -2=estimated stray light negative, -3=signal before stray light correction negative	X=300, 302.5, 305, 310, 320, 350 or 400
Number of iterations needed to reach tolerance goal at wavelength change determination, -9=no wavelength change determination	See also section 6.4

Column name	Remark
Wavelength change fitting result index: 0,1,2=no error or warning, 3=warning, -1 or >3=error	See also section 6.4
Normalized rms of fitting residuals weighted with independent instrumental uncertainty, -9=fitting not successful or no fitting done	See also section 6.4
Number of pixels included in the wavelength correction, -9=no wavelength correction	See also section 6.4
Mean wavelength correction applied [%], -9=no wavelength correction	See also section 6.4
Standard deviation of wavelength correction applied [%], -9=no wavelength correction	See also section 6.4
Minimum wavelength correction applied [%], -9=no wavelength correction	See also section 6.4
Maximum wavelength correction applied [%], -9=no wavelength correction	See also section 6.4
Expected wavelength shift based on effective temperature [nm], -9=no effective temperature given	See also section 6.4
Retrieved wavelength change, order X, -9=no wavelength change determination	X=0 until the largest order listed in ICF entries "Wavelength change retrieval parameters for FUNCFILT"
Temperature at detector X [°C], 999=no temperature signal	X=1, 2 or empty
Temperature at electronics board X [°C], 999=no temperature signal	X=1, 2 or empty
Spectrometer control temperature X [°C], 999=no temperature signal	X=1, 2 or empty
Auxiliary spectrometer temperature X [°C], 999=no temperature signal	X=1, 2 or empty
Temperature in head sensor [°C], 999=no temperature signal	
Azimuth motor temperature [°C], 999=no temperature signal	
Azimuth driver temperature [°C], 999=no temperature signal	
Zenith motor temperature [°C], 999=no temperature signal	
Zenith driver temperature [°C], 999=no temperature signal	
Humidity in head sensor [%], -9=no humidity signal	Relative humidity
Pressure in head sensor [hPa], -9=no pressure signal	
Scale factor for data and uncertainties, to obtain unscaled output divide them by this number	
Indicator for uncertainty and atmospheric variability (see manual for exact meaning)	See table 36 and section 6.3.4
L1 data type, data are... 1=corrected count rate [s^{-1}], 2=radiance [W/m^2/nm/sr], 3=irradiance [W/m^2/nm]	
L1 data for each pixel, 0 is NOT a 'true' zero if the corresponding value in the uncertainty is -2, -3, -4 or -5	
Atmospheric variability of L1 data for each pixel [%], 101=no atmospheric variability was measured and pixel is inside the range of the filter, 102=no atmospheric variability was measured and pixel is outside the range of the filter, 103=atmospheric variability was measured, but pixel is outside the range of the filter, 104=saturated data, 105=the wavelength is inside the valid range, but the sensitivity at this wavelength equals 0, 109=no atmospheric variability was determined since no dark correction was attempted	See section 6.3.4
Independent instrumental uncertainty of L1 data for each pixel, -2=pixel is outside the range of the filter, -4=saturated data	See section 6.3.4

Table 36: Meaning of column 'Indicator for uncertainty and atmospheric variability'

Number	Description
0	No bright count was measured and dark count was measured for one cycle only. No atmospheric variability was determined. Independent instrumental uncertainty is based on theoretical dark count independent instrumental uncertainty.
1	No bright count was measured and dark count plus standard deviation of dark count was measured. No atmospheric variability was determined. Independent instrumental uncertainty is based on theoretical dark count independent instrumental uncertainty.
2	Bright count was measured for one cycle only and no dark count was measured. No atmospheric variability was determined. Independent instrumental uncertainty is based on theoretical bright count independent instrumental uncertainty.
3	Both bright and dark count were measured for one cycle only. No atmospheric variability was determined. Independent instrumental uncertainty is based on theoretical independent instrumental uncertainties of bright and dark count.
4	Bright count was measured for one cycle only and dark count plus standard deviation of dark count was measured. No atmospheric variability was determined. Independent instrumental uncertainty is based on theoretical independent instrumental uncertainties of bright and dark count.
5	Bright count plus standard deviation of bright count was measured and no dark count was measured. No atmospheric variability was determined. Independent instrumental uncertainty is based on theoretical independent instrumental bright count uncertainty.
6	Bright count plus standard error to a straight line fitted in the data was measured and no dark count was measured. Atmospheric variability is based on the measured bright count standard error to a straight line and theoretical dark count independent instrumental uncertainty. Independent instrumental uncertainty is based on theoretical independent instrumental bright count uncertainty.
7	Bright count plus standard deviation of bright count was measured and dark count was measured for one cycle only. No atmospheric variability was determined. Independent instrumental uncertainty is based on theoretical independent instrumental uncertainties of bright and dark count.
8	Bright count plus standard error to a straight line fitted in the data was measured and dark count was measured for one cycle only. Atmospheric variability is based on the measured bright count standard error to a straight line and theoretical dark count independent instrumental uncertainty. Independent instrumental uncertainty is based on theoretical independent instrumental uncertainties of bright and dark count.
9	Bright count plus standard deviation of bright count was measured and dark count plus standard deviation of dark count was measured. No atmospheric variability was determined. Independent instrumental uncertainty is based on theoretical independent instrumental uncertainties of bright and dark count.
10	Bright count plus standard error to a straight line fitted in the data was measured and dark count plus standard deviation of dark count was measured. Atmospheric variability is based on the measured bright count standard error to a straight line and measured dark count standard deviation. Independent instrumental uncertainty is based on theoretical independent instrumental uncertainties of bright and dark count.

5.13 L2Fit Files

BlickP converts the L1 data into L2Fit data by applying the L2Fit algorithm (see section 6.5). L2Fit files are daily ASCII-text files with a header, which includes meta data (see section 5.1), a description of the data columns and the L2Fit data. L1 data with a "Data processing type index" of 0 (processing type "ONLYL1", see section 4.1.12) are not converted to L2Fit data.

L2Fit files are called `PandoraXsY_LLL_YYYYMMDD_L2Fit_fFFFFcCdDpP.txt`. X, Y, LLL, YYYYMMDD are as for the L0 file (section 5.7). The segment "fFFFFcCdDpP" is the "Data file version". C, D and P are as for the L1 file (section 5.12). FFFF is the 4-character "f-code" or "Fitting setup", that was used for the spectral fitting (see section 5.10.3). Only those L1 data are used for a specific L2Fit file, which have a "Data processing type index" (see section 4.1.12), that is the one required by the r-code (see section 5.10.4). Obviously, if L1 data are processed with different data file versions, different L2Fit data files are produced, i.e. more than one L2Fit file can exist for a given f-code.

L2Fit files usually occupy less space than the corresponding L1 file, since the fitting window includes in general less pixels than exist on the spectrometer. Table 37 lists the maximum possible data columns in the L2Fit file. The real number of columns varies with the instrument, s-code and f-code. E.g. if the f-code does not have absolute wavelength limits (see entries "WL-starts" and "WL-ends" in table 25), then no residuals are written. The meaning of each column is described in the header after the meta data.

Column "Effective GAS fitting wavelength" gives the wavelength, which we consider representative for this trace gas for the respective f-code. It is calculated by equation 17:

$$\lambda_{EFFj} = \frac{\sum_i \lambda_i \cdot \tau_{ji}/\sigma_i^2}{\sum_i \tau_{ji}/\sigma_i^2} \tag{17}$$

λ_{EFFj} is the effective fitting wavelength for trace gas j, the λ_i are the wavelength centers for each pixel i inside the fitting window, τ_{ji} are the absorption cross sections for gas j at pixel i and σ_i are the measurement uncertainties (in log-space) at pixel i.

All polynomial coefficients given in the L2Fit data are to be evaluated at scaled wavelengths based on equation 4 with x_{MIN} and x_{MAX} given in columns "Lower limit used for wavelength scaling [nm]" and "Upper limit used for wavelength scaling [nm]" respectively. The only exception are entries "L1 based wavelength change coefficient ...", which are scaled as in the L1 data.

As for L1 data, the "L2Fit data quality flag" can have values DQ0, DQ1 and DQ2 for QA data and DQ10, DQ11 and DQ12 otherwise.

Table 37: Columns in L2Fit file

Column name	Remark
Two letter code of measurement routine	See section 4.1
UT date and time for center-time of measurement, yyyymmddThhmmssZ (ISO 8601)	
Fractional days since 1-Jan-2000 UT midnight for center-time of measurement	
Routine count (1 for the first routine of the day, 2 for the second, etc.)	Corresponds to the L0 routine count
Repetition count (1 for the first set in the routine, 2 for the second, etc.)	Corresponds to the L1 repetition count
Total duration of measurement set in seconds	As in L1
Latitude at beginning of measurement [deg], negative=South of equator, positive=North of equator, -999=no latitude retrieved	
Longitude at beginning of measurement [deg], negative=West of Greenwich, positive=East of Greenwich, -999=no longitude retrieved	
Altitude a.s.l. at beginning of measurement [m], -999=no altitude retrieved	
Data processing type index	See table 7
Solar zenith angle for center-time of measurement in degree	
Solar azimuth for center-time of measurement in degree, 0=north, increases clockwise	
Lunar zenith angle for center-time of measurement in degree	
Lunar azimuth for center-time of measurement in degree, 0=north, increases clockwise	
Pointing zenith angle in degree, absolute or relative (see next column), 999=tracker not used	
Zenith pointing mode: zenith angle is... 0=absolute, 1=relative to sun, 2=relative to moon	
Pointing azimuth in degree, increases clockwise, absolute (0=north) or relative (see next column), 999=tracker not used	
Azimuth pointing mode: like zenith angle mode but also fixed scattering angles relative to sun (3) or moon (4)	
Fitting result index: 0=no error or warning, 1,2=warning, >2=error	See table 38
Number of function evaluations used, 0=linear fitting or fitting not successful or no fitting done	
rms of unweighted spectral fitting residuals, -9=fitting not successful	Equation 119
Normalized rms of fitting residuals weighted with independent uncertainty, -9=fitting not successful or no uncertainty used. Note that if fcode entry 'Uncertainty' is set to 'MEAS', then the measured standard error output of the L1 data is used to calculate this uncertainty.	Equation 120
Expected rms based on independent uncertainty, -9=fitting not successful or no uncertainty given. Note that if fcode entry 'Uncertainty' is set to 'MEAS', then the measured standard error output of the L1 data is used to calculate this uncertainty.	Equation 121
Expected normalized weighted rms based on instrumental uncertainty, -9=fitting not successful or no uncertainty given. Note that if fcode entry 'Uncertainty' is set to 'MEAS', then the measured standard error output of the L1 data is used to calculate this uncertainty.	Equation 122

Column name	Remark
GAS slant column amount [GASUNIT], -9e99=fitting not successful	Fitted slant column in unit GASUNIT for gas GAS
Independent uncertainty of GAS slant column amount [GASUNIT], -1=cross section is zero in this wavelength range, -3=spectral fitting was done, but no independent uncertainty could be retrieved, -5=no independent uncertainty input was given, -9=spectral fitting not successful	See section 6.3.5
Structured uncertainty of GAS slant column amount [GASUNIT], -9=spectral fitting not successful	See section 6.3.5
Common uncertainty of GAS slant column amount [GASUNIT], -1=cross section of the gas is zero in this wavelength range, -5=no common uncertainty input was given, -9=spectral fitting was not successful	See section 6.3.5
rms-based uncertainty of GAS slant column amount [GASUNIT], -1=cross section is zero in this wavelength range, -3=spectral fitting was done, but no rms-based uncertainty could be retrieved, -9=spectral fitting not successful	See section 6.3.5
GAS effective temperature [K]	Either the fitted value or a fixed value or taken from the climatology; to distinguish one needs to look at the uncertainty
Independent uncertainty of GAS effective temperature [K], -1=temperature fitting was requested, but cross section is zero in this wavelength range, -2=no temperature fitting was requested and output for effective temperature and structured uncertainty of it is based on f-code, -3=spectral fitting was done, but no independent uncertainty could be retrieved, -4=temperature fitting was requested, but differential optical depth is too small to retrieve the temperature, -5=no independent uncertainty input was given, -9=spectral fitting not successful	See section 6.3.5
Structured uncertainty of GAS effective temperature [K], -1=temperature fitting was requested, but cross section is zero in this wavelength range, -4=temperature fitting was requested, but differential optical depth is too small to retrieve the temperature, -9=spectral fitting not successful	See section 6.3.5
Common uncertainty of GAS effective temperature [K], -1=temperature fitting was requested, but cross section is zero in this wavelength range, -2=no temperature fitting was requested and output for effective temperature and structured uncertainty of it is based on f-code, -3=spectral fitting was done, but no common uncertainty could be retrieved, -4=temperature fitting was requested, but differential optical depth is too small to retrieve the temperature, -6=no common uncertainty input was given, -9=spectral fitting not successful	See section 6.3.5
rms-based uncertainty of GAS effective temperature [K], -1=temperature fitting was requested, but cross section is zero in this wavelength range, -2=no temperature fitting was requested and effective temperature output is based on f-code, -4=temperature fitting was requested, but differential optical depth is too small to retrieve the temperature, -9=spectral fitting was not successful	See section 6.3.5
Effective GAS fitting wavelength [nm], -9=fitting not done or not successful	See equation 17

Column name	Remark
Diffuse correction applied before fitting at effective fitting wavelength for GAS [%], 0=no diffuse correction applied or fitting not done or not successful, >0=measured diffuse correction, <0=(negative value of) calculated diffuse correction	See section 5.10.3
Molecular scattering air mass factor used for molecular scattering subtraction before the fitting	
Estimated uncertainty of molecular scattering air mass factor, -9=molecular scattering was not subtracted before the fitting	
Fitted Ring spectrum, -9e99=no fitting done or fitting not successful	Ring spectrum slant column
Independent uncertainty of fitted Ring spectrum, -9=fitting not successful	See section 6.3.5
Structured uncertainty of fitted Ring spectrum, -9=fitting not successful	See section 6.3.5
Common uncertainty of fitted Ring spectrum, -9=fitting not successful	See section 6.3.5
rms-based uncertainty of fitted Ring spectrum, -9=fitting not successful	See section 6.3.5
Effective Ring fitting wavelength [nm], -9=fitting not done or not successful	See equation 17
Diffuse correction applied before fitting at effective Ring fitting wavelength [%], 0=no diffuse correction applied or fitting not done or not successful, >0=measured diffuse correction, <0=(negative value of) calculated diffuse correction	See section 5.10.3
Lower limit used for wavelength scaling [nm]	
Upper limit used for wavelength scaling [nm]	
Order of smoothing polynomial	
Smoothing polynomial coefficient, order X	X=0 to maximum 10, see 6.5
Independent uncertainty of smoothing polynomial coefficient, order X, -9=fitting not successful	See section 6.3.5
Structured uncertainty of smoothing polynomial coefficient, order X, -9=fitting not successful	See section 6.3.5
Common uncertainty of smoothing polynomial coefficient, order X, -9=fitting not successful	See section 6.3.5
rms-based uncertainty of smoothing polynomial coefficient, order X, -9=fitting not successful	See section 6.3.5
Mean value of measured data inside fitting window [same units as measurements]	$\overline{F}$ from equation 96
Offset polynomial coefficient, order X	X=0 to maximum 5, see 6.5
Independent uncertainty of offset polynomial coefficient, order X, -9=fitting not successful	See section 6.3.5
Structured uncertainty of offset polynomial coefficient, order X, -9=fitting not successful	See section 6.3.5
Common uncertainty of offset polynomial coefficient, order X, -9=fitting not successful	See section 6.3.5
rms-based uncertainty of offset polynomial coefficient, order X, -9=fitting not successful	See section 6.3.5
Wavelength change polynomial coefficient, order X	X=0 to maximum 5, see 6.5
Independent uncertainty of wavelength change polynomial coefficient, order X, -9=fitting not successful	See section 6.3.5
Structured uncertainty of wavelength change polynomial coefficient, order X, -9=fitting not successful	See section 6.3.5
Common uncertainty of wavelength change polynomial coefficient, order X, -9=fitting not successful	See section 6.3.5
rms-based uncertainty of wavelength change polynomial coefficient, order X, -9=fitting not successful	See section 6.3.5

Index	Description
L1 based wavelength change coefficient, order X, -9=no L1 wavelength change determination	As in L1
Resolution change polynomial coefficient, order X	X=0 to maximum 5, see 6.5
Independent uncertainty of resolution change polynomial coefficient, order X, -9=fitting not successful	See section 6.3.5
Structured uncertainty of resolution change polynomial coefficient, order X, -9=fitting not successful	See section 6.3.5
Common uncertainty of resolution change polynomial coefficient, order X, -9=fitting not successful	See section 6.3.5
rms-based uncertainty of resolution change polynomial coefficient, order X, -9=fitting not successful	See section 6.3.5
L2Fit data quality flag: 0=assured high quality, 1=assured medium quality, 2=assured low quality, 10=not-assured high quality, 11=not-assured medium quality, 12=not-assured low quality	
Sum over 2^i using those i, for which the corresponding data quality parameter exceeds the DQ1 limit, 0=L1 data quality above 0, 1=Spectral fitting was not successful, 2=Weighted rms of spectral fitting too large, 3=Wavelength shift too large	See table 28
Sum over 2^i using those i, for which the corresponding data quality parameter exceeds the DQ2 limit (same parameters as for DQ1)	
L1 data quality flag: 0=assured high quality, 1=assured medium quality, 2=assured low quality, 10=not-assured high quality, 11=not-assured medium quality, 12=not-assured low quality	As in L1
Sum over 2^i using those i, for which the corresponding L1 data quality parameter exceeds the DQ1 limit, 0=Saturated data, 1=Too few dark counts measurements, 2=No temperature given or effective temperature too different from the reference temperature, 3=Dark count too high, 4=Unsuccessful dark background fitting, 5=Absolute value of estimated average residual stray light level too high, 6=Although attempted, no wavelength change could be retrieved, 7=Retrieved wavelength shift too large, 8=Retrieved wavelength shift differs too much from the shift predicted by the effective temperature	As in L1
Sum over 2^i using those i, for which the corresponding L1 data quality parameter exceeds the DQ2 limit (same parameters as for DQ1)	As in L1
Atmospheric variability [%], 999=no atmospheric variability was determined	From L1 data for pixel with highest SNR
Wavelength effective temperature [°C], 999=no effective temperature given	As in L1
Estimated average residual stray light level [%] (only valid for stray light correction methods 2 and higher)	
Retrieved wavelength shift from L1 data [nm], -9=no wavelength change determination	As in L1 (constant term)
Retrieved wavelength shift from spectral fitting data [nm], -9=no wavelength change fitting	
Number of bright count cycles	As in L1
Number of dark count cycles	As in L1
Effective position of filterwheel #1, 0=filterwheel not used, 1-9 are valid positions	As in L1
Effective position of filterwheel #2, 0=filterwheel not used, 1-9 are valid positions	As in L1

Index	Description
Sum over 2^i, 0=spectra were interpolated in time, 1=spectra are corrected for off-target signal	See table 25
Integration time [ms]	As in L1
Mean over camera offsets [deg], -9=camera not in automatic mode	As in L1
Maximum of camera offsets [deg], -9=camera not in automatic mode	As in L1
Temperature at detector X [°C], 999=no temperature signal	As in L1
Temperature at electronics board X [°C], 999=no temperature signal	As in L1
Spectrometer control temperature X [°C], 999=no temperature signal	As in L1
Auxiliary spectrometer temperature X [°C], 999=no temperature signal	As in L1
Temperature in head sensor [°C], 999=no temperature signal	As in L1
Azimuth motor temperature [°C], 999=no temperature signal	As in L1
Azimuth driver temperature [°C], 999=no temperature signal	As in L1
Zenith motor temperature [°C], 999=no temperature signal	As in L1
Zenith driver temperature [°C], 999=no temperature signal	As in L1
Humidity in head sensor [%], -9=no humidity signal	As in L1
Pressure in head sensor [hPa], -9=no pressure signal	As in L1
Unweighted slant column residuals for each pixel inside the fitting window multiplied by 1e5, 9e5=pixel was not used for fitting	
Normalized slant column residuals weighted with independent instrumental uncertainty for each pixel inside the fitting window multiplied by 1e5, 9e5=pixel was not used for fitting, 0=no independent instrumental uncertainty was given	

Table 38: Meaning of fitting error indices. 1 and 2 are warnings. 3 to 10 are errors only affecting the non-linear fitting and return the results of the linear fitting. 11 and 12 are errors affecting already the linear fitting, return output, but no uncertainty. 13 to 17 are errors affecting already the linear fitting and return no output at all.

Index	Description
0	No error or warning
1	Warning: Some gases have not been fitted, since their optical depth was zero in the range of the valid data; otherwise successful fitting
2	Warning: No fitting was done since the measurements equal the reference; all differential slant columns are set to zero
3	Error: The number of valid reference data is smaller than then number of fitting parameters for the non-linear fitting; output gives the result from the linear fitting
4	Error: Encountered singular covariance matrix in uncertainty weighted non-linear fitting; output gives the result from the linear fitting
5	Error: Encountered singular covariance matrix in unweighted non-linear fitting; output gives the result from the linear fitting
6	Error: Negative values were in the covariance matrix of the non-linear fitting; uncertainty output is from linear fitting
7	Error: Maximum number of function evaluations reached; output gives the result from the linear fitting
8	Error: Function tolerance is too small, no further reduction in the sum of squares is possible; output gives the result from the linear fitting
9	Error: Output tolerance is too small, no further improvement in the approximate solution is possible; output gives the result from the linear fitting
10	Error: Orthogonality tolerance is too small; the function is orthogonal to the columns of the Jacobian to machine precision; output gives the result from the linear fitting
11	Error: Negative values were in the uncertainty weighted covariance matrix of the linear fitting; no uncertainty output made
12	Error: Negative values were in the unweighted covariance matrix of the linear fitting; no uncertainty output made
13	Error: The number of data in the reference is smaller than the number of fitting parameters
14	Error: The reference data do not fully include the wavelength range of the fitting
15	Error: The number of valid measured data is smaller than the number of fitting parameters for the linear fitting
16	Error: No fitting because of rank deficiency in design matrix
17	Error: Linear pseudo inversion computation did not converge
18	Error: No fitting since no fitting parameters were requested
19	Error: No fitting since not enough data were available

5.14 L2 Files

BlickP converts the L2Fit data into L2 data by applying an L2 algorithm. L2 files contain total vertical column trace gas amounts retrieved from direct sun or moon observations or trace gas profile information such as partial column amounts in different layers, tropospheric vertical column amounts or surface concentrations retrieved from sky observations. L2 data are ASCII-text files with a header, which includes meta data (see section 5.1), a description of the data columns and the data. Differently to L0, L1 and L2Fit files, L2 files are not daily files anymore. They include the whole time series of measurements for a given retrieval code and instrument at a given location.

L2 files are called `PandoraXsY_LLL_L2_rRRRRpP.txt`. X, Y and LLL are as for the L0 file (section 5.7). The segment "rRRRRpP" is the "Data file version". P is as for the L1 file (section 5.12). RRRR is the "r-code" or "retrieval setup", that was used for the retrieval (see section 5.10.4). Note that the data file version does not include information on the ICF version used. This is because the ICF version is "allowed" to vary over time and is therefore listed as a column in the data themselves (see table 39).

The size of the L2 files depends on the length of the data base at a station, but they are usually much smaller than L0, L1 or L2Fit files, since no spectral information is included. Table 39 lists the maximum possible data columns in the L2 file. The real number of columns varies with the instrument and L2 type (see also column "Remark"). The meaning of each column is described in the header after the meta data.

Column "Remark" in table 39 gives additional details on the L2 output data. The following acronyms are used for this column:

- PROF: this refers to profile measurements from sky observations.
- DIR: this refers to direct sun (or moon) observations. It is further split into:
  - DIR1: direct observations using one fcode only
  - DIR2: direct observations using two fcodes
- RSET: for retrievals using more than one measurement set, such as PROF, RSET refers to that measurement set, to which all other are interpolated or referenced (e.g. in our standard sky retrievals the one at the highest pointing zenith angle). For DIR this is the only measured set.
- OSETS: for retrievals using more than one measurement set, OSETS refers to all measurements sets except the RSET. For DIR this has no meaning.
- ASETS: this refers to all measurement sets.

Differently to L1 and L2Fit files, entry "L2 data quality flag" can also be data quality 20 (DQ20), data quality 21 (DQ21) and data quality 22 (DQ22) in addition to DQ0, DQ1, DQ2, DQ10, DQ11 and DQ12. DQ20 to DQ22 are used for unusable trace gas data. Data are unusable if ...

- ... r-code entry "Product status" says "unusable" for the respective output gas (see table 30). This is typically the case for a trace gas that is not the "primary" gas to be fitted, for which the fitting setup, especially the wavelength range, is not optimized.
- ... the synthetic reference spectrum is used, but no calibration was applied to it. This means f-code entry "Reference" starts with "Synt" (see table 26), but no slant column is listed for the respective gas in ICF entry "Slant columns in synthetic reference spectrum for FUNCFILT" (see section 5.11).

In all other aspects, DQ20 equals DQ0, DQ21 equals DQ1 and DQ22 equals DQ2. Hence DQ20 means that the measurement parameters such as temperature anomaly, noise or spectral fitting residuals are very good, but the data in general have very large biases and can therefore not be used without any further treatment.

Since L2 files are not daily files, their content changes over time. Hence differently from L1 and L2Fit files, the content of a L2 file is not "fixed" with a given L2 file name. It is not necessarily only the number of days included in the file, which changes. It is also possible, that a new calibration has been applied to the data and therefore different L2Fit files are used for the L2 file than in a previous run of BlickP. Therefore, if the user wants to compare different calibration versions of the instrument, he needs to rename the existing L2 file or move it in another directory, otherwise it will be overwritten. For official PGN data, previous versions of L2 files are stored on the server adding "disusedYYYYMMDD" to the name, where YYYYMMDD is the date of the last update to the file (`PandoraXsY_LLL_L2_rRRRRpP_disusedYYYYMMDD.txt`).

Table 39: Columns in L2 file

Column name	Remark
UT date and time for measurement center, yyyymmddThhmmssZ (ISO 8601)	"measurement center" is the center-time of RSET
Fractional days since 2000-1-1 UT midnight for measurement center	
Effective duration of measurement [s]	Duration of RSET only
Latitude for measurement center [deg], negative=South of equator, positive=North of equator, -999=no latitude retrieved	
Longitude for measurement center [deg], negative=West of Greenwich, positive=East of Greenwich, -999=no longitude retrieved	
Altitude a.s.l. for measurement center [m], -999=no altitude retrieved	
Solar zenith angle for measurement center[deg]	
Solar azimuth for measurement center [deg], 0=north, increases clockwise	
Lunar zenith angle for measurement center [deg]	
Lunar azimuth for measurement center [deg], 0=north, increases clockwise	
Pointing zenith angle for measurement center [deg]	PROF only
Pointing azimuth for measurement center [deg], 0=north, increases clockwise	PROF only
rms of unweighted spectral fitting residuals, -9=fitting not successful	DIR2: combination of rms from both fcodes, PROF: mean over rms of OSETS; this is the same for all rms-type columns (next 6 rows of this table), Equation 119
Normalized rms of spectral fitting residuals weighted with independent uncertainty, -9=fitting not successful or no uncertainty given	Equation 120
Expected rms of unweighted spectral fitting residuals based on independent uncertainty, -9=fitting not successful or no uncertainty given	Equation 121
Expected normalized rms of weighted spectral fitting residuals based on independent uncertainty, -9=fitting not successful or no uncertainty given	Equation 122
Climatological station pressure [mbar]	
Climatological station temperature [K]	PROF only
Climatological effective O2 height [km]	PROF only
Climatological effective O2O2 height [km]	PROF only
Climatological surface O2 concentration [molc/cm3]	PROF only
Climatological surface O2O2 concentration [molc2/cm6]	PROF only
Climatological total O2 column [molc/cm2]	PROF only
Climatological total O2O2 column [molc2/cm5]	PROF only

Column name	Remark
Data processing type index	See table 7
Calibration file version	The version of the ICF used for this retrieval
Calibration file validity starting date	The validity date of the ICF used for this retrieval in form YYYYMMDD
Mean value of measured data inside fitting window [same units as measurements]	As in L2Fit, mean over ASETS
Wavelength effective temperature [°C], 999=no effective temperature given	Mean over ASETS
Estimated average residual stray light level [%] (only valid for stray light correction methods 2 and higher)	Mean over ASETS
Retrieved wavelength shift from L1 data [nm], -9=no wavelength change determination	Mean over OSETS
Retrieved wavelength shift from spectral fitting [nm], -9=no wavelength change fitting	Mean over OSETS
Integration time [ms]	For RSET
Number of bright count cycles	For RSET
Effective position of filterwheel #1, 0=filterwheel not used, 1-9 are valid positions	For RSET
Effective position of filterwheel #2, 0=filterwheel not used, 1-9 are valid positions	For RSET
Atmospheric variability [%], 999=no atmospheric variability was determined	As in L2Fit, mean over ASETS
L1 data quality flag: 0=assured high quality, 1=assured medium quality, 2=assured low quality, 10=not-assured high quality, 11=not-assured medium quality, 12=not-assured low quality	PROF: maximum of ASETS, DIR2: maximum of fcodes
Sum over 2^i using those i, for which the corresponding L1 data quality parameter exceeds the DQ1 limit, 0=Saturated data, 1=Too few dark counts measurements, 2=No temperature given or effective temperature too different from the reference temperature, 3=Dark count too high, 4=Unsuccessful dark background fitting, 5=Absolute value of estimated average residual stray light level too high, 6=Although attempted, no wavelength change could be retrieved, 7=Retrieved wavelength shift too large, 8=Retrieved wavelength shift differs too much from the shift predicted by the effective temperature	PROF: maximum of ASETS, DIR2: maximum of fcodes
Sum over 2^i using those i, for which the corresponding L1 data quality parameter exceeds the DQ2 limit (same parameters as for DQ1)	PROF: maximum of ASETS, DIR2: maximum of fcodes
L2Fit data quality flag: 0=assured high quality, 1=assured medium quality, 2=assured low quality, 10=not-assured high quality, 11=not-assured medium quality, 12=not-assured low quality	PROF: maximum of OSETS, DIR2: maximum of fcodes
Sum over 2^i using those i, for which the corresponding data quality parameter exceeds the DQ1 limit, 0=L1 data quality above 0, 1=Spectral fitting was not successful, 2=Weighted rms of spectral fitting too large, 3=Wavelength shift too large	PROF: maximum of OSETS, DIR2: maximum of fcodes
Sum over 2^i using those i, for which the corresponding data quality parameter exceeds the DQ2 limit (same parameters as for DQ1)	PROF: maximum of OSETS, DIR2: maximum of fcodes

Column name	Remark
L2 data quality flag for GAS: 0=assured high quality, 1=assured medium quality, 2=assured low quality, 10=not-assured high quality, 11=not-assured medium quality, 12=not-assured low quality, 20=unusable high quality, 21=unusable medium quality, 22=unusable low quality	GAS is an absorber from table 22
Sum over 2^i using those i, for which the corresponding L2 data quality parameter for GAS exceeds the DQ1 limit, 0=L2Fit data quality above 0, 1=Uncertainty too high, 2=Signal to noise ratio too low, 3=Air mass factor too large	See table 31
Sum over 2^i using those i, for which the corresponding L2 data quality parameter for GAS exceeds the DQ2 limit (same parameters as for DQ1)	See table 31
GAS total vertical column amount [GASUNIT], -9e99=retrieval not successful	DIR only, GASUNIT is the unit for GAS used by the BSS
Independent uncertainty of GAS total vertical column amount [GASUNIT], -1=cross section is zero in this wavelength range, -3=spectral fitting was done, but no independent uncertainty could be retrieved, -5=no independent uncertainty input was given, -9=spectral fitting was not successful	DIR only, see section 6.3.6
Structured uncertainty of GAS total vertical column amount [GASUNIT], -1=cross section is zero in this wavelength range, -9=spectral fitting was not successful	DIR only, see section 6.3.6
Common uncertainty of GAS total vertical column amount [GASUNIT], -1=cross section is zero in this wavelength range, -6=no common uncertainty input was given, -9=spectral fitting was not successful	DIR only, see section 6.3.6
Total uncertainty of GAS total vertical column amount [GASUNIT], -1=cross section is zero in this wavelength range, -3=spectral fitting was done, but no independent uncertainty could be retrieved, -5=no independent uncertainty input was given, -6=no common uncertainty input was given, -9=spectral fitting was not successful	DIR only, see section 6.3.6
rms-based uncertainty of GAS total vertical column amount [GASUNIT], -1=cross section is zero in this wavelength range, -3=spectral fitting was done, but no independent uncertainty could be retrieved, -9=spectral fitting was not successful	DIR only, see section 6.3.6
GAS effective temperature [K]	DIR only
Independent uncertainty of GAS effective temperature [K], -1=temperature fitting was requested, but cross section is zero in this wavelength range, -2=no temperature fitting was requested and output for effective temperature and common uncertainty of it is based on f-code, -3=spectral fitting was done, but no independent uncertainty could be retrieved, -4=temperature fitting was requested, but differential optical depth is too small to retrieve temperature, -5=spectral fitting was done without using the independent uncertainty input, -6=no independent uncertainty input was given, -9=spectral fitting was not successful	DIR only, see section 6.3.6
Structured uncertainty of GAS effective temperature [K], -1=temperature fitting was requested, but cross section is zero in this wavelength range, -4=temperature fitting was requested, but differential optical depth is too small to retrieve temperature, -9=spectral fitting was not successful	DIR only, see section 6.3.6

Column name	Remark
Common uncertainty of GAS effective temperature [K], -1=temperature fitting was requested, but cross section is zero in this wavelength range, -2=no temperature fitting was requested and output for effective temperature and common uncertainty of it is based on f-code, -3=spectral fitting was done, but no independent uncertainty could be retrieved, -4=temperature fitting was requested, but differential optical depth is too small to retrieve temperature, -6=no independent uncertainty input was given, -9=spectral fitting was not successful	DIR only, see section 6.3.6
Total uncertainty of GAS effective temperature [K], -1=temperature fitting was requested, but cross section is zero in this wavelength range, -2=no temperature fitting was requested and output for effective temperature and common uncertainty of it is based on f-code, -3=spectral fitting was done, but no independent uncertainty could be retrieved, -4=temperature fitting was requested, but differential optical depth is too small to retrieve temperature, -5=spectral fitting was done without using the independent uncertainty input, -6=no independent uncertainty or common uncertainty input was given, -9=spectral fitting was not successful	DIR only, see section 6.3.6
rms-based uncertainty of GAS effective temperature [K],-1=temperature fitting was requested, but cross section is zero in this wavelength range, -2=no temperature fitting was requested and output for effective temperature and common uncertainty of it is based on f-code, -4=temperature fitting was requested, but differential optical depth is too small to retrieve temperature, -9=spectral fitting was not successful	DIR only and only if temperature-fit is requested in fcode, see section 6.3.6
Direct GAS air mass factor	DIR only, Direct moon air mass factor (AMF) for direct moon data, direct sun AMF otherwise, see equation 129
Uncertainty of direct GAS air mass factor	DIR only, based on the uncertainty of the effective height (see also section 6.6)
Diffuse correction applied before fitting at effective fitting wavelength for GAS [%], 0=no diffuse correction applied or fitting not done or not successful, >0=measured diffuse correction, <0=(negative value of) calculated diffuse correction	DIR only
GAS surface concentration [ppb], -9e99=retrieval not successful	PROF only, see section 6.7.4
Independent uncertainty of GAS surface concentration [ppb], -6=no surface concentration was retrieved since the maximum viewing zenith angle was below 87deg, -7=uncertainty could not be retrieved since slant column uncertainties were missing	PROF only, see section 6.7.4
GAS surface concentration index, 1=Fully mixed case from extrapolation to horizon, 2=Fully mixed case from largest pointing zenith angle, 3=Heterogeneous case from extrapolation to horizon, 4=Heterogeneous case from largest pointing zenith angle, -8=retrieval not successful	PROF only, see section 6.7.4
GAS heterogeneity flag, 0=well mixed conditions, 1=heterogeneous conditions, -8=retrieval not successful	PROF only, see section 6.7.4

Column name	Remark
Climatological GAS stratospheric column amount [GASUNIT]	Only if a climatology for GAS exists
GAS tropospheric vertical column amount [GASUNIT], -9e99=retrieval not successful	PROF: retrieved amount, DIR: estimated amount in case the effective temperature was fitted
Independent uncertainty of GAS tropospheric vertical column amount [GASUNIT], -5=tropospheric column was estimated from direct sun measurements using effective temperature and stratospheric climatology, -7=uncertainty could not be retrieved since slant column uncertainties were missing	See section 6.3.6
Maximum horizontal distance for GAS tropospheric column [km]	PROF only, Equation XXX
Maximum vertical distance for GAS tropospheric column [km]	PROF only, Equation XXX
Top height of GAS layer ILAY [km], -9e99=retrieval not successful	PROF only, ILAY is the layer number; layer 1 starts at the surface and ends at the given top height, higher layers start at the top height of the next lower layer
Partial GAS vertical column amount in layer ILAY [GASUNIT], -9e99=retrieval not successful	PROF only
Independent uncertainty of partial GAS vertical column amount in layer ILAY [GASUNIT], -6=no profile was retrieved since the maximum viewing zenith angle was below 87deg, -8=no uncertainty retrieval implemented yet	PROF only, see section 6.3.6
Top height of aerosol layer ILAY related to GAS [km], -9e99=retrieval not successful	PROF only
Partial aerosol optical depth in layer ILAY related to GAS, -9e99=retrieval not successful	PROF only
Independent uncertainty of partial aerosol optical depth in layer ILAY related to GAS, -6=no profile was retrieved since the maximum viewing zenith angle was below 87deg, -8=no uncertainty retrieval implemented yet	PROF only, see section 6.3.6

5.15 Log Files

BlickO, BlickP and BlickF create log-files, which report specific information, warnings, errors or general information. Those files are in directories `/log/oslog`, `/log/pslog` and `/log/fslog` respectively.

BlickO log files

They are called `PandoraX_LLL_YYYYMMDD_NNNlog.txt`. X is the instrument number, LLL the Short Location Name (see section 5.2), YYYYMMDD is the UT-date for the time of the local noon and NNN can be "info", "warning" or "error" for the info-file, warning-file and error-file respectively. The info-file includes information, warnings and errors. The warning-file includes warnings and errors. The error-file only includes errors. Hence the warning-file is a subset of the info-file and the error-file a subset of the warning-file. Each line in the log-file looks like this example:

```
[Thu 18 Dec 2014, 10:24:47.722] [INFO] [Connected spectrometer 1]
```

It starts with the UT-time, then the error-level, which can be "INFO, "WARNING" or "ERROR" and finally the content of the message. Note that most log-entries are also added to the L0-files, especially all warnings and errors.

BlickF log files
The actual BlickF log-file is called `BlickF_log.txt`. Once the log file has reached 5000 lines, it is renamed to `BlickF_logYYYYMMDDThhmmssZ.txt`, where the time of the last entry in the file is added to the filename. The actual log file is then started with zero lines. The BlickF log-files include all the messages written by BlickF on the command window (see figure 5), except the lines saying 'No action taken', for example:

```
Sat 16 Jan 2016, 08:45:20, Initiated new data pushing to remote server; 2
files still to be pushed (OF=01)
```

BlickP log files
The actual BlickP log-file is called `BlickP.log`. Once the log file has reached 5000 lines, it is renamed to `BlickP_YYYYMMDDThhmmssZ.log`, where the time of the last entry in the file is added to the filename. The actual log file is then started with zero lines. The BlickP log-files include all the messages written by BlickP on the command window. Below are some sample lines. Each line starts with the date and time, followed by INFO, WARNING or ERROR, then in parenthesis the module, from which it is called, and finally the log-message.

```
[2017-01-12 13:25:55,237] INFO(blickp):  BlickP starting up
[2017-01-12 13:25:55,239] INFO(blickp):  Reading configuration
[2017-01-12 13:25:55,278] INFO(blickp):  Processing day:  2016/05/10
[2017-01-12 13:25:55,918] INFO(blickp.l2fitprocessor):  Processing
L1-File:  Pandora110s1_IBK_20160510_L1_sNWLCc3p1-2.txt with F-Code OORI
```

5.16 Alignment Files

BlickO creates so-called alignment files in directory `/data/alignments`. These files are needed to determine the position of the Pandora unit at the current location in order to ensure correct pointing of the system. For more details on the alignment see section 6.1.

The alignment file is called `PandoraX_LLL_alignments.txt`. X is the instrument number and LLL is the Short Location Name (see section 5.2). It is an ASCII-text file with a header, which includes meta data and a description of the data columns, and the "alignment lines". A new line is written each time a successful sun search has been performed.

Each alignment line has $4*n_{SPEC}+4$ entries, where n_{SPEC} is the number of spectrometers in the Pandora system. An alignment line for a system with two spectrometers looks like this example:

```
20141218T112919Z FS 65.72 196.23 65.78 196.25 0.027 1362.33 65.74 196.16
0.027 1362.33
```

After the UT-time (column 1) and the name of the routine used (column 2), there are the "true" solar (or lunar) zenith angle (column 3) and azimuth (column 4). Those true angles are calculated based on time and location using the formulation of *Jensen et al.* [20].

Then there are groups of 4 columns, one for each spectrometer. The first two columns in the group are the

"apparent" solar (or lunar) zenith angle and azimuth respectively for this spectrometer. These are the angles, in which the instrument observed the sun (or moon). The 3rd column in the group is the rms of the field of view fitting for this alignment line for this spectrometer. The 4th column in the group finally is the weighting factor for this alignment line for this spectrometer.

Note that only a maximum of 5000 alignment lines are stored in the alignment file. If this number is exceeded then two things are happening:

1) The alignment file is reduced to the last 5000 entries.

2) The earlier alignments are stored in a "historic alignment file", which is called `PandoraX_LLL_alignments_YYYYMMDDTHHMMSSZ.txt`, where YYYYMMDDTHHMMSSZ is the UT-time of the file creation in ISO 8601 format.

6 Algorithms Theoretical Basis

The Blick Software Suite includes different algorithms for instrument operation and data production, which are described in this section. All Blick Software Suite data production algorithms have several characteristics in common:

- No actual external data are used, i.e. only measurements from Pandora itself and some climatological parameters (see e.g. section 6.8).
- Only data from one single routine (measurement sequence) are used. This means the algorithms can be applied in real time directly after the measurement sequence is finished.
- No radiative transfer calculations (RTC) or iterative convolution processes are performed and consequently the algorithms are very fast.
- No special software license is required and the source code is provided with the standard installation of the Blick Software Suite.

We envision that the number of algorithms being developed for the PGN will grow over time. If any new algorithm fulfills all the criteria listed above, it might be added to the Blick Software Suite. Otherwise it will be considered an "offline algorithm". Offline algorithms may be written in a language other than Python, may require licenses, may include RTC, etc. We believe that e.g. for a very sophisticated ozone profile algorithm, one will likely need to analyze all the measurements from an entire day together as a group and also do RTC, therefore this will probably be an offline algorithm.

6.1 Alignment Algorithm

This section describes the theoretical background (section 6.1.1) and the practical implementation (section 6.1.2) of the Pandora alignment. It also addresses the problem of different FOVs for sun and sky observations and the situation for Pandora units with more than one spectrometer (section 6.1.3).

6.1.1 Theoretical Background

After proper installation of Pandora (at a Northern Hemisphere location) and after a tracker reset, the entrance window of the head sensor should look to the zenith and the head sensor should be at the East of the shaft holding the tracker as shown in figure 9.

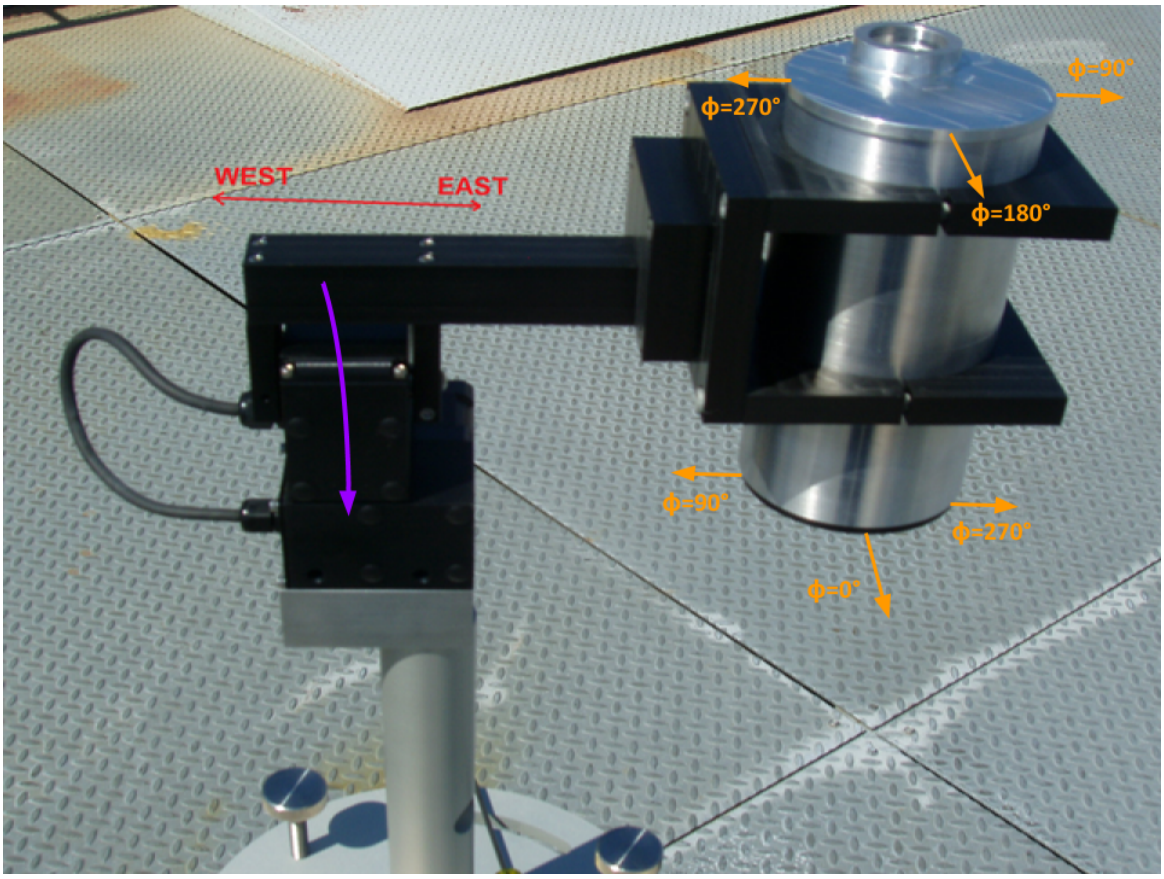


Figure 9: Head sensor position after tracker reset. The purple arrow indicates the direction in which the zenith motor moves.

If we assume that everything is perfectly aligned, i.e. the tracker base plate is perfectly leveled and rotated in the right direction, the tracker's zenith and azimuth motions are perfectly perpendicular to each other and the optical axis inside the head sensor is perfectly parallel to the axis of the zenith motion, then Pandora is in the so-called "horizontal reference frame" (figure 10, left panel). The x-axis goes from South (negative x) to North (positive x), the y-axis goes from East (negative y) to West (positive y) and the z-axis goes from Nadir (negative z) to Zenith (positive z).

To describe a point P in the reference frame (the arrow in the left panel of figure 10, which represents the optical axis of the head sensor), we use Cartesian or spherical coordinates. In the Cartesian system P is characterized by (x,y,z), where x, y and z are the projections of P to the x-, y- and z-axis respectively. In the spherical system P is described by (ρ,θ,φ), where ρ is the distance from the origin, θ is the zenith angle (between 0° and 180°), measured from the positive z-axis, and φ is the azimuth (between 0° and 360°), measured from the positive x-axis to the projection of P on the x-y-plane, clockwise when looking from the zenith to the origin. Note that this definition of φ is different from the standard spherical coordinate convention, where φ is taken counterclockwise. So in our definition φ=0° is North, φ=90° East, φ=180° South and φ=270° West.

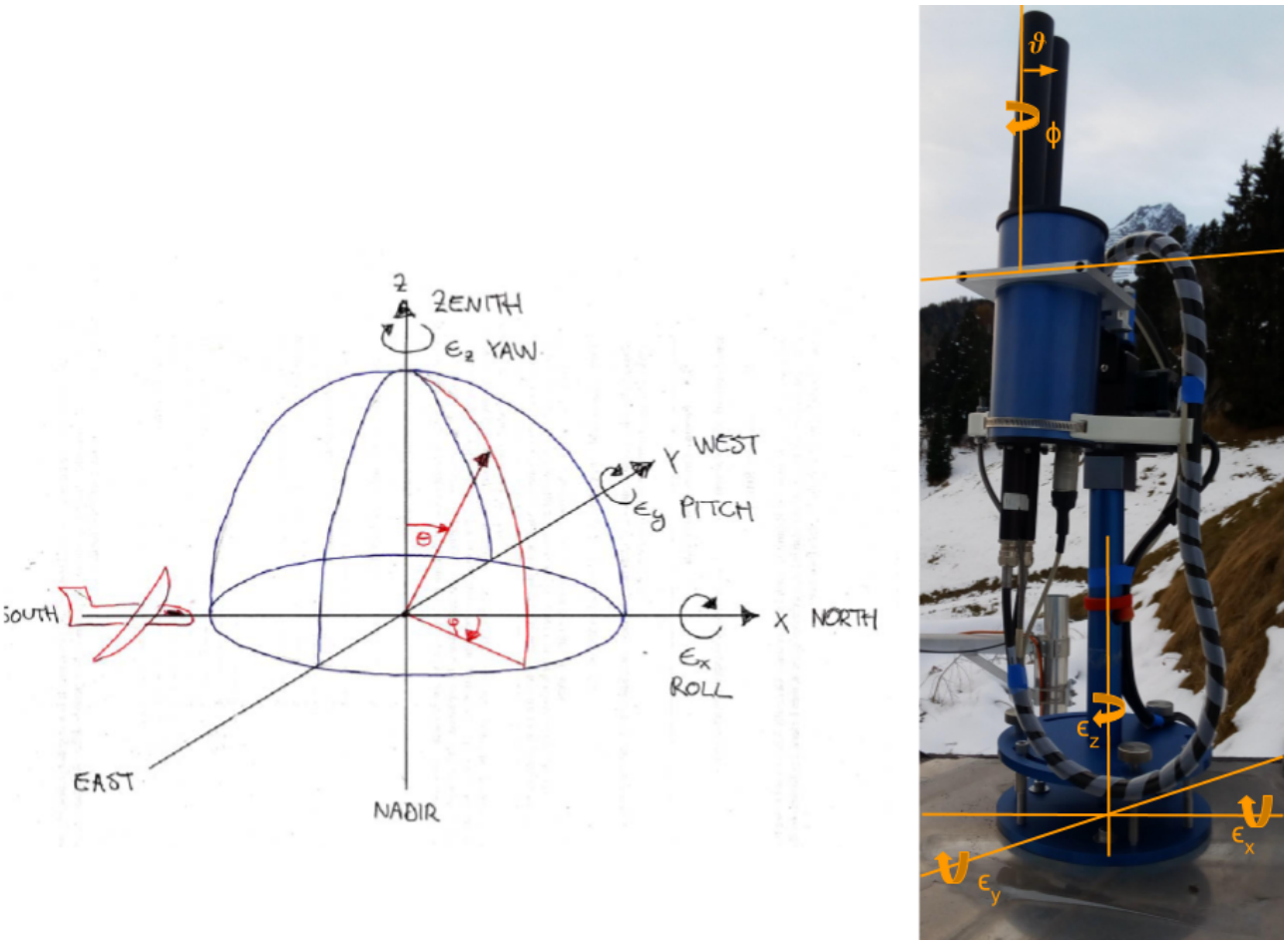


Figure 10: Horizontal frame and leveling angles

Using this definition, the conversion from spherical to Cartesian coordinates is given in equation 18.

$$\begin{aligned} \mathrm{x} &= \rho \cdot \sin\theta \cdot \cos\varphi \\ \mathrm{y} &= -\rho \cdot \sin\theta \cdot \sin\varphi \\ \mathrm{z} &= \rho \cdot \cos\theta \end{aligned} \tag{18}$$

The conversion from Cartesian to spherical coordinates is given in equation 19.

$$\begin{aligned} \rho &= \sqrt{\mathrm{x}^2 + \mathrm{y}^2 + \mathrm{z}^2} \\ \theta &= \arccos\left(\frac{\mathrm{z}}{\sqrt{\mathrm{x}^2 + \mathrm{y}^2 + \mathrm{z}^2}}\right) \\ \varphi &= \begin{cases} \arccos\left(\frac{\mathrm{x}}{\sqrt{\mathrm{x}^2+\mathrm{y}^2}}\right) & \text{if } \mathrm{y} \leq 0 \\ 2\pi - \arccos\left(\frac{\mathrm{x}}{\sqrt{\mathrm{x}^2+\mathrm{y}^2}}\right) & \text{if } \mathrm{y} > 0 \end{cases} \end{aligned} \tag{19}$$

Since in this context we always deal with "directions" rather than "points", ρ equals 1 in all situations and all vectors P introduced are unit vectors.

In practice it is very difficult to have a perfectly aligned instrument. The base plate of the tracker is in general misaligned, i.e. rotated relative to the horizontal reference frame. To describe this we introduce the "tracker reference system", where the x-y-plane is the plane defined by the tracker azimuth motion and the z-axis is simply perpendicular to this plane.

Assume we have the coordinates of a point P_T in the tracker frame. In order to obtain the coordinates of the same point in the horizontal frame P_H, we have to apply a full rotation on vector P_T. A full rotation can be described as a sequence of 3 rotations around the x-, y- and z-axis for angles ϵ_x, ϵ_y and ϵ_z respectively (see figure 10). A positive angle corresponds to a clockwise rotation of the respective axis, when looking from the positive axis towards the origin. Note that in the horizontal reference frame ϵ_x, ϵ_y and ϵ_z correspond to roll, pitch and yaw of an airplane flying along the x-axis to increasing values (from South to North, see figure 10). ϵ_x and ϵ_y are also called West-East correction and North-South correction respectively and ϵ_z is also called Azimuth correction. Equation 20 gives the relationship of P_T and P_H:

$$\mathrm{P}_H = \mathrm{R}_z(\epsilon_z) \cdot \mathrm{R}_y(\epsilon_y) \cdot \mathrm{R}_x(\epsilon_x) \cdot \mathrm{P}_T = \mathrm{R}(\epsilon_x, \epsilon_y, \epsilon_z) \cdot \mathrm{P}_T \tag{20}$$

P_H and P_T are the 3x1-elements vectors with the Cartesian coordinates of the point. R_x, R_y and R_z are 3x3-elements rotation matrices defined in equation 21.

$$\begin{aligned}
\mathrm{R}_x(\epsilon_x) &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\epsilon_x & \sin\epsilon_x \\ 0 & -\sin\epsilon_x & \cos\epsilon_x \end{pmatrix} \\
\mathrm{R}_y(\epsilon_y) &= \begin{pmatrix} \cos\epsilon_y & 0 & -\sin\epsilon_y \\ 0 & 1 & 0 \\ \sin\epsilon_y & 0 & \cos\epsilon_y \end{pmatrix} \\
\mathrm{R}_z(\epsilon_z) &= \begin{pmatrix} \cos\epsilon_z & \sin\epsilon_z & 0 \\ -\sin\epsilon_z & \cos\epsilon_z & 0 \\ 0 & 0 & 1 \end{pmatrix}
\end{aligned} \tag{21}$$

R is simply the product of the 3 matrices (in this order!). So given a point in the tracker frame P_T and knowing the leveling angles ϵ_x, ϵ_y and ϵ_z, we can calculate the coordinates of this point in the horizontal frame P_H. For the opposite, i.e. getting P_T when having P_H, we have to invert equation 20.

$$\mathrm{P}_T = \mathrm{R}^{-1}(\epsilon_x, \epsilon_y, \epsilon_z) \cdot \mathrm{P}_H = \mathrm{R}_x(-\epsilon_x) \cdot \mathrm{R}_y(-\epsilon_y) \cdot \mathrm{R}_z(-\epsilon_z) \cdot \mathrm{P}_H \tag{22}$$

Hence if the optical axis inside the head sensor is perfectly parallel to the axis of the zenith motion or, in other words, after a tracker reset, the instrument's optical axis equals the z-axis of the tracker frame (i.e. the head sensor is not slightly tilted inside its mounting bracket; see figure 9), then we can fully describe the alignment of the instrument by the 3 "leveling" angles ϵ_x, ϵ_y and ϵ_z.

However in practice the instrument's optical axis after a tracker reset is not exactly parallel to the z-axis. It is in general tilted relative to the z-axis. Here we assume the direction of the optical axis after the tracker reset is characterized by zenith angle ϑ and azimuth ϕ (see figure 10, right panel). The "direction" of ϕ is shown in with orange arrows in figure 9. For ϑ>0°, ϕ=0° (90°, 180°, 270°) means that the head sensor is tilted in a way, that after a reset the instrument looks slightly towards North (East, South, West).

Then the position of the optical axis after a zenith motion of θ and an azimuth motion of φ in the tracker reference frame is given by equation 23.

$$\mathrm{P}_T = \mathrm{R}_z(\varphi) \cdot \mathrm{R}_y(-\theta) \cdot \mathrm{R}_z(\phi) \cdot \mathrm{R}_y(-\vartheta) \cdot \mathrm{e}_z = \mathrm{R}(0, -\theta, \varphi) \cdot \mathrm{R}(0, -\vartheta, \phi) \cdot \mathrm{e}_z = \mathrm{R}(0, -\theta, \varphi) \cdot \mathrm{P}_{0\mathrm{AXT}} \tag{23}$$

e_z is the 3x1-elements z-axis-unit-vector (0,0,1). Applying R(0,-ϑ,ϕ) on e_z gives the 3x1-elements vector P_{0AXT}, the direction of the optical axis after the tracker reset. Then applying R(0,-θ,φ) on P_{0AXT} gives P_T, the direction of the optical axis after having moved the zenith motor for θ and the azimuth motor for φ. So given the zenith and azimuth motion angles θ and φ and knowing the position of the optical axis after the tracker reset relative to the z-axes ϑ and ϕ we can calculate the coordinates of the optical axis in the tracker frame P_T. For the opposite, i.e. getting θ and φ when having P_T, we have to invert equation 23, which is not so easy, but can be done.

Combining equations 20 and 23, we obtain P_H as a function of θ, φ, ϵ_x, ϵ_y, ϵ_z, ϑ and ϕ.

$$P_H(\theta, \varphi, \epsilon_x, \epsilon_y, \epsilon_z, \vartheta, \phi) = R(\epsilon_x, \epsilon_y, \epsilon_z) \cdot R(0, -\theta, \varphi) \cdot R(0, -\vartheta, \phi) \cdot e_z \tag{24}$$

So once we have the full set of leveling angles ϵ_x, ϵ_y, ϵ_z, ϑ and ϕ, we can calculate the "true" pointing in the horizontal reference frame P_H for each pair of tracker motion angles θ and φ. And, using the inversion of equation 24, we can calculate the motion angles θ and φ of the tracker needed to point the instrument as close as possible to the absolute position P_H.

Note that it can happen that a "requested" absolute position P_H is not exactly reached. E.g. how close the instrument can point to the zenith depends on the values of ϑ and ϕ (see figure 9). If ϵ_x=ϵ_y=ϵ_z=0°, the minimum zenith angle reached by the instrument, ZA_{min}, is given by equation 25:

$$ZA_{min} = \vartheta \cdot \sin\phi \tag{25}$$

Hence if ϕ=0° or 180°, then the instrument can point exactly to the zenith, even if ϑ>0°, since this offset can be corrected by a motion of the zenith motor. However, for any other values of ϕ, the zenith cannot be reached if ϑ>0°. In the extreme case of ϕ=90° or 270°, the closest the instrument can point to the zenith is exactly ϑ away.

On the other hand there might also be more than one solution for the motion angles that make the instrument point exactly to P_H. E.g. if all leveling angles are zero, any azimuth motion φ will point the instrument in the same direction (zenith), if θ=0°.

6.1.2 Practical Implementation

The Pandora software executes so-called "sun-searches" in a certain frequency over the day (usually every 15 min during the initial days after instrument installation and less frequently afterwards). During a sun-search the instrument moves to the "true" solar position based on astronomical calculations and the geographical coordinates of the location [20], then it scans the sky in zenith direction ("up-down") and in azimuth direction ("left-right") and looks for the position of maximum signal. This position is saved as the "apparent" solar position (see section 5.16). An example for such a sun search is shown in figure 11.

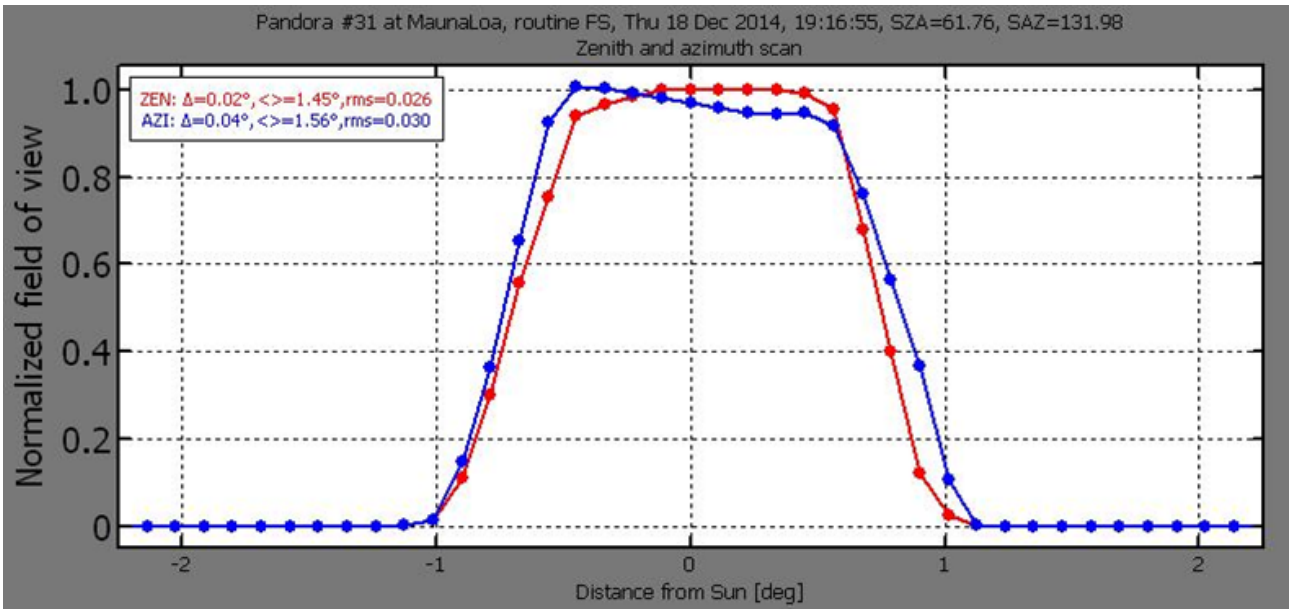


Figure 11: Sun search for Pandora #31 at Mauna Loa on 18 Dec 2014. Red line is the sun scan in zenith direction ("up-down") and blue line in azimuth direction ("left-right"). In this case the apparent angles differ from the true angles by 0.02° in zenith and 0.04° in azimuth.

After a successful sun-search we can calculate angles (θ_H,φ_H), which correspond to point P_H, the position of the sun in the horizontal reference frame, and we have measured angles (θ_T,φ_T), the tracker motion angles of the maximum signal, which correspond to θ and φ in equation 24. Now we try to solve equation 24 with given θ_H, φ_H, θ_T and φ_T to obtain the leveling angles. The technique BlickO uses is based on a linearization of equation 24 and iterations to find the solution. Equation 26 shows the first order approximations of the rotation matrices from equation 21 at position ϵ+$\Delta\epsilon$:

$$
\begin{aligned}
\mathrm{R}_x(\epsilon+\Delta\epsilon) &\approx \begin{pmatrix} 1 & 0 & 0 \\ 0 & cos\epsilon & sin\epsilon \\ 0 & -sin\epsilon & cos\epsilon \end{pmatrix} + \Delta\epsilon \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & -sin\epsilon & -cos\epsilon \\ 0 & cos\epsilon & -sin\epsilon \end{pmatrix} = \mathrm{R}_x(\epsilon) + \Delta\epsilon \cdot \mathrm{V}_x(\epsilon) \\
\mathrm{R}_y(\epsilon+\Delta\epsilon) &\approx \begin{pmatrix} cos\epsilon & 0 & -sin\epsilon \\ 0 & 1 & 0 \\ sin\epsilon & 0 & cos\epsilon \end{pmatrix} + \Delta\epsilon \cdot \begin{pmatrix} -sin\epsilon & 0 & cos\epsilon \\ 0 & 1 & 0 \\ -cos\epsilon & 0 & -sin\epsilon \end{pmatrix} = \mathrm{R}_y(\epsilon) + \Delta\epsilon \cdot \mathrm{V}_y(\epsilon) \\
\mathrm{R}_z(\epsilon+\Delta\epsilon) &\approx \begin{pmatrix} cos\epsilon & sin\epsilon & 0 \\ -sin\epsilon & cos\epsilon & 0 \\ 0 & 0 & 1 \end{pmatrix} + \Delta\epsilon \cdot \begin{pmatrix} -sin\epsilon & -cos\epsilon & 0 \\ cos\epsilon & -sin\epsilon & 0 \\ 0 & 0 & 1 \end{pmatrix} = \mathrm{R}_z(\epsilon) + \Delta\epsilon \cdot \mathrm{V}_z(\epsilon)
\end{aligned}
\tag{26}
$$

The 3-3-elements matrices V_x, V_y and V_z are the first derivatives of the rotation matrices in ϵ. Using equation 26 we can linearize equation 24 at position θ, φ, ϵ_x+$\Delta\epsilon_x$, ϵ_y+$\Delta\epsilon_y$, ϵ_z+$\Delta\epsilon_z$, ϑ+$\Delta\vartheta$ and ϕ+$\Delta\phi$.

$$\begin{aligned}
\mathrm{P}_H \approx\ & \mathrm{R}_z(\epsilon_z)\cdot\mathrm{R}_y(\epsilon_y)\cdot\mathrm{R}_x(\epsilon_x)\cdot\mathrm{R}(0,-\theta,\varphi)\cdot\mathrm{R}_z(\phi)\cdot\mathrm{R}_y(-\vartheta)\cdot\mathrm{e}_z \\
&+\Delta\epsilon_x\cdot\mathrm{R}_z(\epsilon_z)\cdot\mathrm{R}_y(\epsilon_y)\cdot\mathrm{V}_x(\epsilon_x)\cdot\mathrm{R}(0,-\theta,\varphi)\cdot\mathrm{R}_z(\phi)\cdot\mathrm{R}_y(-\vartheta)\cdot\mathrm{e}_z \\
&+\Delta\epsilon_y\cdot\mathrm{R}_z(\epsilon_z)\cdot\mathrm{V}_y(\epsilon_y)\cdot\mathrm{R}_x(\epsilon_x)\cdot\mathrm{R}(0,-\theta,\varphi)\cdot\mathrm{R}_z(\phi)\cdot\mathrm{R}_y(-\vartheta)\cdot\mathrm{e}_z \\
&+\Delta\epsilon_z\cdot\mathrm{V}_z(\epsilon_z)\cdot\mathrm{R}_y(\epsilon_y)\cdot\mathrm{R}_x(\epsilon_x)\cdot\mathrm{R}(0,-\theta,\varphi)\cdot\mathrm{R}_z(\phi)\cdot\mathrm{R}_y(-\vartheta)\cdot\mathrm{e}_z \\
&+\Delta\vartheta\cdot\mathrm{R}_z(\epsilon_z)\cdot\mathrm{R}_y(\epsilon_y)\cdot\mathrm{R}_x(\epsilon_x)\cdot\mathrm{R}(0,-\theta,\varphi)\cdot\mathrm{R}_z(\phi)\cdot\mathrm{V}_y(-\vartheta)\cdot\mathrm{e}_z \\
&+\Delta\phi\cdot\mathrm{R}_z(\epsilon_z)\cdot\mathrm{R}_y(\epsilon_y)\cdot\mathrm{R}_x(\epsilon_x)\cdot\mathrm{R}(0,-\theta,\varphi)\cdot\mathrm{V}_z(\phi)\cdot\mathrm{R}_y(-\vartheta)\cdot\mathrm{e}_z
\end{aligned} \tag{27}$$

$$\mathrm{P}_H \approx \mathrm{P} + \Delta\epsilon_x\cdot\mathrm{C}_x + \Delta\epsilon_y\cdot\mathrm{C}_y + \Delta\epsilon_z\cdot\mathrm{C}_z + \Delta\vartheta\cdot\mathrm{C}_\vartheta + \Delta\phi\cdot\mathrm{C}_\phi$$

All C_x, C_y, etc. in equation 27 are 3x1-element vectors. Rearranging 27 we obtain a system of linear equations:

$$\mathrm{P}_H - \mathrm{P} = \Delta\mathrm{P} = \begin{pmatrix} \mathrm{C}_{xx} & \mathrm{C}_{yx} & \mathrm{C}_{zx} & \mathrm{C}_{\vartheta x} & \mathrm{C}_{\phi x} \\ \mathrm{C}_{xy} & \mathrm{C}_{yy} & \mathrm{C}_{zy} & \mathrm{C}_{\vartheta y} & \mathrm{C}_{\phi y} \\ \mathrm{C}_{xz} & \mathrm{C}_{yz} & \mathrm{C}_{zz} & \mathrm{C}_{\vartheta z} & \mathrm{C}_{\phi z} \end{pmatrix} \cdot \begin{pmatrix} \Delta\epsilon_x \\ \Delta\epsilon_y \\ \Delta\epsilon_z \\ \Delta\vartheta \\ \Delta\phi \end{pmatrix} = \mathrm{C}\cdot\Delta\epsilon \tag{28}$$

Equation 28 cannot be solved in a unique way, since the rank of matrix C is 2, which means there are only 2 independent columns in it. Or in other words we can make many possible choices for the leveling angles that fulfill equation 28. This makes sense, since we are trying to get 5 pieces of information out of equation 28, while putting only 2 pieces of information in. Nevertheless if we combine the results of several sun searches we can add them up and obtain equation 29.

$$\Delta\mathrm{P} = \begin{pmatrix} \Delta\mathrm{P}_1 \\ \Delta\mathrm{P}_2 \\ \ldots \\ \Delta\mathrm{P}_N \end{pmatrix} = \begin{pmatrix} \mathrm{C}_1 \\ \mathrm{C}_2 \\ \ldots \\ \mathrm{C}_N \end{pmatrix} \cdot \Delta\epsilon = \mathrm{C}\cdot\Delta\epsilon \tag{29}$$

N is the number of sun searches used, ΔP is a 3Nx1-elements vector and C is a 3Nx5-elements matrix. For N>2 equation 29 is an overdetermined system of linear equations, which we can solve in a least squares sense with the pseudo-inverse matrix.

$$\Delta\epsilon = [\mathrm{C}^T\cdot\mathrm{C}]^{-1}\cdot\mathrm{C}^T\cdot\Delta\mathrm{P} = pinv(\mathrm{C})\cdot\Delta\mathrm{P} \tag{30}$$

This is how BlickO determines the leveling of the instrument in an iterative process:

1. Read the results of the successful sun searches from the alignments file (see section 5.16).
2. Take a first guess for the leveling angles. At the very beginning the first guess is ϵ(i=0)=(0,0,0,0,0). When a previous determination of the leveling had been done, then this is used as first guess.
3. Calculate ΔP and C using ϵ(i) and the sun search results as in equation 29.
4. Calculate the "cost-function", which is the sum-of-squares over ΔP.
5. Get $\Delta\epsilon$(i) from equation 30.
6. Get the next guess for the leveling angles ϵ(i+1)=ϵ(i)+$\Delta\epsilon$(i).
7. Repeat steps 3 to 6 until the cost function calculated in step 4 changes below a certain tolerance (in BlickO set to 1e-5).

This method usually reaches a solution within a few (<10) iterations and lasts less than 0.2 s. It is possible, that no solution is found and an error message appears saying "Could not calculate leveling angles". This means that the different sun-search results are not mathematically compatible to each other. The reason for this is usually that the instrument has been moved or the tracker has slipped. In such a case the operator needs to investigate the problem in detail.

The more sun search results are available, the better. However, it is even more important that the sun searches are spread over a large range of zenith angles and azimuths. I.e. 3 sun search, one from the morning, one from noon and one from evening, work better than 10 sun searches measured within 10 min. Therefore we recommend to run an instrument, which has been installed at a new location, for about one day in schedule "align", which focuses on sun searches (see section 4.2). In principle one could also use moon searches to improve the instrument alignment, but we do not do this for two reasons:

1. The accuracy of the formulas to calculate the lunar position is 0.14° and comparable to our tracking accuracy, while for the solar position it is 0.02° [20].

2. When the moon is not entirely full, the moon search gives a small offset, since the illuminated area is not centered around the center of the moon.

A special case is when only one sun search is available (as in equation 28). Then BlickO puts some constraints on the leveling angles. It sets ϑ=0 and ϕ=0 and fixes the relationship between ϵ_x and ϵ_y.

$$\frac{\epsilon_x}{\epsilon_y} = tan(\varphi_H) \quad \text{with} \quad \left|\frac{\epsilon_x}{\epsilon_y}\right| < 1000 \tag{31}$$

So e.g. if the solar azimuth is 180° (=South), then ϵ_x is set to zero or if the solar azimuth is 225° (=South-West), then ϵ_x=ϵ_y. With these constraints equation 28 reduces to equation 32, which can be solved with the iterative method described above.

$$\Delta \mathrm{P} = \begin{pmatrix} \mathrm{C}_{xx} + tan(\varphi_H) \cdot \mathrm{C}_{yx} & \mathrm{C}_{zx} \\ \mathrm{C}_{xy} + tan(\varphi_H) \cdot \mathrm{C}_{yy} & \mathrm{C}_{zy} \\ \mathrm{C}_{xz} + tan(\varphi_H) \cdot \mathrm{C}_{yz} & \mathrm{C}_{zz} \end{pmatrix} \cdot \begin{pmatrix} \Delta\epsilon_y \\ \Delta\epsilon_z \end{pmatrix} \tag{32}$$

6.1.3 Multiple FOVs

The theoretical concept and practical implementation described in sections 6.1.1 and 6.1.2 work well if there is only "one" FOV. However Pandora has actually two separate FOVs for each spectrometer, one for direct sun observations (SunFOV) and one for sky observations (SkyFOV).

The FWHM of the SunFOV is about 2.5° and is determined by the diameter of the aperture on top of the collimator, the diameter of the aperture behind the diffuser and the distance of these two apertures (see figure 12). The FWHM of the SkyFOV is about 1.5° and is determined by the diameter of the fiber and the distance between lens and fiber (see figure 12).

If the centers of the aperture on top of the collimator, the aperture behind the diffuser, the lens and the fiber are not perfectly aligned along a straight line, then the centers of the SkyFOV and the SunFOV will not be the same. Since they are also not necessarily the same for different spectrometers, we actually have four different pointing positions in the sky for Pandora-2S systems: a SunFOV and SkyFOV for spectrometer 1 and the same for spectrometer 2.

The tolerance for co-aligning the different FOVs in the manufacturing process is 0.3°. This means that the centers of the FOVs can vary by as much as this angle.

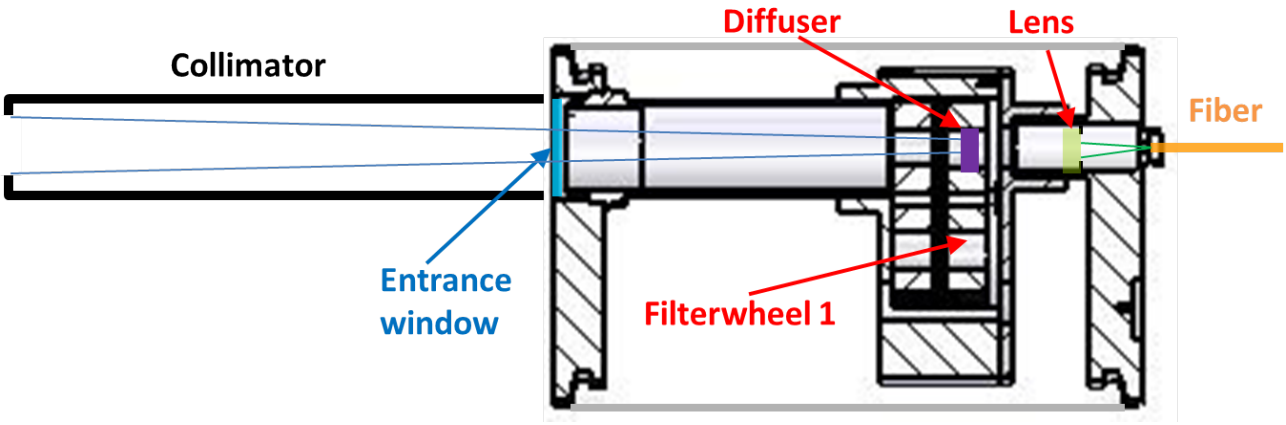


Figure 12: Schematics of the Pandora head sensor. The SunFOV is determined by the aperture on top of the collimator and the aperture behind the diffuser (thin blue lines). The SkyFOV is determined by the focal length of the lens and the diameter of the fiber (thin green lines).

This issue of different FOVs is solved in BlickO in the following way: first the best leveling is determined separately for each FOV using sun searches with different filter settings. Then an average SkyFOV is determined using the SkyFOVs from all spectrometers. Then we determine the angular difference for each individual SkyFOV from the average value. The pointing of the instrument is always done using the leveling to optimize the pointing of the average SkyFOV, but when the data are reported, each individual SkyFOV is used to calculate the pointing position. Here an example: if a Pandora-2S unit is commanded to point to a certain position in the sky, e.g. pointing zenith angle (PZA) 80.0° and pointing azimuth (PAZ) 180.0°, then the true pointing angles (and the numbers written in the raw data file) for spectrometer 1 and 2 will be slightly different, e.g. PZA=80.11°, PAZ=179.97° for spectrometer 1 and PZA=79.94°, PAZ=180.20° for spectrometer 2.

6.2 Signal to Noise Ratio Optimization

This section describes what technique is applied by BlickO to maximize the signal to noise ratio (SNR) for the Pandora measurements.

The first correction from L0 to L1 is the dark correction (see section 6.4.2), where an estimation for the dark counts (DC) is subtracted from the measured bright counts (BC). Pandora can measure DC by setting the filterwheels in a position to block the light input. The question of when and how often DC, i.e. measurements with no light input, should be measured with a photometer to obtain the highest SNR for the final L1 data is not trivial. We distinguish two situations:

- "Immediate dark measurements": immediately after the BC have been measured, DC measurements are taken at the same integration time and are used to correct the BC.
- "Dark map": at a more distant time from the BC measurements, many DC measurements over the full range of possible integration times and temperatures are made and analyzed to create a so-called "Dark map". This map either describes the full dark measurements or parts of it (e.g. the dark count fine structure, see below) and is used either by itself or in combination with immediate dark measurements to correct the BC.

The advantage of the immediate dark measurements is that the conditions (temperature, state of the instrument, etc.) are basically the same as for BC measurements. The disadvantage is that in order to optimize the SNR of the L1 data, the system needs to spend quite some time doing DC measurements, which could be better used to take more BC data.

For the dark mapping it is the opposite. One spends much less time in doing DC measurements, but runs the risk that the dark map is not entirely representative for the BC data, since the conditions (temperature, state of the instrument, etc.) might have changed between the time the dark map was created and the time of the BC measurements. Nevertheless this possible issue can be reduced by combining the dark map with some measured DC.

6.2.1 Theoretical Background

Since "true" noise is uncorrelated from pixel to pixel, all equations given in this section are for one pixel and photons from wavelengths falling in this pixel only. The number of electrons accumulated in a pixel is given by

$$\begin{aligned} N_e &= N_{eT} + N_{e\gamma} \\ &= N_{eT} + N_\gamma \cdot QE \\ &= I_{eT} \cdot \Delta t + I_\gamma \cdot QE \cdot \Delta t \end{aligned} \tag{33}$$

Δt	Exposure time (or integration time) [s]
N_e	Total number of electrons accumulated within Δt [1]
N_{eT}	Number of thermal electrons accumulated within Δt [1]
$N_{e\gamma}$	Number of electrons produced by incident photons within Δt [1]
N_γ	Number of incident photons within Δt [1]
QE	Detector quantum efficiency for this wavelength, number of electrons per number of photons [1]
I_{eT}	Mean rate of thermal electrons during Δt, electrons per second [1/s]
I_γ	Mean rate of incident photons during Δt, photons per second [1/s]

The value in square brackets is a possible unit for each parameter. The amplifier in the readout electronics (ROE) converts the accumulated charge in the output voltage. Here we assume a linear response of the amplifier.

$$\begin{aligned} V &= N_e \cdot q_e \cdot \frac{A}{C_0} + OFFSET_V \\ &= N_e \cdot GAIN_V + OFFSET_V \end{aligned} \tag{34}$$

V	Output voltage [V]
q_e	Electron charge [C]
C_0	Output node capacitance [F=C/V]
A	Amplifier voltage gain [1]
$OFFSET_V$	Electrical offset added by the amplifier [V]
$GAIN_V$	Voltage gain per electron [V]

The analog-digital converter converts the output voltage in digital counts. Here we assume a linear response of the AD-converter with zero offset (a non-zero offset would not change the principle).

$$\begin{aligned} C &= V \cdot F \\ &= N_e \cdot GAIN_V \cdot F + OFFSET_V \cdot F \\ &= N_e \cdot GAIN + OFFSET \end{aligned} \tag{35}$$

C	Raw counts [DN]
F	Analog-digital conversion factor [DN/V]
$OFFSET$	(Count) offset (=$OFFSET_V$·F) [DN]
$GAIN$	(Count) gain (=$GAIN_V$·F) per electron [DN]

A single dark measurement DC_i and a single bright measurement BC_i are given by:

$$\begin{aligned} DC_i &= OFFSET_i + GAIN_i \cdot N_{eTi} \\ &= OFFSET_i + GAIN_i \cdot I_{eTi} \cdot \Delta t_i \\ BC_i &= OFFSET_i + GAIN_i \cdot [N_{eTi} + N_{e\gamma i}] \\ &= OFFSET_i + GAIN_i \cdot [I_{eTi} + I_{\gamma i} \cdot QE] \cdot \Delta t_i \end{aligned} \tag{36}$$

where i is the measurement index. In the following paragraphs each of the parameters in equation 36 is discussed separately:

Δt

We assume the uncertainty in the exposure time Δt to be negligible and set the variance (σ^2) to zero. There might be a systematic error (bias) in Δt (see section 6.4.6), but we do not assume this bias changing over time.

$$\sigma^2_{\Delta t} = 0 \tag{37}$$

OFFSET

The offset is determined by the ROE, varies in general with temperature, may have a long-term drift due to changes in the electronics and may even depend on N_e. Note that if it depends on N_e, then the parameter $OFFSET_i$ in equation 36 is different for DC and BC and a systematic error is introduced, if the measured dark counts are used to apply "dark correction" on the bright counts. This case is discussed in section 6.2.6. Here we limit ourselves to the statistical uncertainty of the offset over a short time period (<1 min). The (short-term) uncertainty in the measured offset is called read noise or electronic noise (see e.g. `http://en.wikipedia.org/wiki/Electronic_noise`).

$$\sigma^2_{\mathrm{OFFSET}}(\text{SHORT-TERM}) = \sigma^2_{\mathrm{READ}} \tag{38}$$

GAIN

The gain is determined by the ROE, may vary with temperature and may also have a long-term drift due to changes in the electronics. Over a short time period (<1 min) we consider the variation of GAIN negligible.

$$\sigma^2_{\mathrm{GAIN}}(\text{SHORT-TERM}) = 0 \tag{39}$$

QE

The quantum efficiency depends on the wavelength and may have a long-term drift due to changes in the detector. Over a short time period (<1 min) we consider the variation of QE negligible.

$$\sigma^2_{\mathrm{QE}}(\text{SHORT-TERM}) = 0 \tag{40}$$

N_{eT}

The number of thermal electrons is the product of I_{eT} times Δt. The (short-term) uncertainty in the measured number of thermal electrons follows a Poisson distribution (see e.g. `http://www.photomet.com/pm_solutions/library_encyclopedia/library_enc_signal.php`). The variance of a Poisson distributed variable with mean value N equals N (see e.g. `http://en.wikipedia.org/wiki/Poisson_distribution`). For the (short-term) uncertainty of N_e follows

$$\sigma^2_{\mathrm{NeT}}(\text{SHORT-TERM}) = N_{eT} \tag{41}$$

$N_{e\gamma}$

The number of electrons produced by incident photons is the product of I_γ times QE times Δt. The rate of incident photons I_γ depends on the light source. For a constant light source, e.g. a stable lamp, I_γ will not vary over a short time period (<1 min). In such case, the (short-term) uncertainty in the measured $N_{e\gamma}$ also follows a Poisson distribution (see e.g. `http://en.wikipedia.org/wiki/Shot_noise`).

$$\sigma^2_{\mathrm{Ne}\gamma}(\text{SHORT-TERM,stable}) = N_{e\gamma} \tag{42}$$

For solar radiation, the input is in general changing, even over a short time period and even for perfectly stable atmospheric conditions, since the solar angles are changing. For variable atmospheric conditions (e.g. clouds), the rate of incident photons changes even more over the duration of the measurement time. Such variation of I_γ does not give a purely statistical uncertainty for $N_{e\gamma}$. If several identical instruments would measure the solar radiation at the same time, they all would see the same systematic variation in I_γ. The total (short-term) uncertainty of $N_{e\gamma}$ is therefore a combination of the photon noise and the input rate variation.

$$\begin{aligned}\sigma^2_{\mathrm{Ne}\gamma}(\text{SHORT-TERM}) &= N_{e\gamma} + \sigma^2_{\mathrm{I}\gamma} \cdot \mathrm{QE}^2 \cdot \Delta t^2 \\ &= N_{e\gamma} + \sigma^2_{\mathrm{eINPUT}}\end{aligned} \tag{43}$$

σ_{eINPUT} is the uncertainty of the electrons produced by incident photons due to the input-rate variation. We may neglect σ_{eINPUT} for a short-term stable input such as a lamp on a very stable power supply.

From equations 34 to 43 we can compose the total short-term (<1 min) uncertainties of $\mathrm{BC_i}$ and $\mathrm{DC_i}$ respectively:

$$\begin{aligned}
\sigma^2_{\mathrm{DCi}} &= \sigma^2_{\mathrm{READi}} + \mathrm{GAIN}^2_{\mathrm{i}} \cdot \mathrm{N_{eTi}} \\
&= \sigma^2_{\mathrm{READi}} + \mathrm{GAIN}^2_{\mathrm{i}} \cdot \mathrm{I_{eTi}} \cdot \Delta \mathrm{t_i} \\
\sigma^2_{\mathrm{BCi}} &= \sigma^2_{\mathrm{READi}} + \mathrm{GAIN}^2_{\mathrm{i}} \cdot \left[\mathrm{N_{eTi}} + \mathrm{N_{e\gamma i}} + \sigma^2_{\mathrm{eINPUTi}}\right] \\
&= \sigma^2_{\mathrm{READi}} + \mathrm{GAIN}^2_{\mathrm{i}} \cdot \left[\mathrm{I_{eTi}} + \mathrm{I_{\gamma i}} \cdot \mathrm{QE_i}\right] \cdot \Delta \mathrm{t_i} + \sigma^2_{\mathrm{INPUTi}}
\end{aligned} \tag{44}$$

σ_{INPUT} is the product of σ_{eINPUT} times GAIN, i.e. the uncertainty due to input-rate variation expressed in counts. This equation is for single DC or BC measurements. In practice we average several detector readings to reduce the noise. For the next equation we assume having $\mathrm{n_{BC}}$ repetitions of BC-measurements $\mathrm{BC_i}$ and $\mathrm{n_{DC}}$ repetitions of DC-measurements $\mathrm{DC_i}$, all at the same integration time Δt. The total time of bright measurements $\mathrm{n_{BC}} \cdot \Delta$t or dark measurements $\mathrm{n_{DC}} \cdot \Delta$t is less than 1 min, so all equations from the theory for short time periods are valid.

The average over the DC- and BC-measurements is given by

$$\begin{aligned}
\mathrm{DC} &= \frac{1}{\mathrm{n_{DC}}} \cdot \sum_{\mathrm{i=1}}^{\mathrm{n_{DC}}} \mathrm{DC_i} = \mathrm{OFFSET} + \mathrm{GAIN} \cdot \mathrm{I_{eT}} \cdot \Delta \mathrm{t} \\
\mathrm{BC} &= \frac{1}{\mathrm{n_{BC}}} \cdot \sum_{\mathrm{i=1}}^{\mathrm{n_{BC}}} \mathrm{BC_i} = \mathrm{OFFSET} + \mathrm{GAIN} \cdot \left[\mathrm{I_{eT}} + \mathrm{I_{\gamma}} \cdot \mathrm{QE}\right] \cdot \Delta \mathrm{t}
\end{aligned} \tag{45}$$

We have removed index i from all parameters, since the integration time Δt is the same for all scans, OFFSET, GAIN and QE have presumably not changed and $\mathrm{I_{eT}}$ and $\mathrm{I_{\gamma}}$ are defined as the average values over the $\mathrm{I_{eTi}}$ and $\mathrm{I_{\gamma i}}$. We can calculate the standard deviation over the DC-measurements as best estimation for σ_{DCi}:

$$\sigma^2_{\mathrm{DCi}} = \frac{1}{\mathrm{n_{DC}} - 1} \cdot \sum_{\mathrm{i=1}}^{\mathrm{n_{DC}}} (\mathrm{DC_i} - \mathrm{DC}) \tag{46}$$

If we assume an input without drift (e.g. lamp measurements over a short time period), we can calculate the standard deviation over the BC-measurements as best estimation for σ_{BCi} (first line of equation 47). If we assume an input changing linearly in time (e.g. solar radiation over a short time period at perfectly stable atmospheric conditions) we calculate the rms to a fitted straight line through the BC-measurements as best estimation for σ_{BCi} (second line of equation 47). In the latter case the points on the fitted straight line are called $\mathrm{BC_{iFIT}}$.

$$\begin{aligned}
\sigma^2_{\mathrm{BCi}} &= \frac{1}{\mathrm{n_{BC}} - 1} \cdot \sum_{\mathrm{i=1}}^{\mathrm{n_{BC}}} (\mathrm{BC_i} - \mathrm{BC}) \\
\sigma^2_{\mathrm{BCi}} &= \frac{1}{\mathrm{n_{BC}} - 2} \cdot \sum_{\mathrm{i=1}}^{\mathrm{n_{BC}}} (\mathrm{BC_i} - \mathrm{BC_{iFIT}})
\end{aligned} \tag{47}$$

From equations 44 and 45 we can derive the noise in the averaged dark measurements σ_{DC}:

$$\sigma_{DC}^2 = \frac{\sigma_{DCi}^2}{n_{DC}} = \frac{1}{n_{DC}} \cdot \left[\sigma_{READ}^2 + GAIN^2 \cdot I_{eT} \cdot \Delta t\right] \tag{48}$$

Here we apply that for the standard uncertainty of the mean value (also called standard error), the statistical components in the uncertainties are reduced by the square root of the number of measurements (see e.g. `http://en.wikipedia.org/wiki/Standard_error`).

For the uncertainty of the averaged bright measurements σ_{BC} we use the same equations and distinguish two cases. The first line in equation 49 is for the case that σ_{INPUT} is purely statistical and the variance scales with $1/n_{BC}$ (e.g. a lamp with a white noise flicker). The second line in equation 49 is for the case that σ_{INPUT} is not purely statistical and includes a systematic component, which means it does not scale with $1/n_{BC}$ (e.g. an atmospheric change while the measurement is taken).

$$\begin{aligned} \sigma_{BC}^2(STAT) &= \frac{1}{n_{BC}} \cdot \left[\sigma_{READ}^2 + GAIN^2 \cdot (I_{eT} + I_\gamma \cdot QE) \cdot \Delta t + \sigma_{INPUT}^2\right] = \frac{\sigma_{BCi}^2}{n_{BC}} \\ \sigma_{BC}^2(SYS) &= \frac{1}{n_{BC}} \cdot \left[\sigma_{READ}^2 + GAIN^2 \cdot (I_{eT} + I_\gamma \cdot QE) \cdot \Delta t\right] + \sigma_{INPUT}^2 > \frac{\sigma_{BCi}^2}{n_{BC}} \end{aligned} \tag{49}$$

6.2.2 Single Scan Dark Correction

Here we look at the case, where exactly one bright and one dark measurement is given. For the dark corrected counts CC_i we obtain from equation 36:

$$CC_i = BC_i - DC_i = GAIN \cdot I_{\gamma i} \cdot QE \cdot \Delta t \tag{50}$$

We assume that DC_i and BC_i were measured at the same temperature and exposure time and that all parameters such as OFFSET, GAIN, QE, etc. have not changed. Therefore, we write for the uncertainty of CC_i based on equation 44:

$$\begin{aligned} \sigma_{CCi}^2 &= \sigma_{DCi}^2 + \sigma_{BCi}^2 \\ &= 2 \cdot \sigma_{READ}^2 + GAIN^2 \cdot [2 \cdot I_{eT} + I_\gamma \cdot QE] \cdot \Delta t + \sigma_{INPUT}^2 \\ &= 2 \cdot \sigma_{READ}^2 + 2 \cdot GAIN^2 \cdot I_{eT} \cdot \Delta t + GAIN \cdot CC_i + \sigma_{INPUT}^2 \\ &= 2 \cdot \sigma_{DCi}^2 + GAIN \cdot CC_i + \sigma_{INPUT}^2 \\ &= \sigma_{INSTR}^2 + \sigma_{INPUT}^2 \end{aligned} \tag{51}$$

In this equation we have split the uncertainty of the corrected counts in the "instrumental noise" σ_{INSTR} and the "input variation" σ_{INPUT}. If we assume no input variation (σ_{INPUT}=0) and furthermore neglect I_{eT}, which can be done for low exposure times and/or low temperatures, then equation 51 reduces to:

$$\sigma_{CCi}^2 = 2 \cdot \sigma_{READ}^2 + GAIN \cdot CC_i \tag{52}$$

Figure 13 shows the estimated σ_{CCi} from equation 52 for two cases: the "CMOS-system" is characterized by low gain and high read noise (red lines) and is typical for CMOS detectors as used in the first Pandora units, which could only measure in direct sun mode. The "CCD-system" is characterized by high gain and low read noise (blue lines) and is typical for CCD detectors as used in the newer Pandora systems. Note that currently all Pandora systems use a 16-bit AD converter, i.e. the nominal saturation limit is 2^{16}-1=65535 counts, which means a read noise of 20 (40) counts corresponds to 0.03% (0.06%) of saturation.

The solid lines in the figure are the total noise (combination of read noise and photon noise), the dashed lines represent the photons noise only. The total noise is driven by the read noise for low counts and by the photon noise for high counts.

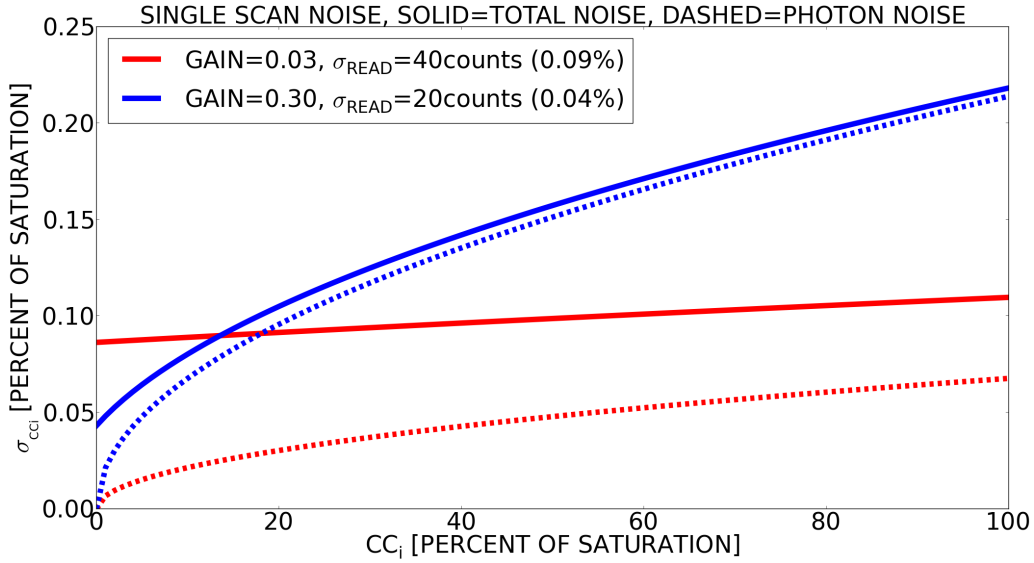


Figure 13: Noise of dark corrected counts for a single bright and dark measurement as a function of the corrected counts, expressed as a fraction of saturation.

The SNR of CC_i based on equation 52 is given by:

$$SNR_i = \frac{CC_i}{\sigma_{CCi}} = \frac{CC_i}{\sqrt{2 \cdot \sigma_{READ}^2 + GAIN \cdot CC_i}} \tag{53}$$

This is shown in figure 14. At 80% of saturation (black dashed vertical line), the SNR for the CMOS-system (red) is about 760:1 and for the CCD-system (blue) about 410:1.

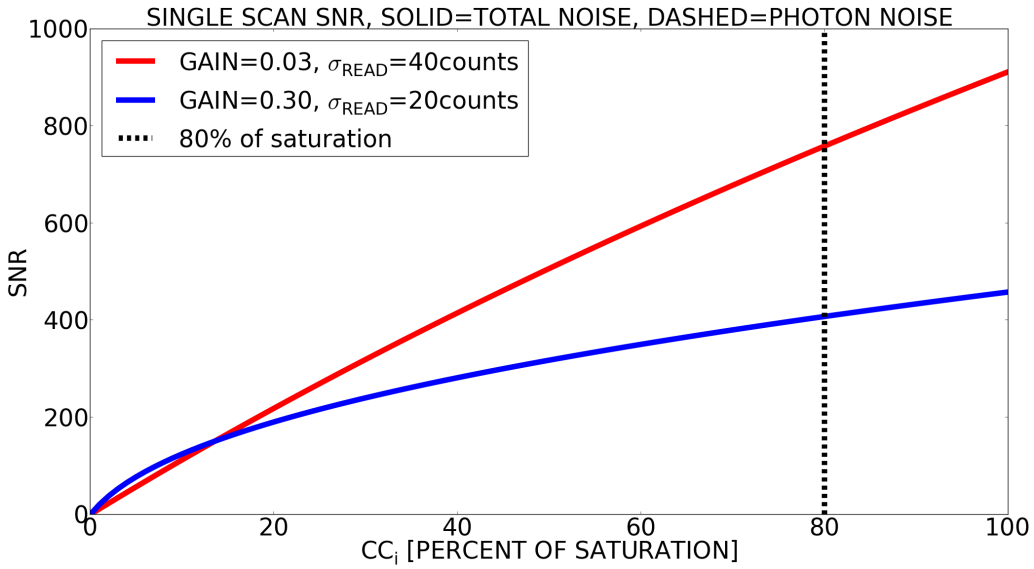


Figure 14: SNR of dark corrected counts for a single bright and dark measurement as a function of the corrected counts, expressed as a fraction of saturation.

6.2.3 Multiple Scans Dark Correction

Here we use the same assumptions as in the previous section, but allow multiple measurements of DC_i and BC_i. From equation 45 we get for the corrected counts CC:

$$CC = BC - DC = GAIN \cdot I_\gamma \cdot QE \cdot \Delta t \tag{54}$$

For the uncertainty of CC follows from equations 48 and 49:

$$\begin{aligned}\sigma^2_{CC} &= \sigma^2_{DC} + \sigma^2_{BC} \\ &= \left(\frac{1}{n_{DC}} + \frac{1}{n_{BC}}\right) \cdot \left[\sigma^2_{READ} + GAIN^2 \cdot I_{eT} \cdot \Delta t\right] + \frac{1}{n_{BC}} \cdot \left[GAIN^2 \cdot I_\gamma \cdot QE \cdot \Delta t\right] \\ &= \left(\frac{1}{n_{DC}} + \frac{1}{n_{BC}}\right) \cdot \sigma^2_{DCi} + \frac{1}{n_{BC}} \cdot GAIN \cdot CC \\ &= \sigma^2_{INSTR}\end{aligned} \tag{55}$$

Here we assume no input variation (σ_{INPUT}=0), in which case the uncertainty of CC is the instrumental noise only.

We can ask ourselves the question, what the best split between the number of bright and dark measurements is to get the highest SNR in the corrected counts. We can rewrite equation 55 using the "Dark fraction" f_{DC}, which is the number of dark count repetitions relative to the total number of repetitions (so e.g. f_{DC}=0.5 means the same number of repetitions for bright and dark counts).

$$\sigma^2_{INSTR} = \frac{\sigma^2_{DCi}}{n \cdot f_{DC}} + \frac{\sigma^2_{DCi} + GAIN \cdot CC}{n \cdot (1 - f_{DC})} \tag{56}$$

n is the sum of n_{DC} and n_{BC}. Deriving equation 56 for f_{DC} yields:

$$\frac{\partial \sigma^2_{INSTR}}{\partial f_{DC}} = \frac{-\sigma^2_{DCi}}{n \cdot f^2_{DC}} + \frac{\sigma^2_{DCi} + GAIN \cdot CC}{n \cdot (1 - f_{DC})^2} \tag{57}$$

For the extreme conditions, we obtain this solution:

$$f_{DCOPT} = \frac{-\sigma^2_{DCi}}{GAIN \cdot CC} \pm \sqrt{\left(\frac{\sigma^2_{DCi}}{GAIN \cdot CC}\right)^2 + \frac{\sigma^2_{DCi}}{GAIN \cdot CC}} \tag{58}$$

f_{DCOPT} must be positive and we call it the "Optimized dark ratio" ODR:

$$f_{DCOPT} = ODR = \sqrt{q^2 - q} - q \tag{59}$$

where q is given by

$$q = \frac{\sigma^2_{DCi}}{GAIN \cdot CC} \geq \frac{\sigma^2_{READ}}{GAIN \cdot CC} \tag{60}$$

If we neglect I_{eT}, which can be done for low exposure times and/or low temperatures, we can replace σ_{CCi} by σ_{READ}. ODR as a function of q is shown in figure 15.

For high values of q (low gain and high read noise systems), ODR approaches 0.5, i.e. to optimize the SNR, one needs to measure bright and dark counts for nearly the same duration. For a typical CMOS-system, the ODR ranges from 0.41 at 80% of saturation to 0.47 at 20% of saturation (red line in figure).

For low values of q (high gain and low read noise systems), ODR approaches 0, i.e. to optimize the SNR one needs to dedicate much more measurement time for BC than for DC. For a typical CCD-system, the ODR ranges from 0.14 at 80% of saturation to 0.23 at 20% of saturation (blue line in figure).

For the IOF-entry "Optimized dark ratio" (see section 5.3) we use the ODR at 50% of saturation, which would be 0.44 for the typical CMOS-system and 0.16 for the typical CCD-system (red and blue dots in figure respectively). Hence for "Immediate dark measurements", the best split between BC and DC is given by the ODR.

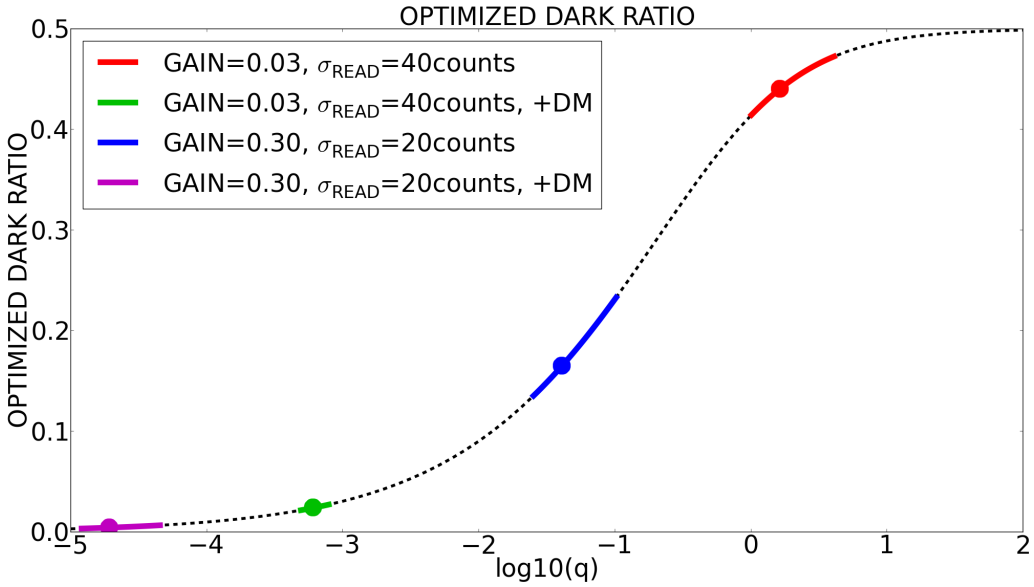


Figure 15: Optimized dark ratio as a function of q from equation 60 or 62 for q-values ranging from 1e-5 to 1e2. The colored lines are for CC-values ranging from 20% to 80% of saturation for typical CMOS- and CCD-systems respectively. The colored dots are for CC-values at 50% of saturation. Red and blue data are for the case of not using a dark map, while green and magenta data assume the use of a dark map.

6.2.4 Dark Map

If instead or in addition to the immediate dark measurements, a dark map is used, the noise in the dark estimation is reduced. As described in details in section 6.4.2 we are not creating a full dark map at present. Instead the dark count is split into a "DC background" and "DC fine structure".

Since the background consists of a few fitting parameters only and we assume no noise in the dark fine structure parameters, the noise in DC_E is reduced to approximately σ_{DCi} divided by square root of the number of pixels $\sqrt{npix}$. Including this reduction, equation 56 becomes

$$\sigma^2_{INSTR} = \frac{\sigma^2_{DCi}}{n \cdot n_{PIX} \cdot f_{DC}} + \frac{\sigma^2_{DCi} + GAIN \cdot CC}{n \cdot (1 - f_{DC})} \tag{61}$$

and consequently q changes to

$$q = \frac{\sigma^2_{DCi}}{\sigma^2_{DCi} \cdot [n_{PIX} - 1] + n_{PIX} \cdot GAIN \cdot CC} \tag{62}$$

Using the dark map the values of q are much smaller causing ODR to drop significantly to 0.03 for low gain and even <0.01 for high gain (see figure 15).

Figure 16 compares the immediate dark method and the dark mapping method. For this example we have used a total number of scans of n=1000. The solid lines show the dark mapping method, where most of the 1000 scans are spent taking BC data. The dashed lines refer to the immediate dark method, where the number of dark measurements is much larger. The improvement of the dark mapping method over the immediate dark method is especially pronounced for the CMOS-case.

Based on this figure we can say that if we believe that the dark map represents all instrumental parameters such as OFFSET, GAIN and QE accurately enough, it is the preferred method for the dark correction.

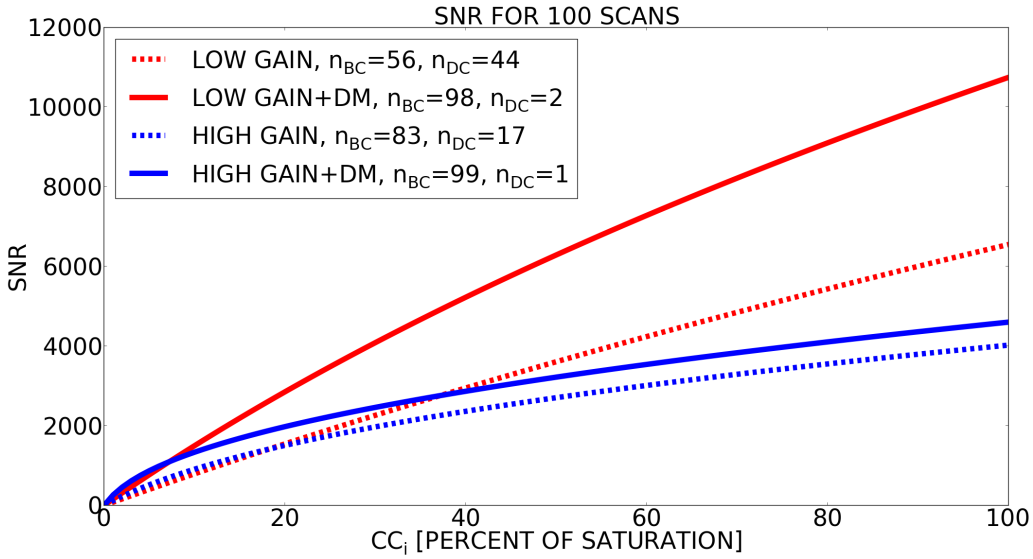


Figure 16: SNR of averaged dark corrected counts for a total number of 1000 single scans as a function of the corrected counts, expressed as fraction of saturation. Solid lines show dark mapping method, where all 1000 scans are spent taking BC data. Dashed lines refer to the immediate dark method, where the 1000 scans are split between DC and BC measurements.

6.2.5 Optimized SNR

The optimized SNR as a function of the number of scans is shown in figure 17, where we assume corrected counts at 50% of saturation. For the retrieval of weaker absorbers in the atmosphere using the spectral fitting technique, we consider a SNR of 10000:1 as the desired minimum (black dashed line) to avoid being noise-limited in the retrieval. In order to exceed this limit, we need at least 250 scans for CMOS-systems and 960 scans for CCD-systems. These scan-numbers can be obtained by Pandora for direct sun observations, except for measurements near twilight or with clouds in the solar direction. For sky radiance measurements (only possible with CCD-systems), the integration times are usually 20 to 500 ms (depending on the wavelength range, solar angles, etc.). This means that we would have to acquire spectra for 20 s to 500 s in order to not be noise-limited. While 20 s works from a practical point of view, 500 s is definitely too long and Pandora data are noise limited for some applications in this case.

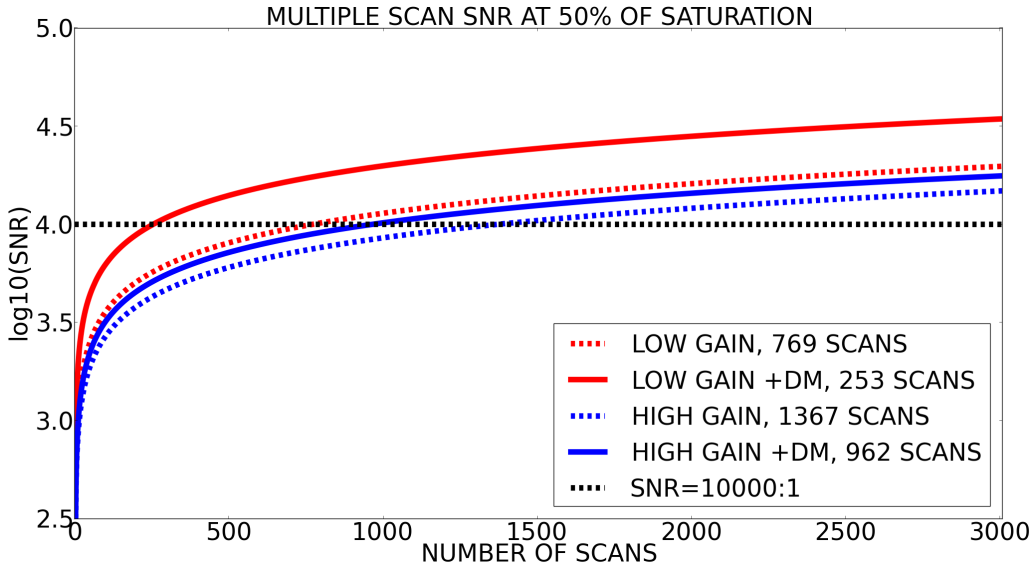


Figure 17: SNR of averaged dark corrected counts at 50% of saturation as a function of the number of scans averaged with (solid) and without (dashed) using a dark map. The black dashed line is for SNR=10000:1. Values listed in the legend give the number of scans needed to exceed an SNR of 10000:1.

6.2.6 Blind Pixels

This section is not directly related to the SNR, but discusses an important systematic issue in the dark correction.

All previous sections were based on the assumption that the dark offset does not depend on N_e, i.e. the parameter OFFSET in equation 36 is the same for DC and BC. However, we noticed that this is in general not the case for most Pandora systems. Instead, we observed that OFFSET is reduced when N_e increases, i.e. BC measurements have systematically a smaller OFFSET than DC measurements.

We were not able to determine the magnitude of this effect in the laboratory in a consistent way, which means we could not develop a technique to correct for it with some mathematical algorithm. We could only determine that the OFFSET bias increases with the total photon energy falling on the detector (or the sum over the N_e for all pixels) and can be >50 counts (for a 16-bit unit) at high signal levels.

This problem affects both the dark mapping and the immediate dark method. Fortunately it is a small effect that has negligible significance in regular field operation. However, it is a large problem in the characterization of the instrument's spectral stray light. For the stray light characterization, the instrument is illuminated by a laser line and the distribution of the signal over the whole detector is analyzed. We know that the pixels in the far field (>10 nm away from the maximum signal at the laser wavelength) have signals relative to the signal at the maximum in the order of <3e-5 for "good units" (with low amount of stray light) and >1e-4 for "bad units" (with high amount of stray light). Hence, if the maximum is at 60000 counts, then the far field pixels have <2 counts for good units and >6 counts for bad units. Since the OFFSET bias is in this order of magnitude or even larger, the determination of the stray light level is not possible.

It turns out that most detectors have a feature, which can be used to reduce this problem, the "Blind pixels". Blind pixels are pixels that do not receive any light input even if the detector is illuminated. All newer Pandoras with CCD-detectors have at least 6 such blind pixels, of which at least 3 are read during the data acquisition. The blind pixels allow to estimate OFFSET for the lowest pixels (those adjacent to the blind pixels) during the BC measurements, which is a big help in the determination of the instrument's stray light in the laboratory.

The blind pixels are included in the dark correction in a way that the average of them is subtracted from both the BC and DC data before the corrected counts CC are build (see also section 6.4.2). This correction assumes that the systematic OFFSET change is a constant value, affecting all pixels in the same way. We know

that this is not the case, but applying this correction is better than not applying it.

6.3 Data uncertainty

6.3.1 Overview

The main output products of BlickP are spectra (L1), slant columns (L2Fit) and total and tropospheric column amounts or profiles or surface concentrations (L2). Most of these data come with associated uncertainties. For the naming and meaning of the uncertainties the Blick Software Suite follows the guidelines laid out by *Mittaz et al.* [27]. Three types of errors are distinguished, which differ from each other by the correlation length of the associated error along a certain "dimension". In the Blick Software Suite this dimension is wavelength for L1 data and time for L2Fit and L2 data.

- Independent uncertainty: the correlation length along the dimension for the independent error is zero. An example for L1 data is the read noise in a certain pixel (i.e. at a certain wavelength), which is totally uncorrelated to the read noise in any other pixel (wavelength). An example for L2Fit data is the photon noise propagated into the slant column amount measured at a certain moment, which is totally uncorrelated to the propagated photon noise for measurements taken at any other time. The uncertainty associated with an independent error is called "Independent uncertainty" and is symbolized with U_I.

- Common uncertainty: the correlation length along the dimension for the common error is infinite. An example for L1 data is a bias in the radiometric calibration due to a faulty current for the calibration lamp in the laboratory. While this bias affects smaller wavelengths more than higher wavelengths, there is nevertheless full correlation between the error in one wavelength and the error in any other wavelength. An example for L2Fit data is an error in the assumed slant column in the reference spectrum. This error affects all retrieved slant columns using the same reference spectrum in the same way, hence the error at a certain measurement is fully correlated to the error for measurements taken at any other time. The uncertainty associated with a common error is called "Common uncertainty" and is symbolized with U_C.

- Structured uncertainty: the correlation length along the dimension for the structured error is larger than zero, but not infinite. An example for L1 data is an error in the flat field correction around a certain wavelength region. Such an error affects all the pixels inside this wavelength region in the same way, but is uncorrelated to pixels at a different part of the spectrum. An example for L2Fit data is a difference between the effective temperature of a trace gas used in the spectral fitting (assuming that the temperature is NOT fitted itself) and the true effective temperature of this gas in the atmosphere. This introduces an error in the retrieved slant column, which is highly correlated to measurements taken around the same time, but in general not correlated to measurements taken at times farther away. E.g. if an effective ozone temperature of 225 K is used in the spectral fitting, but the true effective ozone temperature is 228 K at 10:00 in the morning of 27 October, this causes approximately a -1% error in the retrieved ozone slant column. The next measurement on this day at 10:02 will still suffer nearly exactly the same error, since the true temperature has hardly changed in the 2 minutes. However a few days later, on 3 November, the true temperature has in general changed and might be 225 K, which means the error due a mismatch of the effective temperature is then 0 and not correlated to the error from 27 October at 10:00. The uncertainty associated with a structured error is called "Structured uncertainty" and is symbolized with U_S.

For the total uncertainty U of a single (L1, L2Fit or L2) data point, we simply combine U_I, U_C and U_S as shown in equation 63:

$$U = \sqrt{U_I^2 + U_C^2 + U_S^2} \tag{63}$$

When the data are averaged, e.g. by building the mean spectrum over a certain wavelength range, or the mean column amount over a certain time interval, the combined uncertainty associated with the mean is a combination of the individual $U_I(i)$, $U_C(i)$ and $U_S(i)$. i=1 to n is the index for a single data point out of the n data points averaged. Here we look at the two "extreme" cases.

In the first situation the structured errors are fully correlated along the dimension. In this "short" case the total uncertainty of the mean value, called U(n,short), is given by:

$$U(n,short) = \frac{1}{n} \cdot \sqrt{\sum_{i=1}^{n} \left[U_I(i)^2\right] + \left[\sum_{i=1}^{n} U_C(i)\right]^2 + \left[\sum_{i=1}^{n} U_S(i)\right]^2} \tag{64}$$

Hence the independent uncertainty of the mean is "reduced" compared to the individual values, but the common and structured uncertainties are not. An example for this would be the mean column amount over a rather short time period, e.g. 10 min, in which we assume the data with respect to mismatch of the true and assumed effective trace gas temperature to be fully correlated.

The other extreme case assumes the structured uncertainties to be uncorrelated along the dimension. In this "long" case the total uncertainty U(n,long), is given by:

$$U(n,long) = \frac{1}{n} \cdot \sqrt{\sum_{i=1}^{n} \left[U_I(i)^2\right] + \left[\sum_{i=1}^{n} U_C(i)\right]^2 + \sum_{i=1}^{n} \left[U_S(i)^2\right]} \tag{65}$$

Here the structured uncertainty "behaves" like the independent uncertainty. An example for this would be the mean column amount over a long time period, e.g. one year, when we assume that the temperature used in the spectral fitting is from a climatology that represents very well the average true effective temperature over this year. Then we could say that the temperature errors are a mixture of over- and underestimations and can therefore be approximated as uncorrelated overall.

It is important to note that not all possible uncertainty sources are included in the Blick Software Suite at this moment and therefore even the total uncertainty is still incomplete and likely to be underestimated. Therefore the output product also include data quality flags (DQF), which are described in the next section.

The plan is to add the uncertainty sources not taken into account at later versions of the software. More details on the uncertainty outputs of the Blick Software Suite, and which uncertainty sources are (not) included are given in the remaining part of section 6.3 and also in the algorithm descriptions.

6.3.2 Data quality flags

In addition to uncertainty information, the different data products also include DQFs (see also sections 5.10 and 5.12 to 5.14), which are needed, since the uncertainty does not cover all sources that may contribute to a decrease in the data quality. In other words, there are effects, which we know are affecting the data quality, that are either not being taken into account at all in the current Blick Software Suite retrieval version, or which are not quantitatively estimated within the software. Here some examples of such effects:

- We know that if the temperature of the spectrometer is different from the reference temperature, i.e. the one present during the calibration, then the L1 data change. This effect is considered in the L1

algorithm (see section 6.4). However the Blick Software Suite does currently not "know" how much such a temperature change increases the uncertainty. Therefore the qs-code (table 24) includes entry "Eff temp diff limits", which changes the DQ if the temperature variation exceeds a certain threshold. This example is actually representative for most entries of the qs-code, which refer to L1 corrections that are applied to the data, but where no uncertainty is associated to this correction.

- If the measurements are modified by an "unwanted" spectral signal, which arises from instrumental issues like a non-perfect pointing during direct sun observations, then this increases the rms of the fitting residuals (see section 6.5). However the Blick Software Suite does currently not "translate" such a change in the rms into an increased uncertainty. Therefore the qf-code (table 28) includes entry "wrms limits".

- The fraction of diffuse light entering the instrument in addition to the direct beam for direct sun or moon observations increases with the (solar or lunar) zenith angle and the amount of aerosols in the atmosphere. Since the direct algorithm (section 6.6) is based on the assumption that only direct light is measured, a systematic error in the L2 data is introduced, which grows with this "diffuse fraction". This causes e.g. total ozone columns to be biased low. However the Blick Software Suite does currently not take this effect into account at all. Therefore the qr-code (table 31) includes entry "AMF limits".

- A similar situation happens, when clouds are in the direct light path. In this case the AMF calculated by the direct algorithm (section 6.6) underestimates the "true" AMF and systematically changes the data and e.g. total NO_2 columns are biased high. Again the Blick Software Suite does currently not take this effect into account at all. Since the Blick Software Suite uses the atmospheric variability to detect clouds, the qr-code includes entry "AtmVar limits", so that the data quality is reduced when clouds are present.

Currently there are 9 possible DQFs: DQ0, DQ1, DQ2, DQ10, DQ11, DQ12, DQ20, DQ21 and DQ22. The unit position 0, 1 or 2 has the following meaning:

- Unit position 0, "High quality": no data quality indicator exceeds the data quality 1 (DQ1) limit and therefore there are no indications that the data might not be of the highest possible quality. Once quality assured, those data can be used with high confidence and the uncertainty associated with these additional effects is negligible, i.e. the provided uncertainty can be assumed to represent the true uncertainty.

- Unit position 1, "Medium quality": at least one data quality indicator exceeds the DQ1 limit and therefore the quality of the data might be reduced. Depending on the application, the user should decide whether to use these data. Note that the reduced quality can originate from instrumental sources (e.g. too large wavelength shift) or atmospheric sources (e.g. clouds in direct sun measurements). This also means that the reported data underestimates the true uncertainty by a small amount.

- Unit position 2, "Low quality": at least one data quality indicator exceeds the data quality 2 (DQ2) limit and therefore the quality of the data is strongly reduced. For most purposes, the user should not use these data. As for unit position 1, the low quality can originate from instrumental or atmospheric sources. In this case it is nearly certain that reported data uncertainty underestimates the true uncertainty.

The decade of the DQF can be 0, 1 or 2 and has the following meaning:

- Decade 0, "Quality assured": this means that quality control (QC) has already been applied to the data. QC consists of a semi-automatic inspection of the obtained L2 data to determine, whether the instrument was monitoring correctly over a certain measurement period. With this procedure one can possibly detect factors influencing the data quality, which are not reflected in the uncertainty and not captured by the DQF. An example would be a dirty entrance window. This reduces the overall throughput of the

system and is interpreted by the algorithm as an increased aerosol load in the atmosphere. Since this effect causes usually a non-physical dependence of the AOD on the SZA, it can often be detected in the QA process. After the QC has been performed, the unit position will not change anymore.

- Decade 1, "Not quality assured": the quality flag in the unit position is based on an initial estimate and formal QC has not been carried out. It is possible that the unit position changes after that happens.
- Decade 2, "Unusable data": this means the data are not usable, which can have different reasons, e.g. no calibration for a specific trace gas has been included in the ICF. These data will not undergo QC. For more details see section 5.14.

It is also important to note, that the unit position of the DQF can only stay the same or increase through the different processing levels, but never go down. Hence if the L2Fit data DQ11, the L2 data also stay DQ11 even when none of the qr-code parameters exceeds the DQ1-threshold.

6.3.3 L0 Uncertainty

Since in most cases a measurement set is comprised of several individual spectrometer readings, i.e. the "number of cycles" is above 1, the L0 data contain the "Uncertainty of raw counts for each pixel divided by the square root of the number of cycles", $U_M(L0_i)$, in addition to the "Mean over all cycles of raw counts for each pixel" (see table 18). $U_M(L0_i)$ does not represent one single error type as introduced in section 6.3.1, since it is in general a mixture of types. Therefore we use index "M" for "Measured".

Mathematically $U_M(L0_i)$ is simply the standard deviation over the individual spectra in case L0-output "Uncertainty indicator" equals 1, or the rms to a straight line fitted into the individual spectra in case the "Uncertainty indicator" equals 2. In both cases it is also divided by the square root of the number of cycles.

Physically $U_M(L0_i)$ is a combination of the independent instrumental uncertainty (i.e. read noise and photon noise, see section 6.2.1), possible other instrumental uncertainty (maybe caused by faulty pointing during part of the measurement), and the variability of the input radiation over the duration of the measurement set. For a light source, which is considered stable, like a calibration lamp, the Blick Software Suite uses uncertainty indicator 1. Solar radiation reaching the Earth's surface over a short time interval (typically <1 min) is considered to have a linear intensity change with time in case the atmospheric transmission is constant, simply because the solar zenith angle is changing. Therefore the Blick Software Suite uses uncertainty indicator 2 for field measurements.

Hence when the variability of the input radiation is small and there are only insignificant systematic instrumental errors in the measurement, $U_M(L0_i)$ is mostly an independent instrumental uncertainty. The more input variability is present, the more $U_M(L0_i)$ includes a common component, since this input change will affect all pixels in a correlated way. For field measurements we call the variability of the input radiation "Atmospheric Variability" (AtmVar), which is defined in the next section.

6.3.4 L1 Uncertainty

In the current version of the Blick Software Suite, there are two L1 outputs related to uncertainty. The "Independent instrumental uncertainty of L1 data for each pixel", $U_I(L1_i)$, and the "Atmospheric variability of L1 data for each pixel [%]", AtmVar($L1_i$).

$U_I(L1_i)$ is first determined after L1 correction step "Dark correction" is applied (see section 6.4.2). It is calculated based on equation 55, here written in a slightly different way:

$$U_I(L1_i) = \sqrt{\left(\frac{1}{n_{DC} \cdot n_{PIX}} + \frac{1}{n_{BC}}\right) \cdot \sigma^2_{DCi} + \frac{1}{n_{BC}} \cdot GAIN \cdot L1_i} \tag{66}$$

The $L1_i$ are the corrected counts at pixel i from equation 73, GAIN is ICF-entry "Gain [counts per electron]" and the dark variance σ^2_{DCi} is given from the L0 data, i.e. $U_M(L0_i)$ for the dark measurements. n_{DC} and n_{BC} are the number of cycles for dark and bright counts respectively. n_{PIX} is set to 1 for the "Immediate dark method" and is the number of pixels on the detector for the "Dark map method" (see also section 6.4.2 and equation 61). Then $U_I(L1_i)$ is propagated through all other correction steps listed in section 6.4.

AtmVar($L1_i$) is defined by equation 67:

$$\text{AtmVar}(L1_i) = \left[1 - \frac{U_I(L1_i)^2}{U_M(L1_i)^2}\right] \cdot 100 \tag{67}$$

$U_M(L1_i)$ is initialized with $U_M(L0_i)$ as defined in section 6.3.3 and then propagated through all correction steps from section 6.4 just as it is done for $U_I(L1_i)$. AtmVar($L1_i$) is a percentage <100% indicating the magnitude of the atmospheric variability during the measurement interval. Small numbers mean the atmosphere was very stable. In practice the numbers can also be negative. Higher numbers mean there was more and more variability in the atmosphere. Numbers close to 100% are typically obtained, when a cloud moves in or out of the beam during a direct sun measurement.

There are special situations, where the L1 uncertainty output is not exactly as described in this section. This happens e.g. if only one cycle is measured and therefore no $U_M(L0_i)$ is given for the dark measurements. In this case the uncertainty is calculated in a different way, e.g. calculating the dark variance σ^2_{DCi} as shown in equation 6 based on ICF-entry "Dark variance power fit coefficients". The different cases are indicated by L1 output "Indicator for uncertainty and atmospheric variability (see manual for exact meaning)" and described in table 36. In the vast majority of situations the indicator will have the value 10, which means there were more than one cycle for both the bright and dark measurements and the description given in this section applies.

There is no common or structured uncertainty given for L1 in the current version of the Blick Software Suite. The reason is that at this moment there are no uncertainties associated to the different calibration parameters given in the ICF.

6.3.5 L2Fit Uncertainty

The L2Fit data include independent, U_I(L2Fit), common, U_C(L2Fit), and structured, U_S(L2Fit), uncertainties for the following parameters retrieved by the Blick spectral fitting algorithm (BlickSFA):

- Slant column amounts for each fitted gas
- Effective temperatures for each fitted gas
- Ring spectrum pseudo-slant column in case it was fitted
- Each coefficient of the smoothing polynomial used in the fitting
- Each coefficient of the offset polynomial used in the fitting
- Each coefficient of the wavelength change polynomial used in the fitting
- Each coefficient of the resolution change polynomial used in the fitting

Additionally, the L2Fit output also gives a so-called "rms-based uncertainty", denoted U_{rms}(L2Fit), for each of the parameters listed above. The detailed mathematics for the retrieval of all uncertanties is given in section 6.5.10. An overview of the error sources affecting L2Fit and whether they are included in the BlickSFA is given in table 40.

Table 40: Uncertainty output in L2Fit data. Column "Output" lists that L2Fit uncertainty output, in which the respective error source is taken into account. If this column is empty, then this source is not included in the BlickSFA yet. The error source "Reference spectrum" is split into different cases, depending on the choice of FSE "Reference" (see section 26).

Error source	**Remark**	**Output**
L1 data	U_I(L1) is propagated into L2Fit as shown in section 6.5.10 and contributes to U_I(L2Fit). Since no U_C(L1) or U_S(L1) is given in this software version, the L1 data do not contribute to U_C(L2Fit) or U_S(L2Fit) yet.	U_I(L2Fit)
Cross sections	Neither the choice of the cross sections nor their uncertainty is taken into account	
Algorithm deficiencies	The BlickSFA is an approximation and "suffers" from intrinsic deficiencies. Those are mostly caused by the use of pre-convoluted parameters, e.g. the cross sections, and cross-correlation among the fitted gases. These effects are not considered in the current software version.	
Reference "Ext*"	No uncertainty is associated with this reference. This means that any systematic issues arising from using a reference not measured by the instrument itself are neglected.	
Reference "Synt*"	ICF-entry "Independent instrumental uncertainty of synthetic reference spectrum for FUNCFILT" contributes to U_I(L2Fit), and the uncertainties in ICF-entry "Slant columns in synthetic reference spectrum for FUNCFILT" contribute to U_C(L2Fit) as shown in section 6.5.10. Potential errors from a possible "mismatch" of the reference, e.g. when using a solar reference for lunar data, are not considered. Any error in ICF-entry "Wavelengths for synthetic reference spectrum for FUNCFILT [nm]" is not considered either.	U_I(L2Fit) U_C(L2Fit)
Reference "Meas*"	As for uncertainties associated with L1 data only the U_I(L1) from the selected reference U_I(L2Fit) measurement is included and contributes to U_I(L2Fit).	
Reference "Ref_*"	If the external reference includes independent and/or common uncertainties, then they are propagated and contribute to U_I(L2Fit) and/or U_C(L2Fit).	U_I(L2Fit) U_C(L2Fit)
Effective temperature	If the effective temperature of a gas is NOT fitted, then the given uncertainty from FSE "Gas temps" is propagated through the BlickSFA and contributes to output U_S(L2Fit). Hence if FSE "Gas temps" contains totally unreasonable values, then unreasonable values for U_S(L2Fit) are produced too.	U_S(L2Fit)
Molecular scattering	If FSE "Mol scatt" is NOT set to "NO", then the Blick Software Suite takes an estimation for the uncertainty of the surface pressure from a climatology, propagates it through the BlickSFA, and adds it to output U_S(L2Fit).	U_S(L2Fit)
"Known" slant OD	If one or more heritage f-codes are used in the spectral fitting (see section 5.10.3), then the output from those calculations is subtracted as "known" slant OD in the BlickSFA, the respective uncertainties are propagated and added to the final L2Fit output uncertainties.	U_I(L2Fit) U_S(L2Fit) U_C(L2Fit)

6.3.6 L2 Uncertainty

L2 data based on the "L2 Direct Algorithm" (see section 6.6), i.e. total vertical column amounts and effective temperatures for each output gas, include independent, U_I(L2), common, U_C(L2), structured, U_S(L2), total, U(L2), and "rms-based", U_{rms}(L2), uncertainties. The Blick Software Suite propagates the uncertainties coming from the L2Fit output and also adds uncertainty raising from the estimation of the direct AMF. Figure 18 shows as an example the different uncertainty contributions for total vertical NO_2 columns of Pandora 67 for a period of 15 min.

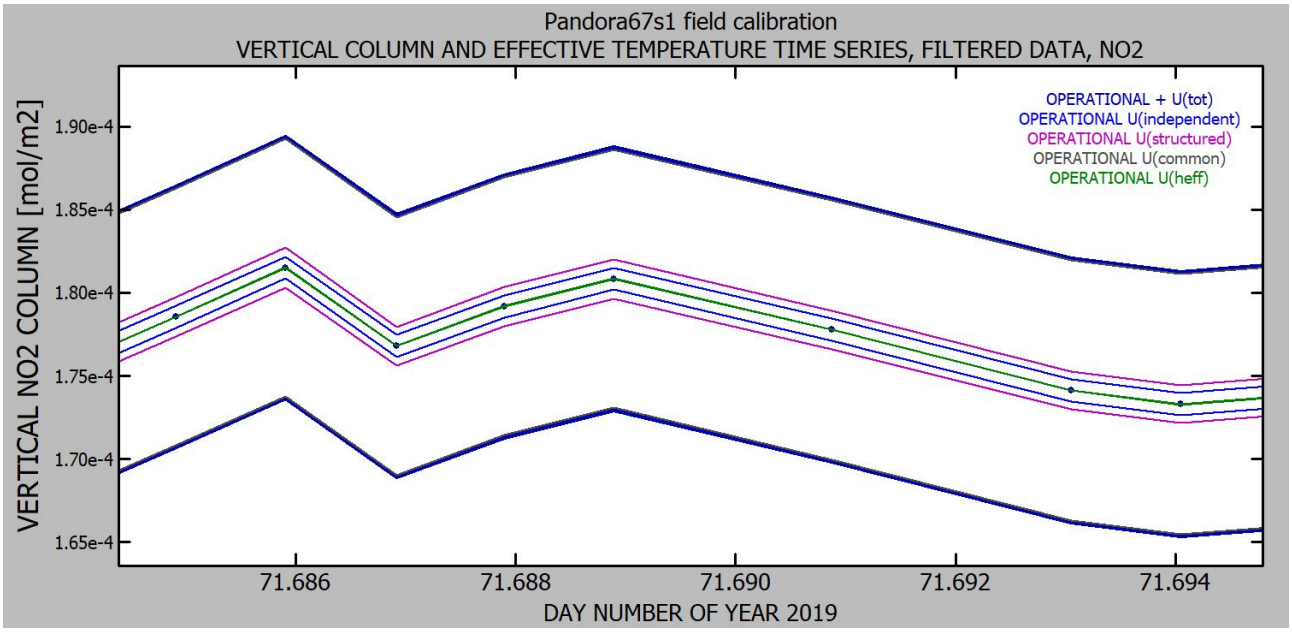


Figure 18: Vertical NO_2 column amount from Pandora 67 for a period of about 15 min on 12 Mar 2019 (dots) and different uncertainties as lines: AMF-uncertainty (green), independent uncertainty (light blue), structured uncertainty (purple), common uncertainty (grey, mostly hidden under the dark blue line) and total uncertainty (thick dark blue).

For the tropospheric columns and surface concentrations obtained by the Air-Ratio Sky Algorithm, the Blick Software Suite produces an independent uncertainty output by simply propagating the independent uncertainties from the L2Fit data through equations listed in section 6.7. No other (common or structured) uncertainties are produced yet in the software version. For the profile data (section 6.7.5) no uncertainty information at all is given.

6.4 L1 Algorithm - Data Correction

6.4.1 Overview

A maximum of 9 processing steps can be applied to the Pandora L0 data to produce L1 data.

1. Dark correction
2. Non-linearity correction
3. Latency correction
4. Flat field correction
5. Conversion to count rates
6. Temperature correction
7. Stray light correction
8. Sensitivity correction
9. Wavelength correction

Each step is described in the following sections. The mathematical equations describe how L0 data at pixel i, $L0_i$, are converted into L1 data at pixel i, $L1_i$. By default BlickP applies all correction steps to the L0 data, but it also allows to only apply a subgroup of correction steps for research purposes (see section 5.10.2). Note that the order of the correction steps cannot be changed since they are not commutative. If no correction steps are applied, then the L1 data equal the L0 data.

$$L1_i = L0_i \tag{68}$$

We will use this equation as a starting point for all equations to come, which means $L1_i$ "evolves" through the correction steps. In order to make the equations more readable, we will call the L1 data, which have been processed for all previous correction steps, $L1_i^*$ (at the right side of the equation) and the L1 data with the new correction step added $L1_i$ (at the left side of the equation).

6.4.2 Dark Correction

The theory of the dark count is described in section 6.2. It is the sum of the dark offset (given by an electronic bias of the ROE) and the dark slope (charge produced by thermal electrons). The Pandora dark count depends on the detector it is using. Most instruments have a dark count behavior as shown in figure 19. The dark offset is about 1-2 % (of the saturation value) and the dark slope is about 1-2 % per second at the current operational temperature. For our standard 16-bit AD converter, this corresponds to about 1000 counts dark offset and 1000 counts/s dark slope at a detector temperature of about 25°C.

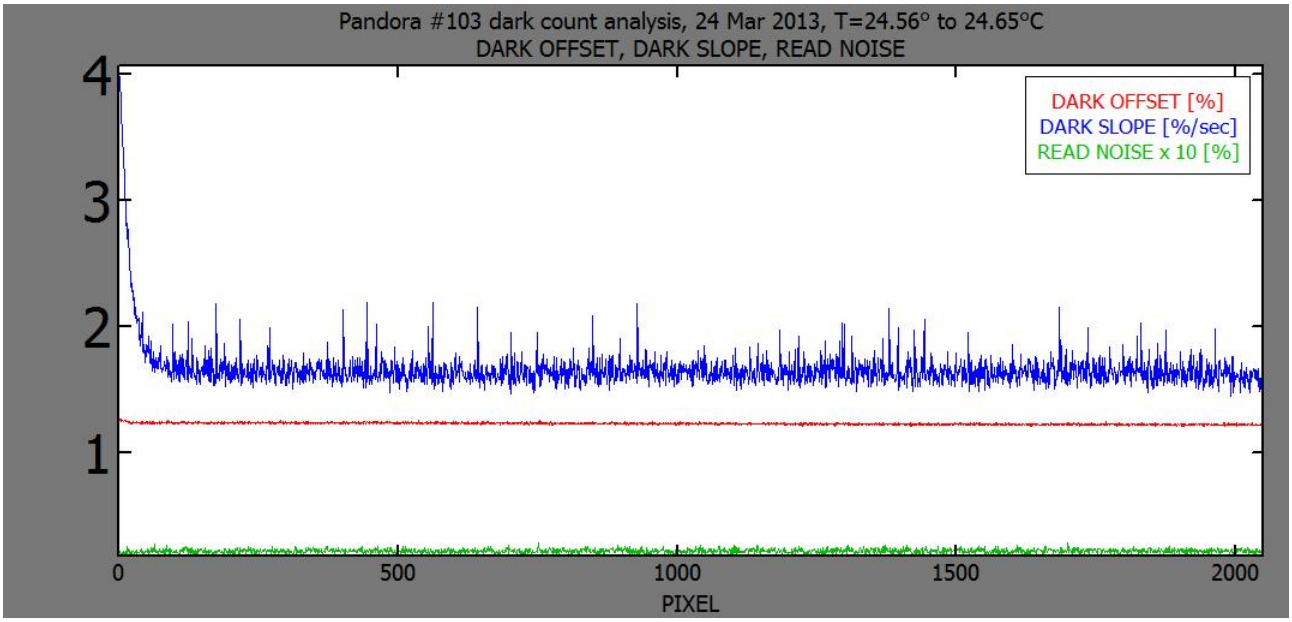


Figure 19: Dark offset (red), dark slope (blue) and read noise (green) of Pandora 103 as a function of pixel. Data are for a set temperature of 20 °C. The electronics board temperature is about 25 °C.

As explained in section 6.2, there are two methods to estimate the dark count. For the "Immediate dark method", only the dark count measured immediately after the regular measurements (with light input) is used to estimate the dark count included in the regular data. In that case the estimated dark count at pixel i, DC_{Ei}, is identical to the immediate dark measurements DC_i:

$$DC_{Ei} = DC_i \tag{69}$$

For the "Dark map method", the immediate dark measurements are used in combination with the "dark fine structure map", which has been determined during calibration. In that case the dark count is estimated as follows:

First the dark count fine structure DC_{FINEi} is calculated:

$$DC_{FINEi} = A_{ICi} \cdot \exp^{B_{ICi} \cdot (T_{RE} - T_{RR})} + A_{SLi} \cdot \exp^{B_{SLi} \cdot (T_{RE} - T_{RR})} \cdot IT \tag{70}$$

T_{RE} is the radiometric effective temperature during the bright measurement, T_{RR} is the dark count reference temperature, IT is the integration time and A_{ICi}, B_{ICi}, A_{SLi} and B_{SLi} are the so-called A- and B-parameters for the dark fine structure intercept and slope respectively. All those parameters are determined during calibration.

Then the dark count fine structure is subtracted from the immediate dark measurements and the dark background DC_{BGi} is obtained by fitting the "dark background function" in the difference DC_i minus DC_{FINEi}. The dark background function is the sum of an exponential function and an Nth order polynomial as shown in equation 71:

$$\mathrm{DC_{BG}}_i = \mathrm{E_0} \cdot \exp^{-\mathrm{E_1} \cdot pixind} + \mathrm{C_0} + \mathrm{C_1} \cdot pixind + ... + \mathrm{C_{N+1}} \cdot pixind^{\mathrm{N}} \tag{71}$$

pixind are the indices of the regular pixels divided by 1000 (starting to count at 0), i.e. for the first regular pixel pixind=0, for the second pixind=0.001, etc. $\mathrm{E_0}$ and $\mathrm{E_1}$ are the parameters of the exponential part and $\mathrm{C_0}$, $\mathrm{C_1}$, etc. are the coefficients of the polynomial. By adding the exponential term, the function is able to follow the "hockey stick" in the dark count (see figure 19). Note that the fitting includes the uncertainty in the measured dark count.

The dark count fine structure is added to the fitted dark background to obtain the estimated dark count $\mathrm{DC_E}_i$:

$$\mathrm{DC_E}_i = \mathrm{DC_{BG}}_i + \mathrm{DC_{FINE}}_i \tag{72}$$

If the detector has blind pixels, they can also be included in the dark correction by subtracting their mean value from both the regular measurements and the dark measurements. The $\mathrm{L1}_i$ after dark correction are given by:

$$\mathrm{L1}_i = \left(\mathrm{L1}_i^* - \frac{1}{\mathrm{n_{BLIND}}} \cdot \sum_{j=1}^{\mathrm{n_{BLIND}}} \mathrm{L1}_j^* \right) - \left(\mathrm{DC_E}_i - \frac{1}{\mathrm{n_{BLIND}}} \cdot \sum_{j=1}^{\mathrm{n_{BLIND}}} \mathrm{DC}_j \right) \tag{73}$$

$\mathrm{DC_E}_i$ is from equation 69 or 72 and $\mathrm{n_{BLIND}}$ is the number of blind pixels in the detector (see section 6.2.6). The '$\mathrm{n_{BLIND}}$-terms' in equation 73 are not included if the detector has no blind pixels or if no 'blind correction' is requested in the data processing.

6.4.3 Non-Linearity Correction

Image sensors are in general not linear, i.e. they do not return a doubled signal when they are illuminated by the double amount of light. A typical non-linearity curve is shown in figure 20. The non-linearity of Pandora is typically a few percent for not too low counts. For very low counts, the non-linearity leaves the range of a few percent correction, i.e. the instrument returns significantly more signal than it should if it was linear. The linearity is characterized in the laboratory and is not dependent on the temperature. To fit the non-linearity the Blick software uses an equation of this type:

$$\mathrm{NLC}_i = \mathrm{E}_0 \cdot \exp^{-\mathrm{E}_1 \cdot (\mathrm{L1}_i^*)^{\mathrm{E}_2}} + \mathrm{C}_0 + \mathrm{C}_1 \cdot \mathrm{L1}_i^* + ... + \mathrm{C}_{\mathrm{N+1}} \cdot (\mathrm{L1}_i^*)^{\mathrm{N}} \tag{74}$$

The order N of the polynomial depends on the detector of the specific Pandora unit, but in general a first or second order polynomial is sufficient. To correct for the non-linearity, the measured counts are divided by the non-linearity. The $\mathrm{L1}_i$ after non-linearity correction are given by:

$$\mathrm{L1}_i = \frac{\mathrm{L1}_i^*}{\mathrm{NLC}_i} \tag{75}$$

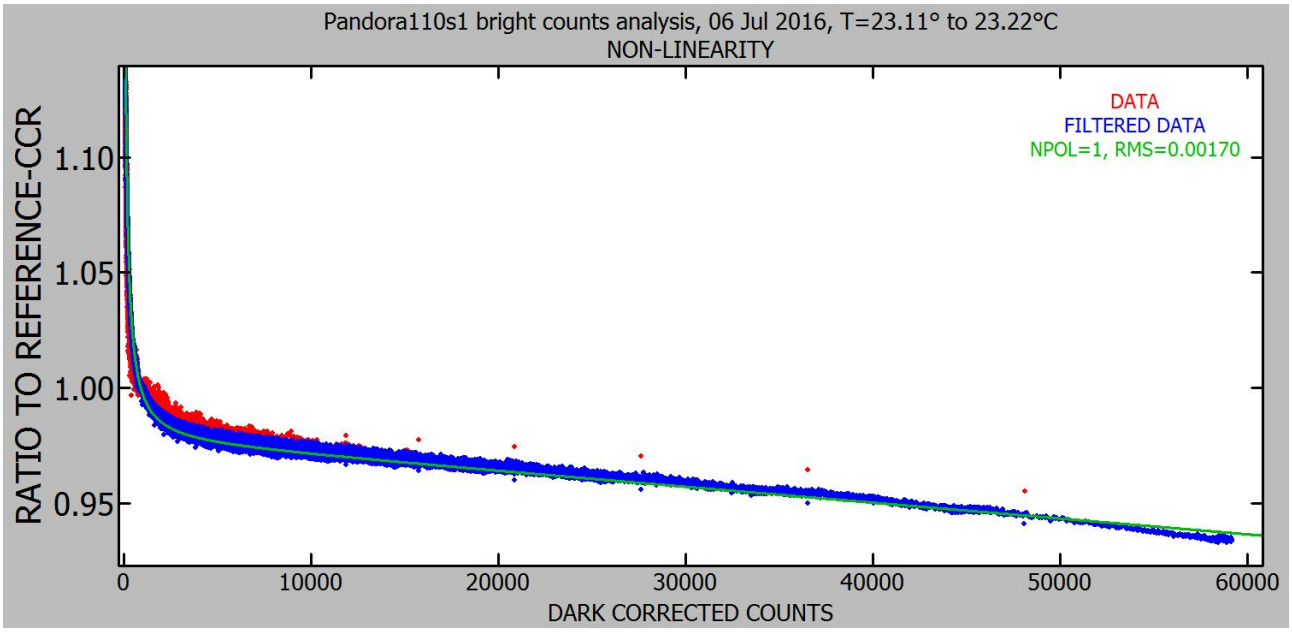


Figure 20: Non-linearity effect for Pandora 110. Data are in red, the data passing the filter criteria in blue and the fit in the blue data is in green.

6.4.4 Latency Correction

Latency effects in the ROE of CCD detectors can cause the readings in a pixel to be influenced by the readings in the previously read pixels. E.g. if there are many subsequent high readings followed by very low readings, then the first low readings are biased high, since a residual charge from the previous readings is still in the ROE capacitor. This is shown in figure 21 for measurements with Pandora 106. For this test the detector was removed from the spectrometer, about a quarter of the pixels on each side were covered and data were taken, where only the central pixels were illuminated (blue line in figure). Then the detector was 'reversed' (rotated by 180°) keeping the illumination constant and the measurements repeated (red line). Hence the only difference between the blue and red line in the figure is that the CCD is read from left to right in one case (blue line) and from right to left in the other case (red line). One can see that for the first pixels read after the high

signal region the values are biased high, therefore blue line exceeds the red line around pixels 1500 and higher, while the red line exceeds the blue line around pixels 550 and lower.

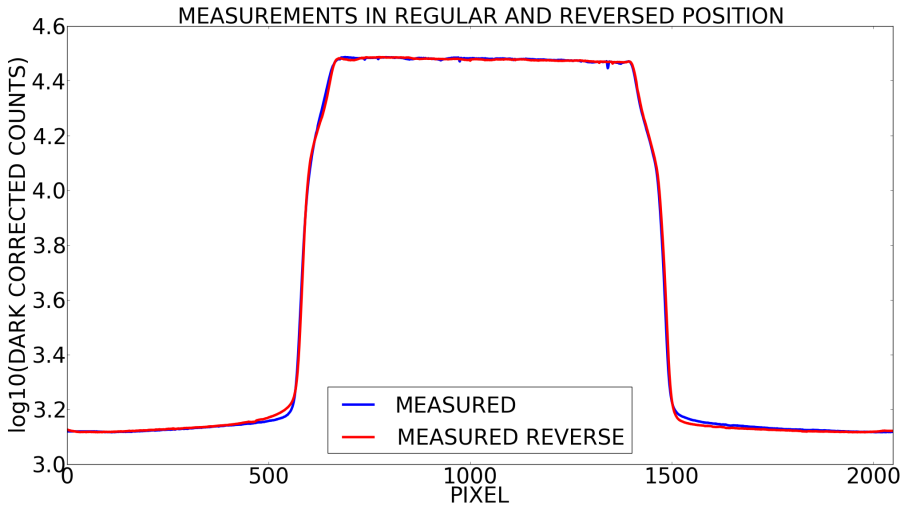


Figure 21: Logarithm of dark corrected counts as a function of the pixel number for measurements, where only the central part of the detector (pixels 600 to 1500) was illuminated and the left and right side blocked. Blue line is for the detector in regular orientation. Red line shows the same illumination on the reversed detector. Reading direction is left to right for the regular orientation (blue line) and right to left for the reversed orientation (red line).

The $L1_i$ after latency correction are given by:

$$L1_i = L1_i^* - \Delta LAT_i \tag{76}$$

ΔLAT_i is the latency correction vector. If is determined in a recursive way as shown in equation 77.

$$\begin{aligned} \Delta LAT_1 &= 0 \\ \Delta LAT_{i+1} &= \Delta LAT_i \cdot (1 - c_{DECAY}) + L1_i^* \cdot c_{GAIN} \end{aligned} \tag{77}$$

c_{DECAY} and c_{GAIN} are the latency decay and latency gain constants respectively. i=1 is the first pixel to be read by the ROE, i=2 the seconds one, etc. For Pandora 106, these constants were determined to c_{DECAY}=6.3e-3 and c_{GAIN}=1.8e-5. Figure 22 is a zoom of figure 21 in linear scale. The black line are the latency corrected counts.

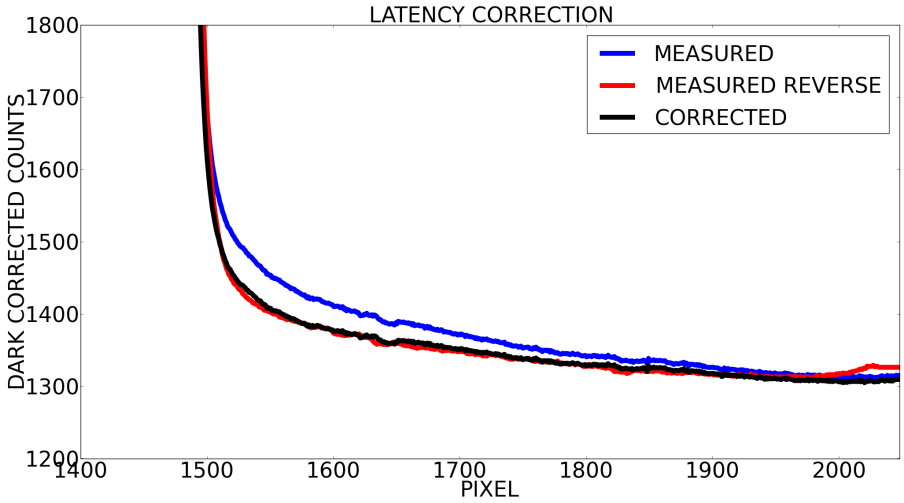


Figure 22: Zoom of figure 21 in linear scale. Blue line are the regular measurements, black line the regular measurements with the latency correction applied.

While the latency correction algorithm is incorporated in the L1 algorithm, it is currently not applied to most instruments, since the actual technique to determine the latency constants c_{DECAY} and c_{GAIN} is extremely risky, difficult and time-consuming as the detector has to be removed from the spectrometer.

6.4.5 Flat Field Correction

Even when each pixel is illuminated by the same amount of light, they all return slightly different signals. This is called "Pixel Response Non Uniformity" (PRNU) and is caused by physical differences in the pixels. The PRNU is determined during the radiometric calibration and is expressed in percent (figure 23). Note that if the lamp signal is not smooth as a function of wavelength, lamp features might falsely be interpreted as PRNU. Therefore only selected lamps can be used for the radiometric calibration.

The PRNU is typically on the order of ± 1 %. Some detectors used in Pandora are 2D image arrays, where N vertical pixels are read in binned mode. This means that the returned value is in reality the sum over N pixels and therefore the measured PRNU is the "true" PRNU divided by $\sqrt{N}$. E.g. Pandora 39 uses a N=16 detector, reducing the measured PRNU from about ± 1 % to ± 0.25 % (figure 23). During radiometric calibration we only determine the PRNU for the binned pixels.

The $L1_i$ after flat field correction are given by:

$$L1_i = \frac{L1_i^*}{PRNU_i} \tag{78}$$

$PRNU_i$ is the 1+PRNU/100 for pixel i.

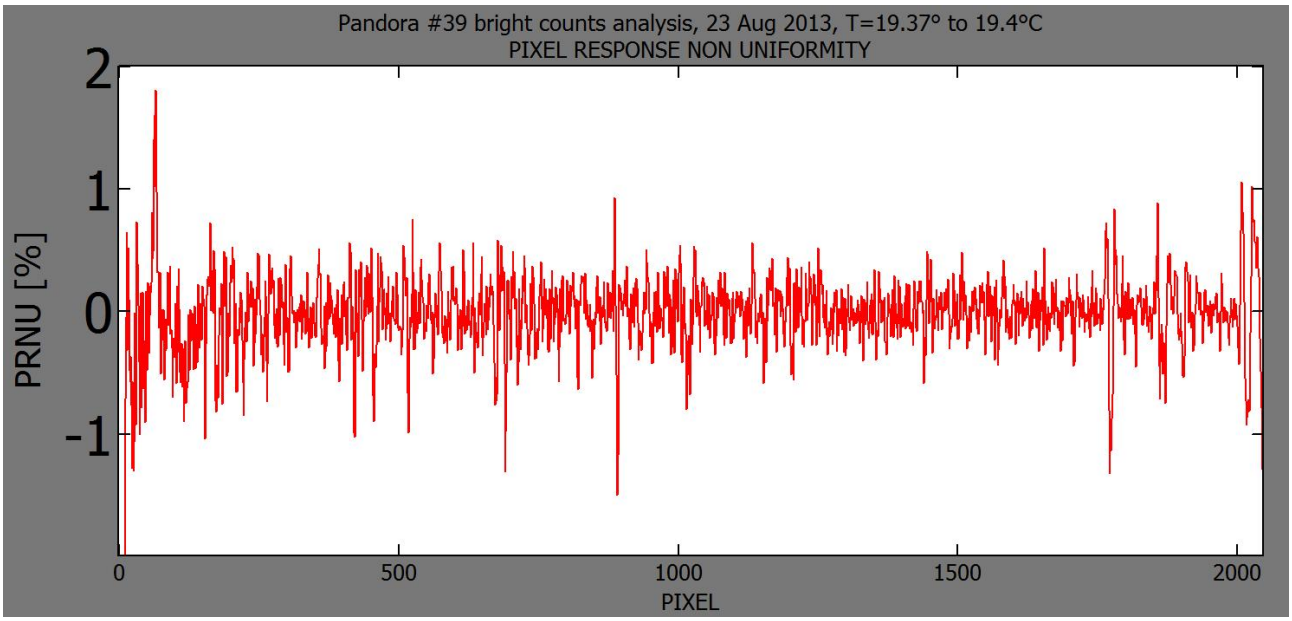


Figure 23: PRNU for Pandora 39 as a function of pixel. Note that the detector for this unit is binning 16 pixels at each scan, which reduces the "single pixel" PRNU by a factor of 4.

6.4.6 Conversion to Count Rates

In this correction step the data are divided by the integration time, which changes their unit from "counts" or "DN" to "counts/s" or "DN/s". For earlier generation Pandoras we noticed that the nominal integration time (the one requested by the user) and the effective integration time (the "true" number) often had a small bias relative to each other. This bias causes very irregular features in the final figure of the linearity calibration (figure 20 in section 6.4.3) and can therefore be detected during calibration. Newer Pandoras show no difference between the nominal and effective integration time.

The $L1_i$ after the conversion to count rates are given by:

$$L1_i = \frac{L1_i^*}{t - \Delta t} \tag{79}$$

t is the nominal integration time and Δt the difference between the nominal and effective integration time. Both are given in seconds resulting a unit of "counts/s" for the $L1_i$ after this step.

6.4.7 Temperature Correction

In order to determine the temperature sensitivity of Pandora, the radiometric calibration is performed in the laboratory at three different spectrometer temperatures. Our experience has shown that a Pandora in good condition does only have very small radiometric temperature sensitivity, which means no temperature correction is applied to the data. In the case a signal change as a function of temperature is noted, the instrument will give false calibration results in the other tests as well, thus leading to an investigation of a hardware problem, e.g. moisture inside the optical bench.

The C_{1i} after temperature correction are given by:

$$L1_i = \frac{L1_i^*}{TC_i} \tag{80}$$

TC_i is the temperature correction polynomial evaluated at pixel i.

6.4.8 Stray Light Correction

The different options for stray light correction are listed in table 23. NO means that no stray light correction is applied to the data. SIMPLE means a "simple" stray light correction is applied, which consists of subtracting the average signal below 290 nm from the spectra. The logic behind this method is that no solar light reaches the Earth's surface in these wavelengths, thus we can attribute such residual signals to stray light. In this case the $\mathrm{L1}_i$ are given by:

$$\mathrm{L1}_i = \mathrm{L1}_i^* - MEAN(\mathrm{L1}_i^* \quad for \quad \lambda_i < 290nm) \tag{81}$$

The Pandora data processing software is also set up to apply so-called "matrix stray light correction methods" MM and CORRMM to the spectra, which are based on the knowledge of the instrument's slit function, typically obtained from laser measurements [57]. Note that the determination of the slit function outside the region near the target pixel was not possible until spring of 2015 due to a problem with the dark offset (for more details see section 6.2.6). If no stray light calibration exists for a unit, methods MM and CORRMM cannot be applied and BlickP switches to method SIMPLE.

MM and CORRMM are the uncorrected and corrected matrix method respectively. The stray light corrected data are obtained applying a "stray light correction matrix" on the uncorrected data.

$$\overrightarrow{L1} = \mathbf{M} \cdot \overrightarrow{L1^*} \tag{82}$$

$\overrightarrow{L1}$ is the (npix,1) vector of the L1 data, $\mathbf{M}$ is the (npix,npix) stray light correction matrix. npix is the number of regular pixels on the detector and the dot stands for a matrix multiplication in this case. For Method MM, no additional correction to the stray light correction matrix is applied. For CORRMM, equation 81 is applied after the stray light correction matrix is applied. This method is typically used when light contribution outside the unit's spectral range is expected.

The L1 and L2 data also report a parameter called "Estimated average residual stray light level [%]". This parameter is the ratio of the average signal below 290 nm over the average signal over all wavelengths. Note that for method SIMPLE this ratio is taken before the stray light correction, since after the correction it would be 0 by default after it. For method MM it is taken after the stray light correction and for method CORRMM it is taken after the matrix is applied, but before the signal below 290 nm is subtracted.

Another parameter reported in the L1 data is the "Estimated stray light in the signal before correction at X nm [%]", with X=300, 302.5, 305, 310, 320, 350 or 400. This gives an estimation of what fraction of the signal at a certain wavelength was due to stray light. These parameters are not determined for method NO.

6.4.9 Sensitivity correction

In this step the spectra are converted to "what would have been measured if open hole had been in both filter wheels". The radiometric calibration of an instrument is done using an ANSI standard 1000 watt quartz halogen lamp (FEL lamp). If a certificate exists for this lamp, which gives the absolute output of the lamp for a given input current and at a given distance from it, then the sensitivity correction applies absolute calibration to the data and the unit of the L1 data changes from [counts/s] to $\left[\mathrm{W/m^2/nm}\right]$ for direct sun or direct moon data and to $\left[\mathrm{W/m^2/nm/sr}\right]$ for sky observations. If there is no certificate, then the calibration is used to determine the filter transmission and the unit after the correction stays [counts/s].

Figure 24 shows measured transmissions for the filters in filterwheel 1 of Pandora 103. Note that the filter transmission determined in the laboratory is also affected by stray light. If no or insufficient stray light correction is applied, the transmission values in the short UV will be biased high.

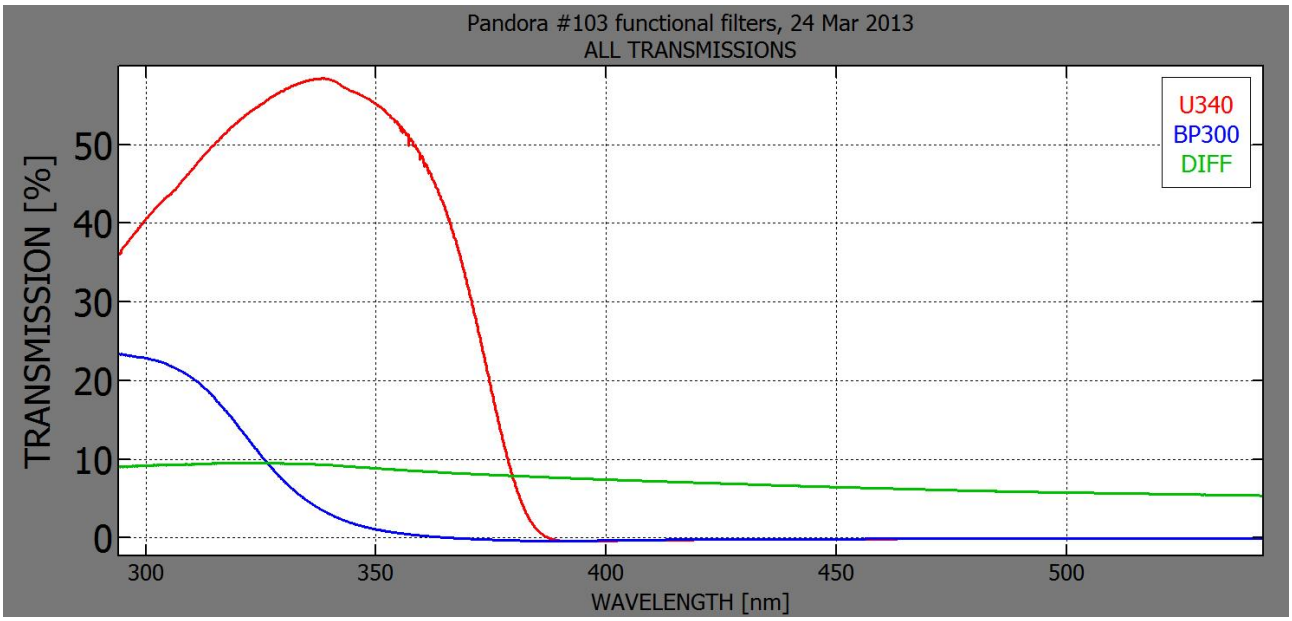


Figure 24: Measured transmissions for filters in Pandora 103 as a function for wavelength. U340 is a colored glass bandpass filter with peak transmission at 340 nm (red line). BP300 is an interference bandpass filter with peak transmission at 300 nm. DIFF is a ground quartz diffuser. Note that the fact that the blue line is increasing to the left of 300 nm is not due to a peak transmission of the BP300 filter shifted to the left of 300 nm. This is caused by the instrument's stray light. That means the measured transmission values in the region around 300 nm are overestimated, in the case only the simple stray light correction method is applied (see section 6.4.8).

Figure 25 shows the absolute spectral sensitivity of Pandora 30 for direct sun setting, i.e. with a diffuser in the filterwheels. It reaches around 16 $\frac{\text{counts/s}}{\text{W/m}^2\text{/nm}}$ at 430 nm. Different lines refer to different alignment methods and different calibration lamps used in the laboratory setup. We still notice differences in the results based on the exact laboratory setup. For this reason we still investigate how we can improve the absolute calibration technique.

The shape of the absolute sensitivity of Pandora is basically a combination of all optical elements involved, mainly the fiber transmission, grating efficiency and quantum efficiency of the detector. The L1_i after the sensitivity correction are given by:

$$\text{L1}_i = \frac{\text{L1}_i^*}{\text{SENS}_i} \tag{83}$$

SENS_i is the sensitivity (or calibration function) of the instrument at pixel i.

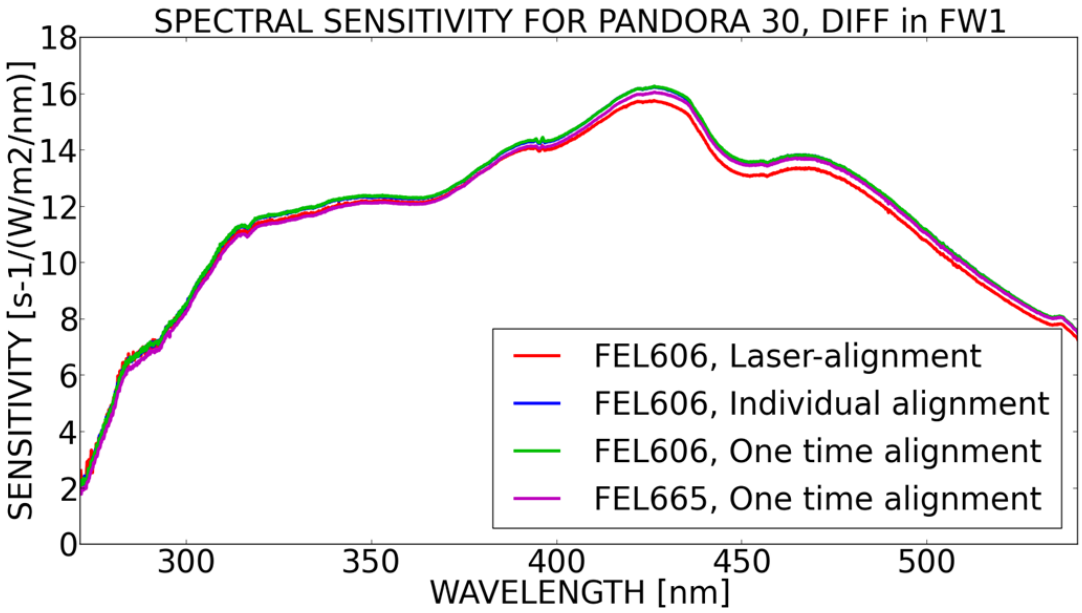


Figure 25: Absolute sensitivity of Pandora 30 for direct sun observations (i.e. with a diffuser in the filterwheels). Different lines refer to different alignment methods and different calibration lamps.

6.4.10 Wavelength Correction

An optional last data correction step is the wavelength correction. This is only needed for users which require the L1 data to be on a fixed wavelength grid. It is not necessary for the current operational PGN data products. In this step the measured spectra are shifted to the nominal wavelength grid using the corresponding "Standard spectrum for FUNCFILT" from the ICF. Note that the wavelength change retrieval is done using the spectral fitting technique (see section 6.5) with the fitting parameters set by ICF-entry "Wavelength change retrieval parameters for FUNCFILT".

6.5 L2Fit Algorithm - Spectral Fitting

The L2Fit data are the result of applying the BlickSFA on the L1 data, which is described in this section.

6.5.1 Lambert-Beer's law

BlickSFA is based on Lambert-Beer's law.

$$F(\lambda) = F_0(\lambda) \cdot \exp\left(-\sum_{j=1}^{n_{EX}} \tau s_j(\lambda)\right) \tag{84}$$

λ	Wavelength
$F_0(\lambda)$	Spectrum at wavelength λ reaching the top of the atmosphere; that is the "Extraterrestrial spectrum" adjusted for the Sun-Earth distance
$F(\lambda)$	Spectrum at wavelength λ reaching the instrument's entrance window
n_{EX}	Number of extinction processes in the atmosphere
$\tau s_j(\lambda)$	Slant optical depth at wavelength λ for extinction process j

The slant optical depth $\tau s_j(\lambda)$ is given by:

$$\begin{aligned} \tau s_j(\lambda) &= qs_j^*(\lambda) \cdot \sigma_j(\lambda, T_j) \\ &= qs_j(\lambda) \cdot \tau_{STDj}(\lambda, T_j) \\ &= m_j(\lambda) \cdot q_j \cdot \tau_{STDj}(\lambda, T_j) \end{aligned} \tag{85}$$

$qs_j^*(\lambda)$	Absolute slant column amount for extinction process j at wavelength λ [units e.g. mol/m^2]
T_j	Effective temperature of extinction process j [K] (see equation 3)
$\sigma_j(\lambda,T_j)$	Cross section for extinction process j at wavelength λ and effective temperature T_j [m^2/mol]
$\tau_{STDj}(\lambda,T_j)$	"Standard vertical optical depth" for extinction process j at wavelength λ [1]
$qs_j(\lambda)$	Relative slant column amount for extinction process j at wavelength λ [1]
$m_j(\lambda)$	AMF (or optical mass) for extinction process j at wavelength λ [1]
q_j	Relative vertical column amount extinction process j [1]

For the standard vertical optical depth $\tau_{STDj}(\lambda,T_j)$, BlickSFA uses the settings as listed in table 22. Note that introducing τ_{STDj} has no other reason than bringing the relative column amounts qs_j or q_j into values around 1, which makes the whole algorithm numerically more stable. Hence using even very different values for τ_{STDj} would not change the results, as long as they are in a similar order of magnitude.

6.5.2 Convolution

Real instruments do not measure a monochromatic $F(\lambda)$, since their slit function extends over a certain band-pass. In the case absolute calibration has been applied, the L1 value at pixel i is given by a convolution of $F(\lambda)$ times the instrument sensitivity $SENS(\lambda)$ with slit function $S_i(\lambda)$ at the center wavelength λ_i of the pixel.

$$L1_i = F_i = \frac{1}{SENS_i} \cdot \int_{\Delta\lambda_i} F(\lambda) \cdot SENS(\lambda) \cdot S_i(\lambda_i - \lambda) \cdot d\lambda \tag{86}$$

$SENS_i$ is the instrument's spectral sensitivity as from the L1 correction step described in section 6.4.9, $\Delta\lambda_i$ is the instrument bandpass at pixel i and F_i is the high-resolution spectra convoluted at pixel i. Applying the same convolution over the entire equation 84 yields:

$$F_i = \frac{1}{SENS_i} \cdot \int_{\Delta\lambda_i} F_0(\lambda) \cdot \exp\left(-\sum_{j=1}^{n_{EX}} \tau s_j(\lambda)\right) \cdot SENS(\lambda) \cdot S_i(\lambda_i - \lambda) \cdot d\lambda \tag{87}$$

Equation 87 is the fundamental equation for another type of trace gas retrieval algorithm, often called "Direct fitting algorithm". In such algorithm all unknowns in equation 87 (the $m_j(\lambda)$, q_j and T_j) are varied in an iterative process until the right and left side of the equation agree within a certain tolerance for all pixels i. These types of algorithms are very time consuming, since the numerical convolution is applied at each iteration step and even nowadays they are not really possible for real time data processing. Therefore the Blick Software Suite uses the following approximation of equation 87:

$$F_i = F_{0i} \cdot \exp\left(-\sum_{j=1}^{n_{EX}} \tau s_{ji}\right) \tag{88}$$

$F_0(\lambda)$ is the convoluted top-of-atmosphere spectrum given by equation 89 and τs_{ji} is the slant optical depth of absorber j for slant column qs_j and effective temperature T_j at pixel i, which is described in the next section.

$$F_{0i} = \frac{1}{SENS_i} \cdot \int_{\Delta\lambda_i} F_0(\lambda) \cdot SENS(\lambda) \cdot S_i(\lambda_i - \lambda) \cdot d\lambda \tag{89}$$

6.5.3 Slant Optical Depth

BlickSFA's method to calculate the slant optical depth for each trace gas j listed in fitting setup entry (FSE) "Fitted Gases" with slant column qs_j and effective temperature T_j at pixel i is done in a two step process.

The first step is to calculate the convoluted the slant optical depth of extinction process j at wavelength λ_i, τs_{ji}, at different relative slant columns qs_j, .

$$\tau s_{ji}(\lambda_i, qs_j) = -\ln\left[\frac{\int_{\Delta\lambda_i} F_0(\lambda) \cdot \exp\left(-qs_j \cdot \tau_{STDj}(\lambda, T_j)\right) \cdot SENS(\lambda) \cdot S_i(\lambda_i - \lambda) \cdot d\lambda}{\int_{\Delta\lambda_i} F_0(\lambda) \cdot SENS(\lambda) \cdot S_i(\lambda_i - \lambda) \cdot d\lambda}\right] \tag{90}$$

All variables are as in equations 85 and 87. Equation 90 is calculated for qs_j values ranging from 1 to 9.

The second step consists in expressing the τs_{ji} as a function of qs_j using so-called OD-fitting parameters A_{ji}, B_{ji} and C_{ji}.

$$\begin{aligned} \tau s_{ji} &= A_j(\lambda_i, T_j) \cdot qs_j^{1+B_j(\lambda_i,T_j)+C_j(\lambda_i,T_j)\cdot ln(qs_j)} \\ &= A_{ji} \cdot qs_j^{1+B_{ji}+C_{ji}\cdot ln(qs_j)} \end{aligned} \tag{91}$$

Equation 91 is a more general approach than what is usually applied in classical Differential Optical Absorption Spectroscopy (DOAS) [32], where only linear absorbers are included. The BlickSFA is also capable to include

stronger extinction processes, for which the relationship between the slant column amount and the slant OD is not linear. We call these species "non-linear absorbers".

Which OD fitting method is used for absorber j by the BlickSFA is decided by FSE "Gas OD Meths". There are four options:

OD Fitting Method	**Description**
OD Fitting Method 0	Here no OD fitting is done and $\tau s_{ji}(\lambda_i,qs_j=1)$ from equation 90 is used as an approximation of τs_{ji}. For this method OD-fitting parameters B and C result zero.
OD Fitting Method 1	A linear fit forced through the point (0,0) is done in the $\tau s_j(\lambda_i,qs_j)$ calculated at qs_j ranging from 1 to 9. Also for this method OD-fitting parameters B and C result zero.
OD Fitting Method 2	A linear fit is done for $ln[\tau s_j(\lambda_i,qs_j)]$ calculated at qs_j ranging from 1 to 9 as a function of $ln[qs_j]$. For this method OD-fitting parameter B differs from zero and C is zero.
OD Fitting Method 3	A quadratic fit is done for $ln[\tau s_j(\lambda_i,qs_j)]$ calculated at qs_j ranging from 1 to 9 as a function of $ln[qs_j]$. For this method OD-fitting parameters B and C differ from zero.

The technique of using non-linear relationships between the slant column and the slant OD has already been applied for filter instruments, where OD fitting method 2 was implemented [42]. Method 3 is an extension of method 2 as a novel approach of BlickSFA.

The different OD-fitting methods are illustrated in figure 26. OD fitting method 0 is the dark blue line, method 1 the green line, method 2 the magenta line and method 3 the light blue line. For this very strong water vapor line at 823 nm, any other OD fitting method than 3 would result in huge errors.

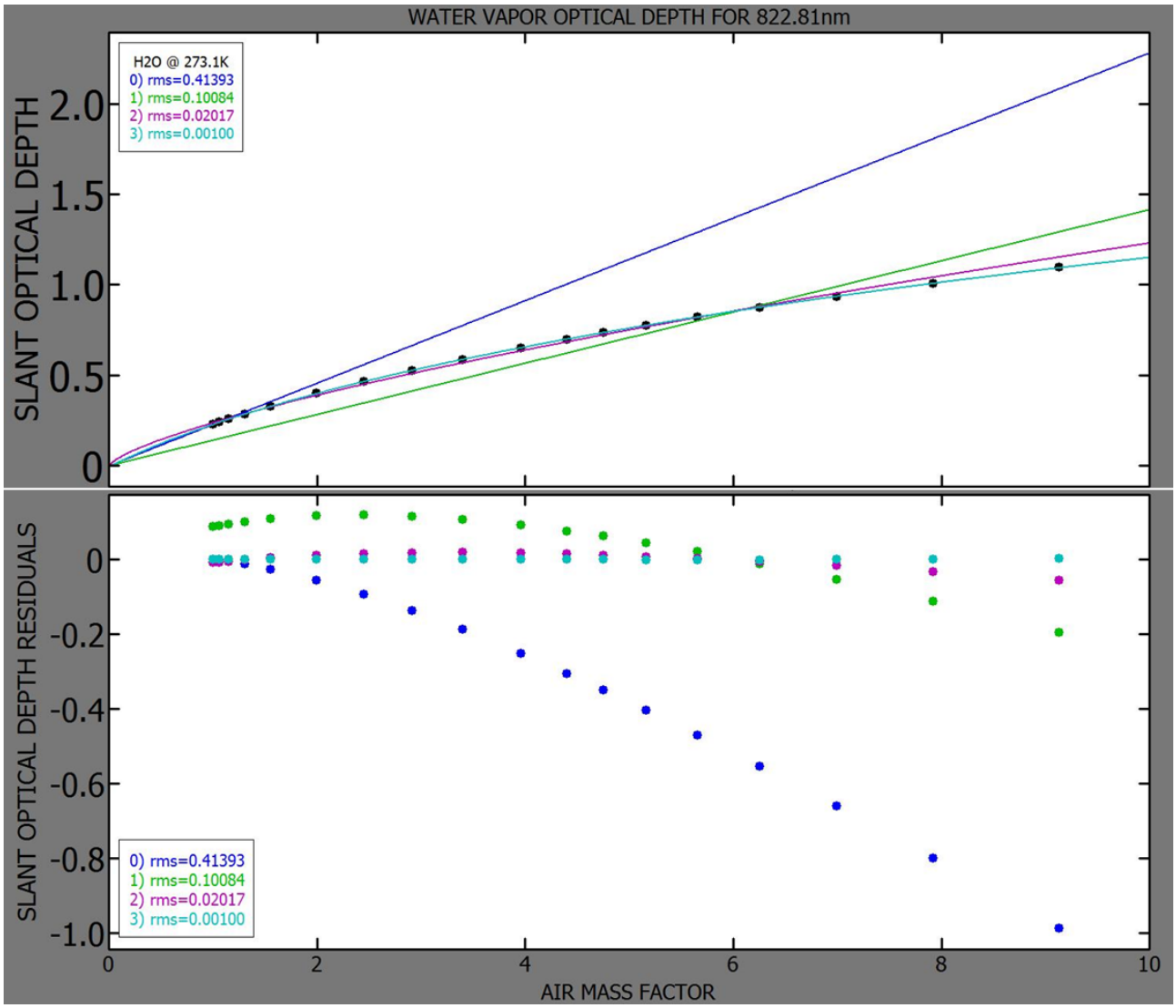


Figure 26: Top: Slant optical depth as a function of the AMF for a vertical column amount of 1 cm precipitable water calculated for AMFs from 1 to 9.3 (black dots) at a strong water vapor line (822.81 nm). Colored lines are different fits in the black dots using 1 (dark blue and green), 2 (magenta) or 3 (light blue) fitting parameters. Bottom: Difference between the black dots and the fitted lines from the top panel. The rms of the difference is given in the figure legend.

OD-fitting parameters A, B and C from equation 91 are in general a function of the effective gas temperature T_j. The BlickSFA allows a temperature dependence up to order 2.

$$A_{ji} = A_{jCi} + A_{jLi} \cdot \frac{T_j - T_{jREF}}{T_{SCALE}} + A_{jQi} \cdot \left(\frac{T_j - T_{jREF}}{T_{SCALE}} \right)^2 \tag{92}$$

A_{jCi}, A_{jLi} and A_{jQi} are the constant, linear and quadratic terms of OD-fitting parameter A in temperature, T_j is the effective gas temperature for gas j, T_{jREF} is the reference temperature of gas j as given in table 27 and T_{SCALE} is a temperature scale factor given in the ICF (usually 50 K). The same equation 92 is used for OD-fitting parameters B and C.

6.5.4 Basic Fitting Equation

Taking the logarithm of equation 88 and rearranging we obtain:

$$\ln F_{0i} - \ln F_i = \sum_{j=1}^{n_{EX}} \tau s_{ji} \tag{93}$$

The following extinction processes are included in the right side of the equation:

- Molecular absorption by gases (see table 22)
- Rayleigh and Raman scattering by air molecules
- Mie scattering and absorption by aerosols

There are instrumental effects, which can alter equation 93, e.g.:

- Stray light can alter $\ln F_i$, if is not fully corrected for in the L1 algorithm.
- If the instrument's dispersion or slit function is different than what the calibration assumes, then all expressions change, since the convolution is wrong.
- If the instrument is not absolutely calibrated, the spectral sensitivity (see e.g. figure 25) has to be added as an additive term to the equation.

The BlickSFA basic fitting equation takes all the effects mentioned above into account and modifies equation 93 accordingly. Details to each term are given in the next section 6.5.5.

$$\ln F_{0i} - \ln (F_i + P_{OFFSi}) - \tau s_{FIXi} = \sum_{j=1}^{n_{GAS}} \tau s_{ji}(qs_j, T_j) + \tau_{RINGi} \cdot qs_{RING} + P_{SMOi} + P_{RESCi} \tag{94}$$

i	Index for pixels inside the limits of the fitting window, i=1 to n; the center-wavelength of pixel i is λ_i
F_{0i}	Reference spectrum at pixel i used in the fitting (see table 26)
F_i	L1 data for pixel i
P_{OFFSi}	Offset polynomial evaluated at pixel i
τs_{FIXi}	"Known" slant optical depth at pixel i
j	Index for atmospheric absorber, j=1 to n_{GAS}
τs_{ji}	Slant optical depth of absorber j for slant column qs_j and effective temperature T_j at pixel i (see section 6.5.3)
qs_{RING}	"Equivalent" slant column amount of the Ring effect
τ_{RINGi}	Standard vertical optical depth of the Ring effect at pixel i
P_{SMOi}	Smooth-part polynomial evaluated at pixel i
P_{RESCi}	Resolution change polynomial evaluated at pixel i

6.5.5 Terms of Basic Fitting Equation

τs_{FIXi}

The "known" slant optical depth τs_{FIXi} is initially set to 0. If FSE "Mol Scatt" is set to "YES", then the estimated molecular (Rayleigh and Raman) scattering extinction slant optical depth $\tau s'_{SCAi}$ for the given conditions is added to τs_{FIXi}. $\tau s'_{SCAi}$ is calculated by:

$$\tau s'_{SCAi} = \frac{p}{p_{STAN}} \cdot \tau s_{SCAi} \tag{95}$$

p is the estimated air pressure at the measurement site (calculated using the station altitude), p_{STAN} is the standard pressure (=1013.25hPa) and τs_{SCAi} is the standard molecular optical depth for pixel i. BlickSFA uses cross sections based on the work of *Bodhaine et al.* [9] and *Owens* [29] for 1 standard atmosphere of dry air molecumolecular scatteringles (2.1533e25 molc/cm^2) containing 400 ppm of CO_2. The effective height (see equation 2) is estimated to h_{SCAEFF}=6.2 km.

If FSE "Fixed Gases" is not empty, then the "known" slant optical depths for all gases listed in FSE "Fixed Gases" are also added to τs_{FIXi}. Those values are taken from L2Fit data from other fitting setups, of which the numbers are listed in FSE "Fixed Numbers".

P_{OFFSi}

The offset polynomial P_{OFFSi} is used to reduce effects of uncorrected stray light in the data. The assumption is that the way stray light alters the measurements can be approximated by a polynomial. While this assumption is clearly not true, we still see some improvement in the spectral fitting results adding such polynomial.

$$P_{OFFSi} = \overline{F} \cdot \sum_{k=0}^{noffs} p_{OFFSk} \cdot \lambda_i^k \tag{96}$$

$\overline{F}$ is the mean over the F_i, the p_{OFFSk} are the coefficients of the offset polynomial and the λ_i are the scaled wavelength-centers for each pixel i (scaling with equation 4 and x_{MIN} and x_{MAX} being the minimum and maximum nominal wavelength of the instrument's total wavelength range).

τ_{RINGi}

If FSE "Ring" is set to "YES", the Ring spectrum [16] is also fitted by the BlickSFA. The standard vertical optical depth of the Ring effect τ_{RINGi} is given in the ICF.

P_{SMOi}

The purpose of the smooth-part polynomial P_{SMOi} is to "absorb" all smooth structures in equation 94, e.g. Rayleigh scattering if it has not been included in τs_{FIXi}, or the instrument spectral sensitivity for the case the unit is not absolutely calibrated.

$$P_{SMOi} = \sum_{k=0}^{nsmo} p_{SMOk} \cdot \lambda_i^k \tag{97}$$

The p_{SMOk} are the coefficients of the smooth-part polynomial and the λ_i are as in equation 96.

P_{RESCi}

The resolution change polynomial P_{RESCi} is given by

$$P_{RESCi} = \Delta_{RESCi} \cdot \sum_{k=0}^{nresc} p_{RESCk} \cdot \lambda_i^k \tag{98}$$

The p_{RESCk} are the coefficients of the resolution change polynomial and the λ_i are as in equation 96. Δ_{RESCi} is the estimated change of equation 94 for a 1 % change in the instrument's resolution. It is calculated by

$$\Delta_{RESCi} = m_i \cdot \Delta\tau_{TOTi} - \Delta \ln F_{0i} \tag{99}$$

$\Delta \ln F_{0i}$ is the relative change (or absolute change of the logarithm) of F_{0i} for a 1 % increase in the instrument's resolution.

$$\Delta \ln F_0(\lambda_i) = \ln F_{0RESC}(\lambda_i) - \ln F_0(\lambda_i) \tag{100}$$

$\ln F_{0RESC}$ is the logarithm of the reference spectrum for a 1 % increased resolution and is given in the ICF. $\Delta\tau_{TOTi}$ is the absolute change of the standard total optical depth for a 1 % increase in the instrument's resolution.

$$\Delta\tau_{TOT}(\lambda_i) = \tau_{TOTRESC}(\lambda_i) - \tau_{TOT}(\lambda_i) \tag{101}$$

τ_{TOTi} and $\tau_{TOTRESCi}$ are the standard total optical depth change and the standard total optical depth for a 1 % increased resolution respectively and are given in the ICF.

6.5.6 Least Squares Minimization

BlickSFA is executed for a given fitting setup as defined in the 'f-codes'-table of the processing setups file (section 5.10). It retrieves n_{PAR} output-variables from n measured data points, which are the L1 data for all pixels inside the fitting window limits. These limits are defined by FSEs "WL-start" and "WL-end" (for all FSEs see table 25). BlickSFA requires $n_{PAR} \leq n$. The total number of output-parameters is given by:

$$n_{PAR} = n_{GAS} + n_{TEMP} + n_{RING} + (n_{PAR} + 1) + (n_{OFFS} + 1) + (n_{WLC} + 1) + (n_{RESC} + 1) \tag{102}$$

n_{GAS}	Number of absorbers, for which slant columns are fitted; this is the length of FSE "Fitted Gases"; $n_{GAS} \geq 0$
n_{TEMP}	Number of absorbers, for which effective gas-temperatures are fitted; this is the length of FSE "Fitted Temps"; $0 \leq n_{TEMP} \leq n_{GAS}$
n_{RING}	=1 if the Ring effect is fitted (FSE "Ring" equals YES); =0 if the Ring effect is NOT fitted (FSE "Ring" equals YES)
n_{SMO}	Order of the smooth-part polynomial; from FSE "npol"
n_{OFFS}	Order of the offset polynomial; from FSE "noffs"
n_{WLC}	Order of the wavelength change polynomial; from FSE "nwlc"
n_{RESC}	Order of the resolution change polynomial; from FSE "nresc"

A value of -1 for n_{SMO}, n_{OFFS}, n_{WLC} or n_{RESC} means the respective polynomial is not used in the fitting process. The residuals ξ_i are the differences between the left side and the right side of the basic fitting equation.

$$\xi_i = \ln F_{0i} - \ln (F_i + P_{OFFSi}) - \tau s_{FIXi} - \sum_{j=1}^{n_{GAS}} \tau s_{ji} - \tau_{RINGi} \cdot qs_{RING} - P_{SMOi} - P_{RESCi} \tag{103}$$

The BlickSFA minimizes the residuals in a least squares sense including an optional "uncertainty weighting", which is further explained in the next section.

$$\sum_{i=1}^{n}\left(\frac{\xi_i}{\sigma_i}\right)^2 \rightarrow Minimum \tag{104}$$

6.5.7 Linear Fitting

BlickSFA consists of a linear and a non-linear part. The linear part is always executed first by linearizing and solving equation 94. If requested and necessary, the results of the linear fitting are then used as first guesses for a non-linear fitting process. The least squares fitting in the BlickSFA follows the description of *Press et al.* [34], chapter 15. In order to linearize equation 94, the "measurement term" is linearized for offset and wavelength change in a way as described by *Beirle et al.* [5] and shown in equation 105:

$$\ln\left[F_i\left(\lambda_i + P_{WLCi}\right) + P_{OFFSi}\right] = \ln F_i + P_{WLCi}\cdot F_i'/F_i + P_{OFFSi}/F_i \tag{105}$$

P_{WLCi} is the wavelength change polynomial:

$$P_{WLCi} = \sum_{k=0}^{nwlc} p_{WLCk}\cdot\lambda_i^k \tag{106}$$

F'$_i$ is the derivative of F_i with wavelength, which is calculated using the reference spectrum. The fully linearized form of equation 94 is finally given by equation 107:

$$\begin{aligned}\ln F_{0i} - \ln F_i - \tau s_{FIXi} = &\sum_{j=1}^{n_{GAS}} A_{jCi}\cdot qs_j + \sum_{j=1}^{n_{TEMP}} A_{jLi}\cdot\Delta T_j\cdot qs_j + \tau_{RINGi}\cdot qs_{RING}\\ &+ P_{SMOi} + P_{RESCi} + P_{OFFSi}/F_i + P_{WLCi}\cdot F_i'/F_i\end{aligned} \tag{107}$$

A_{jCi} and A_{jLi} are the constant and linear terms in temperature of OD-fitting parameter A (see equation 92) and ΔT_j is the scaled temperature difference to the reference temperature.

$$\Delta T_j = \frac{T_j - T_{jREF}}{T_{SCALE}} \tag{108}$$

All variables in equation 108 are as in equation 92. So the linearized version of the fundamental equation assumes a linear dependence of the slant optical depth on the slant column amount (OD-fitting parameters B and C equal 0) and at most a linear dependence of OD-fitting parameter A on the temperature (A_Q=0). Equation 107 can be written in matrix form

$$\vec{Y} = \mathbf{M}\cdot\vec{X} \tag{109}$$

$\vec{Y}$ is a (n,1)-vector. Its elements Y_i are given by

$$Y_i = \ln F_{0i} - \ln F_i - \tau s_{FIXi} \tag{110}$$

$\vec{X}$ is a (n_{PAR},1)-vector

$$\begin{aligned}\overrightarrow{X} =&[qs_1, ..., qs_{nGAS}, \Delta T_1 \cdot qs_1, ..., \Delta T_{nTEMP} \cdot qs_{nTEMP}, qs_{RING}, p_{SMO1}, \cdots, p_{SMOnSMO},\\ &p_{RESC1}, \cdots, p_{RESCnRESC}, p_{OFFS1}, \cdots, p_{OFFSnOFFS}, p_{WLC1}, \cdots, p_{WLCnWLC}]^T\end{aligned} \tag{111}$$

M is a (n,n_{PAR})-matrix. One row of **M** is given by

$$\begin{aligned}\overrightarrow{M_{i:}} =&[A_{1Ci}, ..., A_{nGASCi},\\ &A_{1Li}, ..., A_{nTEMPLi},\\ &\tau_{RINGi}, 1, \lambda_i, \lambda_i^2, ..., \lambda_i^{nSMO},\\ &\Delta_{RESCi}, \Delta_{RESCi} \cdot \lambda_i, ..., \Delta_{RESCi} \cdot \lambda_i^{nRESC},\\ &\overline{F}/F_i, \overline{F}/F_i \cdot \lambda_i, ..., \overline{F}/F_i \cdot \lambda_{nOFFS},\\ &F'_i/F_i, F'_i/F_i \cdot \lambda_i, ..., F'_i/F_i \cdot \lambda_{nWLC}]\end{aligned} \tag{112}$$

Each element of vector $\overrightarrow{Y}$ and each column of matrix **M** is divided by σ_i (see equation 104). **M*** is called the design matrix of the fitting problem [34].

$$Y^*_i = \frac{Y_i}{\sigma_i} \qquad \overrightarrow{M^*_{i:}} = \frac{\overrightarrow{M_{i:}}}{\sigma_i} \tag{113}$$

What exactly is used for σ_i depends on FSE "Uncertainty". According to *Press et al.* [34], σ_i should be "... *the measurement error for each data point that is independently random and distributed as a normal (Gaussian) distribution around the true model ...*". This would mean the correct use for the weightings σ_i in equations 104 and 113 is the independent uncertainty of the Y_i, here called $U_I(Y_i)$, which is the combination of the independent uncertainties from $\ln F_i$, $\ln F_{0i}$ and τs_{FIXi} (see equation 110 and table 41). This is done by the BlickSFA in case FSE "Uncertainty" is set to "INSTR".

$$\text{"INSTR"}: \sigma_i = U_I(Y_i) = \sqrt{U_I(\ln F_i)^2 + U_I(\ln F_{0i})^2 + U_I(\tau s_{FIXi})^2} \tag{114}$$

The BlickSFA allows also other choices for FSE "Uncertainty". Setting it to "NO" means all elements of σ_i are set to 1, i.e. unweighted spectral fitting is done.

$$\text{"NO"}: \sigma_i = 1 \tag{115}$$

Finally FSE "Uncertainty" can also be set to "MEAS". In this case σ_i is the combination of the "measured" uncertainties from parameters F_i and F_{0i} in equation 103:

$$\text{"MEAS"}: \sigma_i = \sqrt{U_M(\ln F_i)^2 + U_M(\ln F_{0i})^2} \tag{116}$$

$U_M(\ln F_i)$ and $U_M(\ln F_{0i})$ correspond to $U_M(L1_i)$ from equation 67 for the measured spectrum and the reference spectrum respectively. Using "MEAS" is mathematically not correct, since the U_M in equation 116 are not

independent uncertainties as explained in section 6.3.4. However this method has been used in previous versions of the Blick Software Suite and is therefore still an allowed option for "historic" reasons. Note that depending on the chosen reference spectrum, $U_I(\ln F_{0i})$ may or may not be given (see table 41).

BlickSFA solves for the output vector $\vec{X}$ in equation 117 using the linalg.lstsq-routine of Python's numpy module (see section 2.4).

$$\vec{Y^*} = \mathbf{M}^* \cdot \vec{X} \tag{117}$$

To obtain the effective gas temperature-difference ΔT_j, BlickSFA divides the output parameter $\Delta T_j \cdot qs_j$ by the corresponding output parameter qs_j. If no non-linear fitting is needed (n_{OFFS}=-1, n_{WLC}=-1, OD parameters B, C and A_q equal 0) or if FSE "Linear Fit" is set to "YES", then the BlickSFA stops here. Otherwise the non-linear spectral fitting is applied.

6.5.8 Non-linear Fitting

The non-linear fitting minimizes the residuals in equation 103 in an iterative way using the optimize.leastsq-routine of Python's scipy module (see section 2.4). The parameters retrieved from the linear fitting are used as first guesses. The number of function evaluations is limited to 1000. While the linear fitting is always a very fast process (<0.1 s per fit), the non-linear fitting can take >1 s per fit in the worst case.

6.5.9 Residuals

The L2Fit data contain two types of residuals. The "unweighted slant column residuals" correspond to the ξ_i from equation 103, i.e. are the difference between the measured and modeled data at each pixel. The "normalized slant column residuals weighted with independent instrumental uncertainty", called $w\xi_i$, are given by:

$$w\xi_i = \frac{\xi_i}{\sigma_i} \cdot \sqrt{\frac{n}{\sum_{i=1}^{n} \left(\frac{1}{\sigma_i}\right)^2}} \tag{118}$$

The L2Fit output also includes 4 types of root mean squares of the spectral fitting residuals:

- "rms": rms of unweighted fitting residuals (equation 119)
- "wrms": Normalized rms of fitting residuals weighted with independent uncertainty (equation 120)
- "rmse": Expected rms based on independent uncertainty (equation 121)
- "wrmse": Expected normalized weighted rms based on independent uncertainty (equation 122)

The "expected" quantities listed above are based on the independent uncertainties of the input only, i.e. are not even using the residuals ξ_i or $w\xi_i$.

Note that the values for the residuals and the various rms depend on the setting of FSE "Reference", which is described in more detail in section 6.5.10.

$$\text{rms} = \sqrt{\frac{\sum_{i=1}^{n} \xi_i^2}{n - n_{PAR}}} \tag{119}$$

$$\text{wrms} = \sqrt{\frac{\sum_{i=1}^{n} w\xi_i^2}{n - n_{PAR}}} \tag{120}$$

$$\text{rmse} = \sqrt{\frac{\sum_{i=1}^{n} \sigma_i^2}{n - n_{PAR}}} \tag{121}$$

$$\text{wrmse} = \sqrt{\frac{n}{\sum_{i=1}^{n} \left(\frac{1}{\sigma_i}\right)^2} \cdot \frac{n}{n - n_{PAR}}} \tag{122}$$

6.5.10 Uncertainty

This section explains how the BlickSFA propagates the input uncertainties from parameters $\vec{Y}$ (equation 110) and $\mathbf{M}$ (equation 112) into independent, structured and common uncertainties for all elements of the output vector $\vec{X}$ (equation 111). Table 41 gives an overview of all the input uncertainties used.

Table 41: BlickSFA input uncertainties. If an uncertainty is not given, it is consequently not included and propagated in BlickSFA.

Symbol	Remark
$U_I(F_i)$	$U_I(L1_i)$ from equation 66
$U_S(F_i)$	Not given (see section 6.3.4)
$U_C(F_i)$	Not given (see section 6.3.4)
$U_I(F_{0i})$	Depends on the choice of FSE "Reference": • "Ext*": not given • "Meas*": $U_I(L1_i)$ from the reference measurement • "Ext_*": included if provided • "Synt*": ICF entry "Independent instrumental uncertainty of synthetic ..."
$U_S(F_{0i})$	Not given
$U_C(F_{0i})$	Depends on the choice of FSE "Reference": • "Ext*": not given • "Meas*": not given • "Ext_*": included if provided • "Synt*": calculated based on ICF-entry "Slant columns in synthetic ...". It consists of 2 times n_{GAS} partial uncertainties, where n_{GAS} is the number of gases listed in table 22. Each element represents the uncertainty in F_{0i} caused by the uncertainty in the slant column (elements 1 to n_{GAS}) or the effective temperature (elements n_{GAS}+1 to 2*n_{GAS}) of the respective gas. If a gas is not calibrated and therefore no slant column and effective temperature uncertainty is given in the ICF, then the Blick Software Suite assumes a conservative slant column uncertainty of half the standard amount listed in table 22, but does not include any uncertainty in the effective temperature.
$U_I(\tau s_{FIXi})$	Given, if a heritage f-code is used (see section 5.10.3)
$U_S(\tau s_{FIXi})$	• Given, if a heritage f-code is used (see section 5.10.3) • Based on an estimation for the uncertainty of the surface pressure from a climatology, if FSE "Mol Scatt" is not set to "NO"
$U_C(\tau s_{FIXi})$	Given, if a heritage f-code is used (see section 5.10.3)
$U_I(\mathbf{M})$	No independent uncertainty of any element of **M** is assumed
$U_S(\mathbf{M})$	For those gases to be fitted, but without fitting the effective temperature, an estimation of the effective temperature uncertainty is made based on climatological values. This uncertainty is translated into an uncertainty of the A-parameters in the design matrix **M**.
$U_C(\mathbf{M})$	No common uncertainty of any element of **M** is assumed

The propagation of the independent uncertainties follows again the description of *Press et al.* [34]. The covariance matrix C* is the inverse of the matrix product of **M*** transposed times **M***.

$$\mathbf{C}^* = inv\left(\mathbf{M}^{*\mathrm{T}} \cdot \mathbf{M}^*\right) \tag{123}$$

The main diagonal elements of C* are the variances of the output parameters X_j and hence the independent uncertainty of X_j, $U_I(X_j)$:

$$U_I(X_j) = \sqrt{C^*_{jj}} \tag{124}$$

Note that only if FSE "Uncertainty" is set to "INSTR" or "NO", the reported L2Fit output is truly the independent uncertainty. In the case FSE "Uncertainty" equals "MEAS", it is something else, since the design matrix has been built with the σ_i from equation 116, which is not an independent uncertainty (see section 6.5.6). In this case also no output for common or structured uncertainties is given.

The propagation of the structured and common uncertainties is done by solving equation 117 several more times with varied values of $\overrightarrow{Y^*}$ or $\mathbf{M}^*$ after the baseline calculation with the unchanged $\overrightarrow{Y^*}$ and $\mathbf{M}^*$. In each variation exactly one element of $\overrightarrow{Y^*}$ or $\mathbf{M}^*$ is replaced by adding the input uncertainty to it. The total number of these variations depends on the choice of the reference, the question whether a heritage code was used, how many gases are fitted without fitting the effective temperature, etc. (see table 41). E.g. when a synthetic reference is used, then there are 2*n_{GAS} variations added. For each of them the uncertainty in F_{0i} caused by the uncertainty in the slant column or the effective temperature of the respective gas is added to $\overrightarrow{Y}$ and equation 117 is solved. Note that these variations are only done for the linear fitting process, hence even if non-linear fitting follows, the common and structured uncertainty outputs will not change compared their values from the linear fitting.

Finally BlickSFA also calculates the so-called "rms-based uncertainty" $U_{rms}(X_j)$:

$$U_{rms}(X_j) = rms \cdot \sqrt{C_{jj}} \tag{125}$$

where rms is from equation 119 and C is given by:

$$\mathbf{C} = inv\left(\mathbf{M}^T \cdot \mathbf{M}\right) \tag{126}$$

6.6 L2 Direct Algorithm

This algorithm is used for direct sun and direct moon measurements and mainly produces total vertical column amounts and effective temperatures for each output gas j requested in the r-code (see section 5.10.4).

The viewing geometry of the direct sun or moon observation mode is outlined in figure 27. The sampled air mass is a circular cone with its apex at the entrance of the instrument and extending into the direction of the sun or moon. This means that for direct sun observations, the measurements sample air towards East in the morning, South or North around noon (depends on the latitude), and West in the afternoon.

The vast majority of the light sampled in direct observation mode comes from an angle of 0.5°, since this is the angular size of both the sun and the moon. The direct light comes from inside these 0.5°, the forward scattered diffuse light is distributed over the entire FOV of the instrument. Only at large ZA and high aerosol content is the diffuse fraction significant (a few percent of the total signal) and can possibly introduce systematic errors in the retrieval. Each trace gas molecule inside the cone is equally "counted", i.e. there is in principle no dependence on the vertical profile in the data.

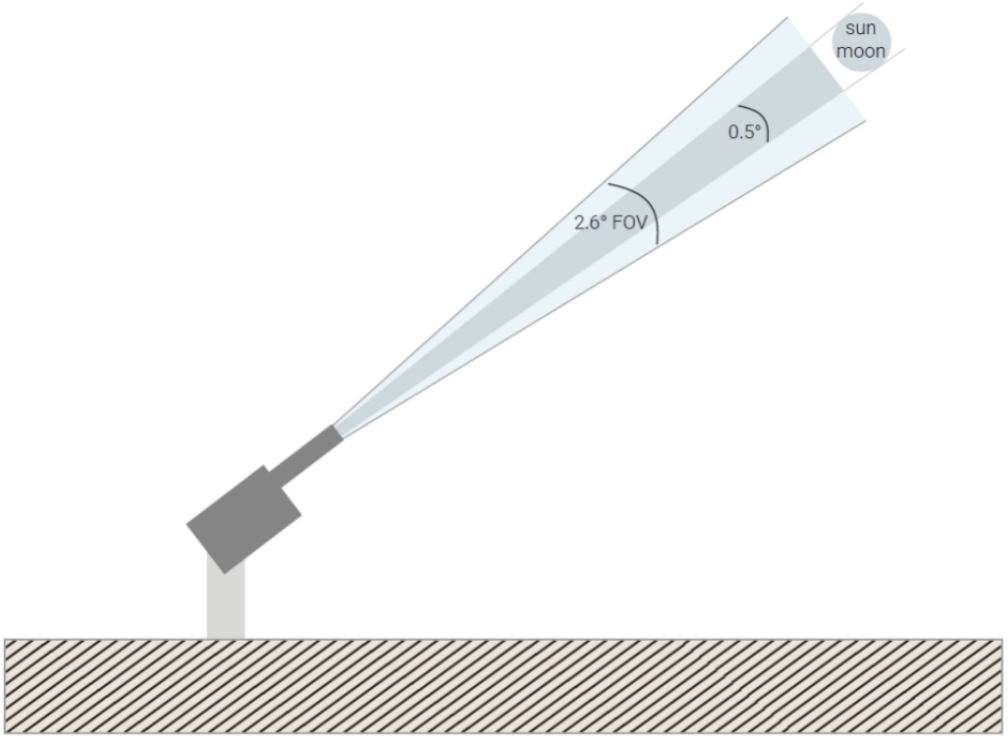


Figure 27: Direct sun or moon observations

Figure 28 shows the situation including the Earth's curvature. R is the distance from the center of the Earth to the measurement location (about 6370 km, refined based on the location's latitude), ZA* is the apparent solar (or lunar) zenith angle (i.e. the geometrical ZA corrected for refraction) and h_{EFFj} is the effective height for trace gas j (from equation 2). Note that if h_{EFFj} is smaller than 10 km ("tropospheric effective height"), the effective height is added to the station height. Otherwise ("stratospheric effective height"), the station height is ignored and the effective height is added to the Earth's surface. ZA'_j is the "reduced" zenith angle for gas j, which can be calculated by equation 127.

$$ZA'_j = \arcsin\left[\left(\frac{R}{R + h_{EFFj}}\right) \cdot \sin(ZA^*)\right] \tag{127}$$

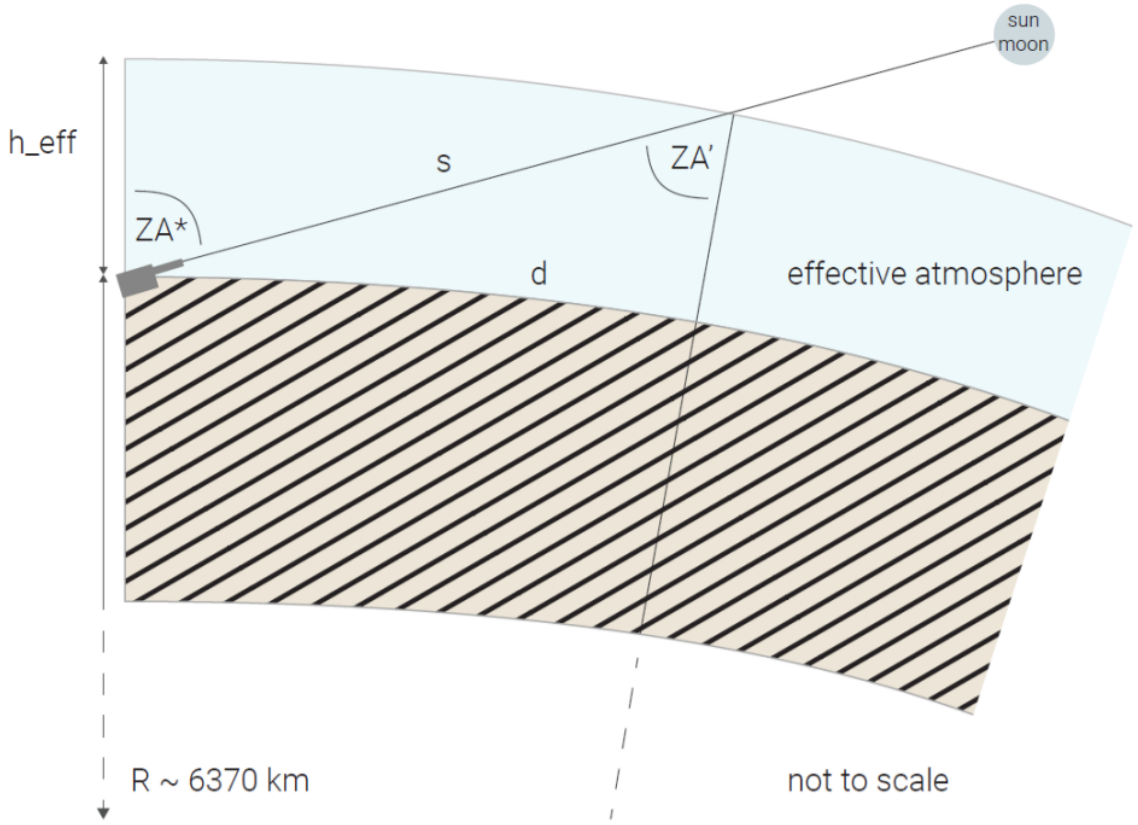


Figure 28: Direct sun or moon viewing geometry

In the simplest case, which is later referred to as "Case 1", the measured qs_j are divided by the direct sun (or moon) AMF m_{DIRj}:

$$q_j = \frac{qs_j}{m_{DIRj}} \tag{128}$$

m_{DIRj} is calculated in the Blick Software Suite by:

$$m_{DIRj} = \sec(ZA'_j) \tag{129}$$

The formula in equation 129 is based on some assumptions, e.g. that the vertical distribution of trace gas j is a delta function at h_{EFFj}. For details on this equation see e.g. *Bernhard et al.* [7].

The main driver for the uncertainty in m_{DIRj} is h_{EFFj}. Uncertainties in R or ZA*, possibly arising from a wrong time registration, are neglected in the Blick Software Suite. Since we assume the "true" effective height changing "slowly" in time, the AMF-uncertainty is basically a structured uncertainty. While for SZAs up to about 70° the error in m_{DIRj} due to an error in h_{EFFj} is rather small, it can increase substantially for higher SZAs in case the estimation of h_{EFFj} is significantly off. Figure 29 shows as examples cases of overestimations of m_{DIRj} due to an extreme underestimation of h_{EFFj}.

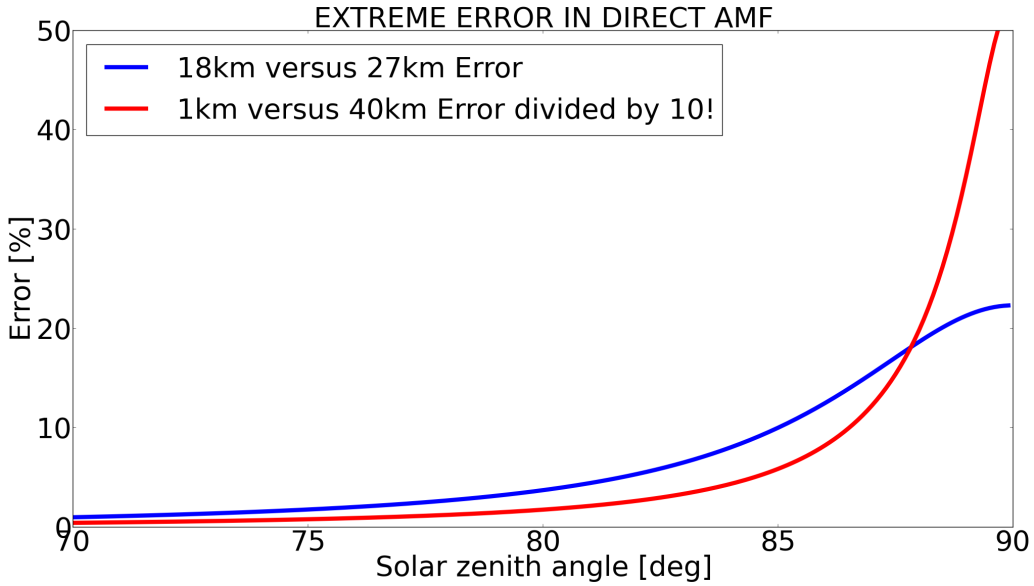


Figure 29: Overestimation of the direct AMF due to a wrong estimation of the effective height as a function of SZA. The blue line represents an extreme case for O_3, where h_{EFF}=18 km is used in the retrieval, typical for high ozone conditions at high latitudes, but the true h_{EFF} was 27 km, typical for low ozone conditions at low latitudes (see figure 35). The red line represents an extreme case for NO_2, where h_{EFF}=1 km is used in the retrieval, typical for highly polluted conditions with the majority of NO_2 near the surface, but the true h_{EFF} was 40 km, typical for a purely stratospheric NO_2 amount at high latitudes in winter (see figure 39). Note that the red line is divided by 10, i.e. the error at SZA=85° is >50%

Hence the key to obtain a good estimation of m_{DIRj} is to have a good estimation of h_{EFFj}, for which the L2 algorithm can make use of the climatologies described in section 6.8.2, if the user sets the r-code in such a way. The specific retrieval of q_j depends on the following questions:

- What are the settings of r-code entry "Effective Heights"?
- Are one or two f-codes listed in r-code entry "f-codes"?
- Was the effective temperature of the output gas fitted?
- Does a stratospheric climatology for the output gas exist (see section 6.8.3)?

The direct algorithm distinguishes 4 different cases, which are summarized in table 42. Note that settings in the r-code, which are not listed in this table, are not allowed by the direct algorithm. This is e.g. for the situation that 2 f-codes are used, but the output gas temperature is fitted for at least one of them, or that 2 height informations are given, but there is no stratospheric climatology for the output gas and the temperature of the output gas was not fitted.

The formulas used for the 4 different cases are described in the paragraphs after the table. Although index j for the output gas is present in all quantities discussed in this section, it is left out in the remaining formulas and descriptions for simplicity.

Table 42: Different cases for direct algorithm. Column "Case No" gives the case-number. Column "Strat Clim" indicates whether a stratospheric climatology for the output gas needs to exist. Column "f-codes" stands for r-code entry "f-codes". "1" means one f-code is used and the temperature of the output gas is not fitted. "FIT" means one f-code is used and the temperature of the output gas is fitted. "2" means two f-codes are used and the temperature of the output gas is not fitted in either of them. Column "No of heights" indicates how many height informations are listed in r-code entry "Effective heights".

Case No	Strat Clim	f-codes	No of heights	Remark
1	No, Yes	1, FIT	1	No stratospheric-tropospheric split is determined. The presence of any existing climatology for the output gas is ignored.
2	No, Yes	FIT	2	A stratospheric-tropospheric split is estimated using the retrieved effective temperature of the output gas and the two entries in r-code "Effective heights". Note that for this case both entries must refer to a climatology, e.g. "BL+STRAT". Something like "BL+25" is not allowed! The presence of any existing stratospheric column climatology for the output gas is ignored.
3	Yes	1	2	A stratospheric-tropospheric split is estimated using the given stratospheric climatology of the output gas.
4	Yes	2	2	A stratospheric-tropospheric split is estimated using the given stratospheric climatology and is adjusted based on the retrieved slant columns from the two requested f-codes.

6.6.1 Case 1

This is the simplest case, where h_{EFF} is taken from the single r-code entry "Effective Heights", used to calculate m_{DIR} with equation 129, which is then inserted in equation 128 to obtain q. The effective gas temperature T is not changed, i.e. the value is equal to the L2Fit output. No stratospheric-tropospheric split is determined.

6.6.2 Case 2

Cases 2 to 4 should be used for species, which have a stratospheric and a tropospheric component. The total vertical column q is split into two parts:

$$q = q_T + q_S \tag{130}$$

q_T is the tropospheric vertical column and q_S the stratospheric vertical column. The total slant column qs is split in the same way:

$$qs = q \cdot m = qs_T + qs_S = q_T \cdot m_T + q_S \cdot m_S \tag{131}$$

m is the "overall" AMF, qs_T the tropospheric slant column, m_T the tropospheric AMF, qs_S the stratospheric slant column and m_S the stratospheric AMF. Finally we also split the slant optical depth at a "representative

wavelength" of the output gas:

$$qs \cdot \tau(T) = qs_T \cdot \tau_T(T_T) + qs_S \cdot \tau_S(T_S) \tag{132}$$

$\tau(T)$ is the optical depth at this wavelength for a standard amount of the output gas at temperature T. T_T and T_S are the tropospheric and stratospheric effective temperatures respectively. We assume a linear dependence of the standard optical depth (or cross section) on the temperature:

$$\tau(T) = \tau(T_0) \cdot [1 + k \cdot (T - T_0)] \tag{133}$$

Inserting equation 133 in 132 and also using 131, we get:

$$qs \cdot T = q \cdot m \cdot T = qs_T \cdot T_T + qs_S \cdot T_S = q_T \cdot m_T \cdot T_T + q_S \cdot m_S \cdot T_S \tag{134}$$

Inserting qs_S from 131 in 134 and solving for qs_T we obtain:

$$qs_T = qs \cdot \frac{T - T_S}{T_T + T_S} = qs \cdot f \tag{135}$$

f is called the "tropospheric fraction" of the total slant column:

$$f = \frac{qs_T}{qs} = \frac{T - T_S}{T_T + T_S} \tag{136}$$

f is between 0 ("purely stratospheric case") and 1 ("purely tropospheric case"). Consequently the stratospheric vertical column is given by:

$$qs_S = qs \cdot (1 - f) \tag{137}$$

Finally we can insert q from 130 in 131 and solve for m using equations 135 and 137:

$$m = \left[\frac{f}{m_T} + \frac{1 - f}{m_S}\right]^{-1} \tag{138}$$

For case 2, the total slant column qs and the effective gas temperature T are measured. We use the overall AMF m from equation 138 to convert qs into the total vertical column q as in equation 128. m_T and m_S are calculated

from equation 129 using the climatological tropospheric and stratospheric effective heights from r-code entry "Effective heights" respectively. f is calculated from 136 with T being the retrieved effective temperature from L2Fit, and T_T and T_S being the climatological tropospheric and stratospheric effective temperatures from r-code entry "Effective heights". Note that f is limited to the range between 0 and 1, hence it is set to 0 in case a negative f is the result of equation 136 and it is set to 1 in case it exceeds 1.

6.6.3 Case 3

While for case 2, the tropospheric fraction f is based on the retrieved and climatological effective temperatures (see equation 136), for cases 3 and 4 it is calculated using a stratospheric column climatology (see section 6.8.3). For case 3 we approximate q_S from equation 131 with the climatological amount q_{CLIM}, solve for qs_T and divide by qs:

$$f = 1 - \frac{q_{CLIM} \cdot m_S}{qs} = 1 - \frac{qs_{CLIM}}{qs} \tag{139}$$

f is calculated from 139 with qs being the retrieved slant column from L2Fit, q_{CLIM} is taken from the stratospheric column climatology and m_S from equation 129 using the climatological stratospheric effective height from r-code entry "Effective heights". Note that as an estimator for q_{CLIM} the Blick Software Suite is not taking the mean value of the stratospheric column climatology, but adding two times the standard deviation of the climatology to it. This means instead of the most likely value for the stratospheric column (based on the climatology), it rather uses an upper limit for it. This has the advantage that situations with elevated stratospheric columns are still captured correctly by the algorithm. On the downside, small tropospheric column amounts on top of normal or low stratospheric columns will falsely be attributed to the stratosphere.

As for case 2, f is limited to the range between 0 and 1 and the "overall" AMF m is calculated with equation 138, where m_T is calculated from 129 using the climatological tropospheric effective height from r-code entry "Effective heights". Finally m is inserted into equation 128 to get the final vertical column amount q.

In case that both pieces of height information in r-code entry "Effective heights" are related to a climatology, then the Direct Algorithm also modifies the L2 output of the effective temperature by solving equation 135 for T:

$$T = f \cdot T_T + (1 - f) \cdot T_S \tag{140}$$

Here T_T and T_S are the climatological tropospheric and stratospheric effective temperatures from r-code entry "Effective heights".

6.6.4 Case 4

Here two f-codes are calculated, which deliver retrieved slant columns amounts qs_{RTT} and qs_{RTS}. "RTT" stands for "retrieved using tropospheric effective temperature T_T" and "RTS" stands for "retrieved using stratospheric effective temperature T_S". qs_{RTT} and qs_{RTS} have in general different values, but the respective slant optical depths at a wavelength representative for the output species must be the same, since they come from the same

data. Therefore we can write:

$$qs_{RTT} \cdot \tau(T_T) = qs_{RTS} \cdot \tau(T_S) \tag{141}$$

Then we can split the slant optical depth into a stratospheric and a tropospheric component using q_{CLIM} as an estimator for the stratospheric vertical column amount:

$$qs_{RTT} \cdot \tau(T_T) = q_{CLIM} \cdot m_S \cdot \tau(T_S) + qs_T \cdot \tau(T_T) \tag{142}$$

Solving equation 142 for qs_T and also using 141 we obtain this expression as best estimation for the true tropospheric slant column qs_T:

$$qs_T = qs_{RTT} \cdot \left(1 - \frac{q_{CLIM} \cdot m_S}{qs_{RTS}}\right) \tag{143}$$

Adding the estimated stratospheric slant column from the climatology to qs_T from equation 143, we obtain the best estimation for the total slant column amount qs:

$$qs = qs_{RTT} \cdot \left(1 - \frac{q_{CLIM} \cdot m_S}{qs_{RTS}}\right) + m_S \cdot q_{CLIM} \tag{144}$$

Dividing equation 143 by equation 144 we get the tropospheric fraction f for case 4:

$$f = \frac{qs_{RTT} \cdot \left(1 - \frac{q_{CLIM} \cdot m_S}{qs_{RTS}}\right)}{qs_{RTT} \cdot \left(1 - \frac{q_{CLIM} \cdot m_S}{qs_{RTS}}\right) + q_{CLIM} \cdot m_S} \tag{145}$$

As for cases 2 and 3, f is limited to the range between 0 and 1. The retrieved qs_{RTT} and qs_{RTS} are from L2Fit, q_{CLIM} is taken from the stratospheric column climatology and m_S and m_T are calculated from equation 129 using the effective heights given in the r-code entry "Effective heights" respectively. As for case 3, the mean value plus two times the standard deviation of the stratospheric column climatology is used as an estimator for q_{CLIM} by the Blick Software Suite. With f we can calculate the overall AMF m from equation 138. Finally the total vertical column is obtained by dividing ss from equation 144 by m. The effective temperature is determined from equation 140, where T_S and T_T are the ones used in the f-codes.

6.6.5 Data averaging

If FSE "Noise levels" is below 100 for all output gases, then BlickP tries to average the different sets of a measurement routine in a way so that the averaged data are below the desired "noise level". The noise level

NoiLev is defined as the percentage fraction of the independent variance, i.e. the square of the independent uncertainty $U_I(i)$, on the total variance, i.e. the square of the total uncertainty U:

$$\text{NoiLev} = \frac{U_I^2}{U^2} \cdot 100 \tag{146}$$

The base for this averaging procedure is equation 64, where parameter n can be chosen to fulfill this condition. Let's assume there is one output gas, 10 sets have been measured in the routine and FSE "Noise levels" is set to '5'. If NoiLev is below 5% for each individual set already, then no averaging will be done and all 10 sets are written out in the L2 data. However if NoiLev is about 10% for each set, then BlickP will notice that averaging three or more sets will bring the noise level of the averaged data below 5%. In this case the L2 output will not report all 10 sets, but instead just have 3 output lines, where the first one is the average over sets 1 to 3, the second one over sets 4 to 6 and the third one over sets 7 to 10 and each of them has a noise level below 5%. In the "worst case", which obviously can also happen, all sets are averaged and only one output line is written, but the desired noise level is still not reached.

6.7 L2 Air-Ratio Sky Algorithm

This algorithm has been developed in collaboration with Elena Spinei and is scientifically explained in Spinei et al., in progress. It calculates the surface concentration, tropospheric vertical column amount and partial column amounts at different layers of the requested trace gas based on sky measurements from different pointing zenith angles (PZA) at a fixed azimuth. In this section the programmatic sequence of the algorithm is described. The following acronyms are used:

q	Absolute vertical column amount
qs	Absolute slant column amount
Δqs	Differential slant column amount. Here differential means relative to the zenith view
n	Concentration
m	Absolute air mass factor
Δm	Differential air mass factor
No index	The quantity refers to the requested output trace gas
Index "AIR"	The quantity refers to the so-called "Air-gas", which is either O_2 or O_2O_2.
Index "CLIM"	The quantity is calculated from a climatology
Index "SURF"	This refers to a surface value
Index "T"	This is a tropospheric amount

6.7.1 Preconditions

The following conditions need to be met for the algorithm to process any data:

- Below are the minimum required PZAs to obtain full output data. Note that if the last two angles in the list are missing, but the others are measured, then the algorithm calculates q_T, but not the other output parameters.
  - A near zenith angle measurement with PZA<5°. In the algorithm description this angle is labeled with 0.
  - One measurement with 59.7°<PZA<60.3°. In the algorithm description this angle is labeled with 60.
  - One measurement with 74.7°<PZA<75.3°. In the algorithm description this angle is labeled with 75.
  - One measurement with PZA>87°, the "largest angle". This angle should be as large as possible, but not having an object other than the sky in the FOV. Since the Pandora Sky-FOV is about 1.5° full width, we recommend staying 1° away from the horizon. I.e. at a flat place, this angle would be 89°. When the horizon is elevated (e.g. trees or nearby mountains in the view) then the largest angle might be <89° and if the instrument is located on a hill it might be even possible to go >89°. In the algorithm description this angle is labeled with MAX.
  - One measurement with PZA between 0.9° and 1.1° smaller than the largest angle. In the algorithm description this angle is labeled with MAXm1.
- The f-codes must include slant columns from the output gas and from a so-called "air-gas", either O_2 or O_2O_2.

6.7.2 Interpolations

If exactly one f-code is used in the retrieval, then the air-gas slant columns are taken from this f-code (see table 29). If two f-codes are used, then the air-gas slant columns are taken from the 2nd f-code. If more than two f-codes are used, then the air-gas slant columns are taken from all the f-codes but the first one and then linearly inter- or extrapolated in wavelength to the effective fitting wavelength of the output gas, using the effective fitting wavelengths of the air-gas slant columns. The goal of this step is to use air-gas slant columns in the algorithm, which are matching as good as possible the 'true' air-gas slant columns at the effective wavelength of the output trace gas (see equation 17). Note that the linear fit is also using the independent uncertainty of the air-gas slant columns.

Although not necessarily required by the algorithm, the measurements should be done in "V-shape", i.e. all angles are measured twice around a central angle. The typical sequence starts with the zenith, then goes down in pointing towards the largest PZA, e.g. 89°, and then the same angles are measured again in upwards direction ending at the zenith. If such a V-shape is used, then the single slant columns (of both the output gas and the air-gas) are interpolated in time to the measurement of the largest angle, which is used as a reference in the spectral fitting. This avoids systematic errors at larger SZAs.

6.7.3 Tropospheric column

The tropospheric column q_T is calculated with equation 147:

$$q_T = \frac{(qs_{75} - qs_0) \cdot q_{CLIM,AIR}}{qs_{75,AIR} - qs_{60,AIR} + 2 \cdot q_{CLIM,AIR}} = \frac{\Delta qs_{75} \cdot q_{CLIM,AIR}}{\Delta qs_{75,AIR} - \Delta qs_{60,AIR} + 2 \cdot q_{CLIM,AIR}} \tag{147}$$

qs_{75} and qs_0 are the absolute slant columns of the output gas at the nominal PZAs 75° and 0° respectively and Δqs_{75} the retrieved differential slant column at the nominal PZA 75°. $qs_{75,AIR}$ and $qs_{60,AIR}$ are the absolute slant columns of the air-gas at the nominal PZAs 75° and 60° respectively. $q_{CLIM,AIR}$ is the total vertical column amount of the air-gas and is calculated using the climatologies (see section 6.8):

$$q_{CLIM,AIR} = n_{SURF,AIR} \cdot h_{EFF,AIR} \tag{148}$$

$h_{EFF,AIR}$ is the effective air-gas height taken from the climatology for O_2 or O_2O_2 (see section 6.8.2). $n_{SURF,AIR}$ is the climatological surface concentration of the air-gas and is calculated by:

$$n_{SURF,O2} = \frac{P_{SURF,AIR} \cdot f_{O2}}{T_{SURF} \cdot k_{Boltz} \cdot n_{Losch}} \tag{149}$$

P_{SURF} is the (dry-air) surface pressure, f_{O2} the O_2 mixing ratio, T_{SURF} the surface temperature, k_{Boltz} the Boltzmann constant and n_{Losch} Loschmidt's number. The Blick Software Suite uses f_{O2}=0.20946 and estimates $P_{SURF,AIR}$ and T_{SURF} from a climatology (see section 6.8.1). In case O_2 is the air-gas, $n_{SURF,O2}$ is used for $n_{SURF,AIR}$. If O_2O_2 is the air-gas, then the squared $n_{SURF,O2}$ is used for $n_{SURF,AIR}$.

The algorithm also estimates the maximum horizontal and vertical distances for the tropospheric column, which is based on an assumption of single scattering and using geometrical path approximations.

$$d_{MAX,HOR} = \frac{qs_{75} - qs_{60}}{n_{SURF,AIR}} \cdot q_{CLIM,AIR} \cdot sin(PZA_{75}) \tag{150}$$

$$d_{MAX,VERT} = \frac{qs_{75} - qs_{60}}{n_{SURF,AIR}} \cdot q_{CLIM,AIR} \cdot cos(PZA_{75}) \tag{151}$$

$d_{MAX,HOR}$ and $d_{MAX,VERT}$ are the maximum horizontal and vertical distances respectively and PZA_{75} is the exact value of the nominal 75° angle.

6.7.4 Surface concentration

Since we actually would like to have PZA_{MAX} at 90°, but in general cannot measure this, the following extrapolation is done to estimate the differential slant column for PZA=90° in the case PZA_{MAX} was below 90°:

$$\Delta qs_{90} = \Delta qs_{MAXm1} + (\Delta qs_{MAX} - \Delta qs_{MAXm1}) \cdot \frac{90 - PZA_{MAXm1}}{PZA_{MAX} - PZA_{MAXm1}} \tag{152}$$

For the surface concentration c we distinguish 4 different cases:

1. Fully mixed case based on the 90° extrapolation, equation 153
2. Fully mixed case based on the largest PZA, equation 154
3. Heterogeneous case based on the 90° extrapolation, equation 155
4. Heterogeneous case based on the largest PZA, equation 156

$$c_{F90} = \frac{\Delta qs_{90}}{\Delta qs_{90,AIR}} \tag{153}$$

$$c_{FMAX} = \frac{\Delta qs_{MAX}}{\Delta qs_{MAX,AIR}} \tag{154}$$

$$c_{H90} = c_{F90} \cdot \frac{\Delta qs_{75}}{q_{CLIM,AIR}} \tag{155}$$

$$c_{HMAX} = c_{FMAX} \cdot \frac{\Delta qs_{75}}{q_{CLIM,AIR}} \tag{156}$$

The final choice for the surface concentration the largest value among all the cases listed above. Output "Surface concentration index" gives the selected case, a number between 1 and 4.

Finally the so-called "heterogeneity flag" is calculated. This flag equals 0, if the ratio of the surface concentration of the selected case over the standard deviation of the surface concentrations from all cases is above 5 OR if the surface concentration index is 1 or 2. In this case it is assumed that there are rather well mixed conditions. Otherwise the flag equals 1 indicating more heterogeneous conditions near the surface.

6.7.5 Vertical profile

The first step in determining the partial column amounts of the output gas in different layers is to estimate the effective height corresponding to a given PZA_i, which is based on the air-gas slant columns using geometrical relationship and assuming single scattering conditions only:

$$h_{CENi} = \frac{\Delta qs_{i,AIR} + q_{CLIM,AIR}}{n_{SURF,AIR}} \cdot \frac{cos(PZA_i)}{2} \tag{157}$$

The measured differential slant columns in n_{PZA} angles (i=1 to n_{PZA}) give us n_{PZA}-1 atmospheric layers. The top height of layer i is given by:

$$h_{TOPi} = 0.5 \cdot (h_{CENi+1} + h_{CENi}) \tag{158}$$

The lowest layer extends from the surface to h_{TOP1}, where the corresponding angles are PZA_{MAX} and PZA_{MAXm1}. The next step is to calculate differential air mass factors for the output gas and the air-gas for each layer, Δm_i and $\Delta m_{i,AIR}$ respectively:

$$\Delta m_i = \frac{qs_i - qs_{i+1}}{q_T} \tag{159}$$

$$\Delta m_{i,AIR} = \frac{qs_{i,AIR} - qs_{i+1,AIR}}{q_{CLIM,AIR}} \tag{160}$$

q_T is the tropospheric column as described in section 6.7.3. The profile shape ps of the partial columns is determined as a variation of the air-gas shape:

$$ps_i = \frac{0.5 + \Delta m_i - \Delta m_{i,AIR}}{1 + \Delta m_{i,AIR}} \cdot q_T \tag{161}$$

For the normalized profile shape psn, the profile shape is divided by its largest element, hence all psn_i are ≤ 1. The average number density of the output gas in layer i, n_i, is then calculated from the following empirical equation:

$$n_i = \frac{2 \cdot (\Delta qs_i - \Delta qs_{i+1}) + 0.5 \cdot q_T \cdot (m_{i,RAYL} - 3 \cdot \Delta m_{i,AIR})}{\Delta qs_{i,AIR} - \Delta qs_{i+1,AIR} + q_{CLIM,AIR}} \cdot n_{SURF,AIR} \cdot psn_i \tag{162}$$

$m_{i,RAYL}$ is the Rayleigh air mass factor for the corresponding PZA. It is calculated from RTC. Further correction due to profile differences are addressed by the correction factor cf_i:

$$cf_i = psn_i \cdot \frac{n_i}{Max(n_i)} \tag{163}$$

Max() refers to the maximum over all i. For those layers with negative values of cf_i the n_i are corrected in the following way:

$$n_i = n_i \cdot (1 + cf_i) \tag{164}$$

Negative values of n_i are set to 0. For the partial column amounts Δq_i, the concentrations n_i are multiplied with the layer width:

$$\Delta q_i = n_i \cdot (h_{TOPi} - h_{TOPi\text{-}1}) \tag{165}$$

For i=1, the lowest layer, $h_{TOPi\text{-}1}$ equals 0. The last step is to normalize the Δq_i with the tropospheric column:

$$\Delta q_i = \Delta q_i \cdot \frac{Sum(\Delta q_i)}{q_T} \tag{166}$$

Sum() refers to the sum over all i.

6.8 Climatologies

In order to obtain real time L2 data, the Blick Software Suite uses climatological estimations for some parameters, which are described in this section. The climatologies include uncertainties, which are propagated in the L2Fit and L2 data and reported as "structured uncertainties" as defined in section 6.3.1.

6.8.1 Surface pressure and temperature

The Blick Software Suite climatology for surface pressure and surface temperature is based on the international reference atmosphere from the Committee on Space Research (COSPAR) [1]. It depends on the season and the latitude and height a.s.l. of the location. The values for sea level are shown in figure 30. Note that the values for latitudes below 60° South are actually not for sea level, but for the average height of the surface in Antarctica.

The uncertainty in the surface pressure is assumed to be 1% of the climatological value, i.e. approximately 10 hPa at sea level. The uncertainty in the surface temperature is assumed to be 20 K.

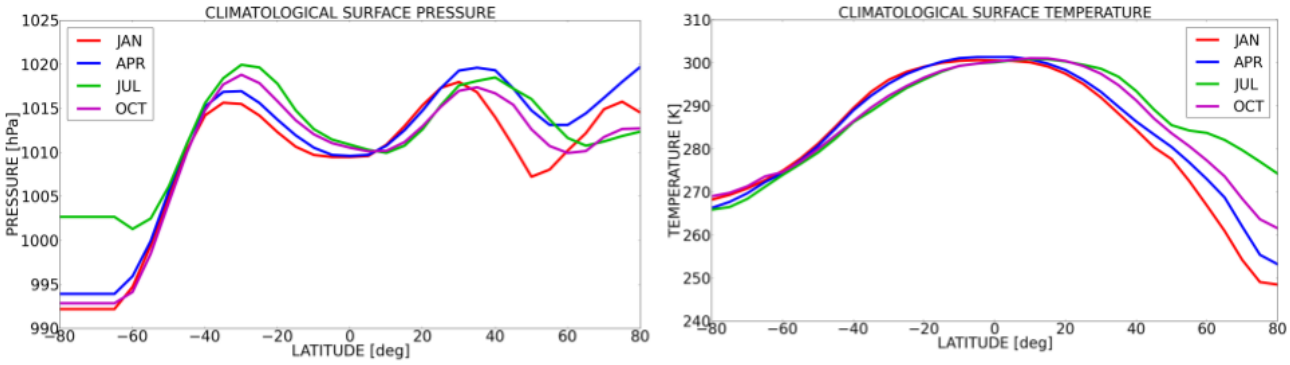


Figure 30: Climatological surface pressure (left panel) and surface temperature (right panel) at sea level for the months of January, April, July and October as a function of latitude.

6.8.2 Effective height and temperature

The climatologies for the effective height and effective temperature for different "profile types" are listed in table 43. The effective heights are calculated from a vertical profile for a given profile type. The effective temperatures are calculated by combining those profiles with the temperature profile from the COSPAR international reference atmosphere [1]. Examples for the climatological effective heights and temperatures are shown in the figures of this subsection.

Table 43: Climatologies for effective temperature and height included in the Blick Software Suite. The values obtained for a given profile type depend on the input parameters listed in column "Depends". "Lat" stands for the geographic latitude of the location, "Long" for the geographic longitude, "Height" for the station height a.s.l., "Season" for the time in the year, "Daytime" for the hour in the day, and "Column" for the total column amount of the respective species.

Type	Depends	Description
O2	Lat Height Season	Air effective height and temperature calculated based on the COSPAR [1] air-pressure and air-temperature profiles (figures 31 and 32). For the uncertainty of the effective height the standard deviation over the months is used (figure 31). For the uncertainty of the effective temperature a combination of the standard deviation over the months (figure 32) with a fixed value of 5 K is used.
O2O2	Lat Height Season	O_2O_2 effective height and temperature calculated in the same way as the air profile, just using the squared values (figures 33 and 34). For the uncertainty of the effective height the standard deviation over the months is used (figure 33). For the uncertainty of the effective temperature a combination of the standard deviation over the months (figure 34) with a fixed value of 10 K is used.
O3	Lat Height Column Season	Ozone effective height and temperature based on data from the TOMS version 8 temperature and ozone profile climatology [8]. The climatologies are shown in figures 35 and 37 for height and temperature respectively. For the uncertainty of the effective height the standard deviation over the months (figure 36, left panel) is used in case the column amount is known, otherwise half of the minimum-maximum range (figure 36, right panel) is used. For the uncertainty of the effective temperature a combination of a third of the standard deviation over the months (figure 36, left panel) with a fixed value of 3 K is used in case the column amount is known, otherwise a combination of half the standard deviation over the months with a fixed value of 3 K is used.
NO2s	Lat Season Daytime	Stratospheric NO_2 effective height and temperature from *Brohede et al.* [12]. The climatologies are shown in figures 39 and 40 for height and temperature respectively. For the uncertainty of the effective height a combination of half of the standard deviation over all months and times of day (figure 41, left panel) with a fixed value of 1 km is used. For the uncertainty of the effective temperature a combination of a quarter of the standard deviation over all months and times of day (figure 41, right panel) with a fixed value of 2 K is used.
BL	Lat Height Season	Effective height and temperature for a species that is well mixed in the "boundary layer", which is assumed 2 km high, and does not exist above it. The effective height is 1 km, with assumed uncertainty of 0.5 km. The climatology for the effective temperature is based on the COSPAR atmosphere [1] and shown in figure 42. For the uncertainty of the effective temperature a fixed value of 20 K is used, just as for the uncertainty in the surface temperature climatology (see section 6.8.1).
STRAT	Lat Season	Effective height and temperature for a species that is well mixed between 13 and 30 km and does not exist elsewhere. The effective height is 18 km with an assumed uncertainty of 5 km. The climatology for the effective temperature is based on the COSPAR atmosphere [1] and shown in figure 43, left panel. For the uncertainty of the effective temperature a combination of a quarter of the standard deviation over all months (figure 43, right panel) with a fixed value of 2 K is used.

Type	Depends	Description
TROPAU	Lat Season	Effective height and temperature for a species that is well mixed between 6 and 15 km and does not exist anywhere else. The effective height is 10 km, with assumed uncertainty of 3 km. The climatology for the effective temperature is based on the COSPAR atmosphere [1] and shown in figure 44, left panel. For the uncertainty of the effective temperature a combination of a third of the standard deviation over all months (figure 44, right panel) with a fixed value of 4 K is used.
WAT	Lat Height Season	Effective height and temperature for a species that is well mixed between 0 and 6 km and does not exist anywhere else. The effective height is 3 km with an assumed uncertainty of 1.5 km. The climatology for the effective temperature is based on the COSPAR atmosphere [1] and shown in figure 45, left panel. For the uncertainty of the effective temperature a combination of the standard deviation over all months (figure 45, right panel) with a fixed value of 10 K is used.

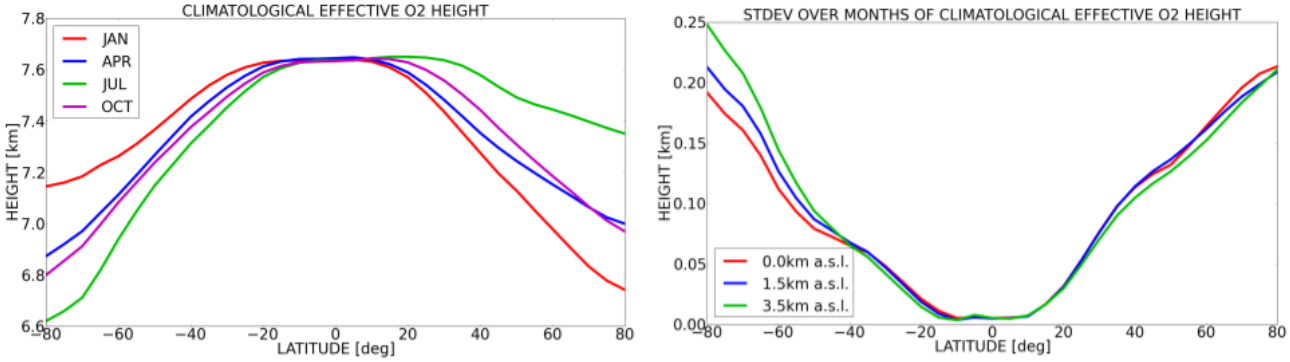


Figure 31: Climatological effective air height for the months of January, April, July and October for a station at sea level (left panel) and its standard deviation over all months for different location heights (right panel) as a function of latitude.

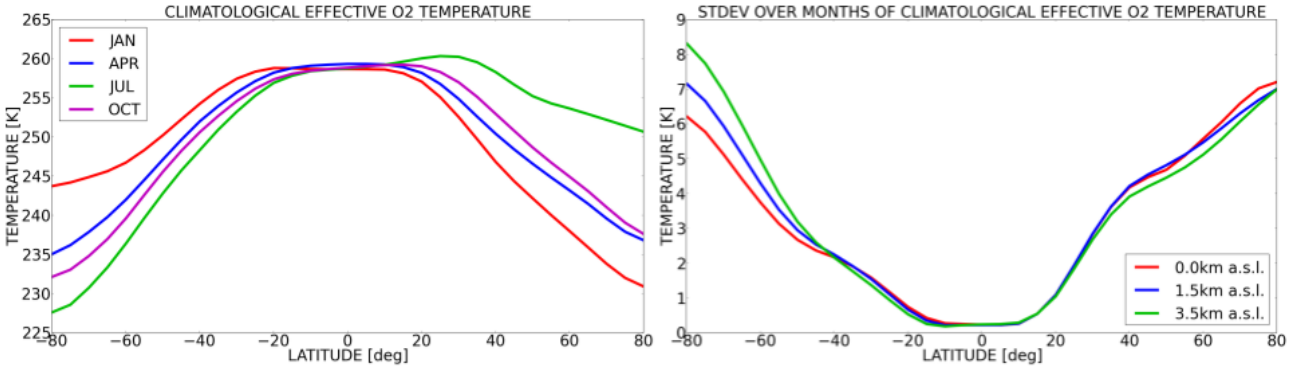


Figure 32: Climatological effective air temperature for the months of January, April, July and October for a station at sea level (left panel) and its standard deviation over all months for different location heights (right panel) as a function of latitude.

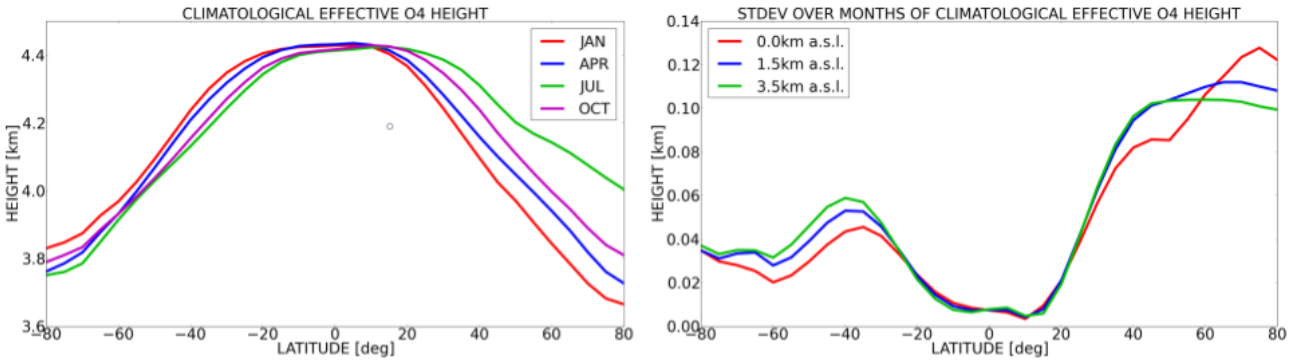


Figure 33: Climatological effective O_2O_2 height for the months of January, April, July and October for a station at sea level (left panel) and its standard deviation over all months for different location heights (right panel) as a function of latitude.

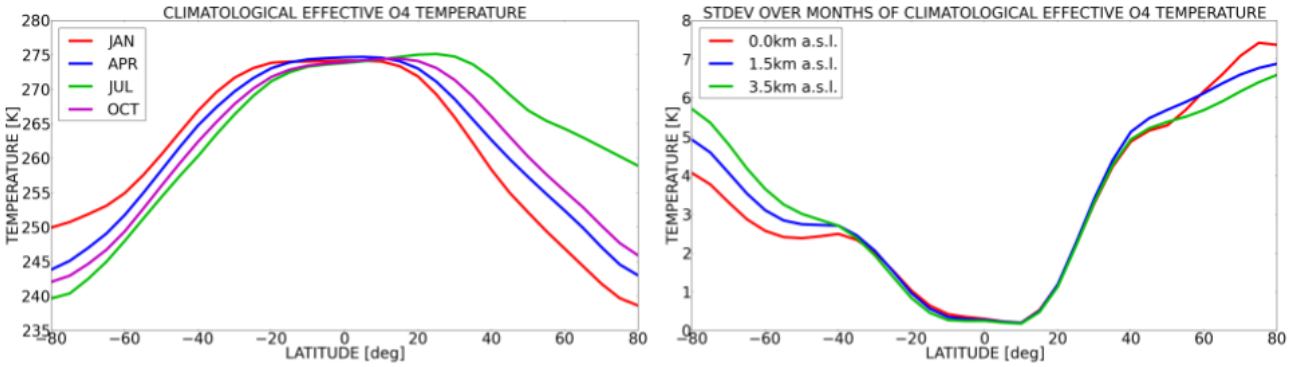


Figure 34: Climatological effective O_2O_2 temperature for the months of January, April, July and October for a station at sea level (left panel) and its standard deviation over all months for different location heights (right panel) as a function of latitude.

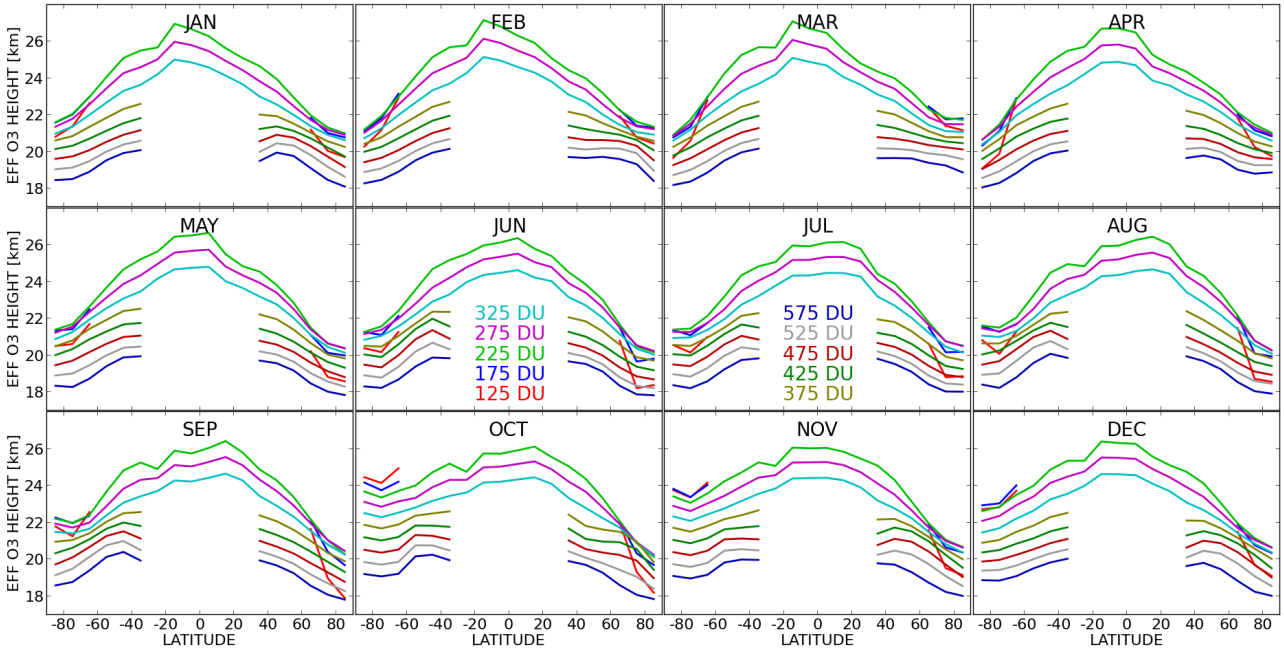


Figure 35: Climatological effective ozone height for a station at sea level for each month and different total ozone column amounts in DU as a function of latitude.

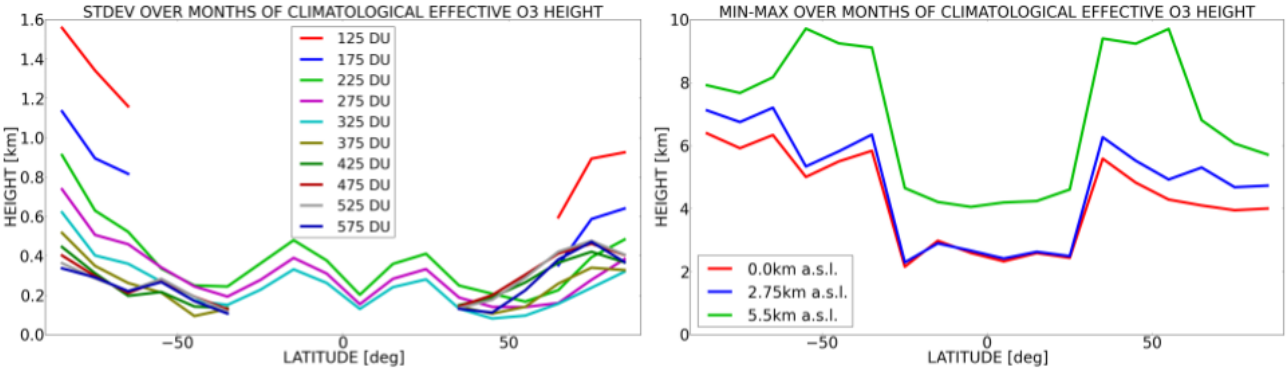


Figure 36: Standard deviation over all months for a station at sea level and different total ozone columns amounts (left panel) and minimum-maximum-range over all months and total column amounts at different station heights (right panel) of the climatological effective ozone height as a function of latitude.

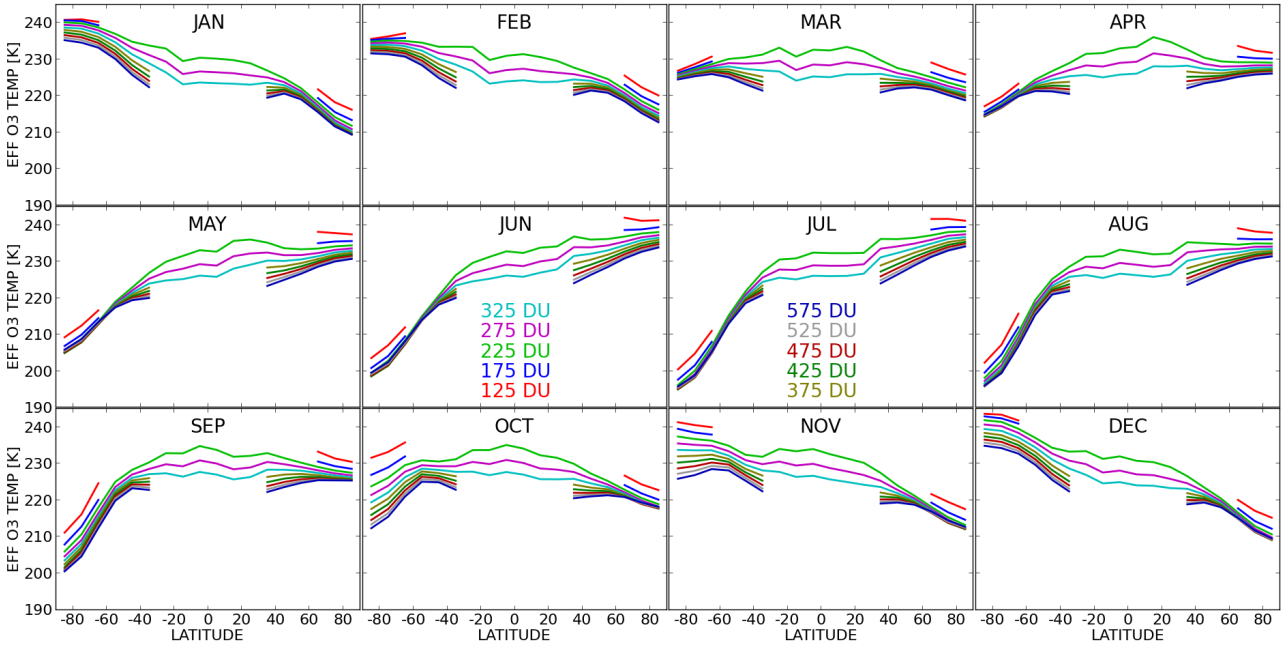


Figure 37: Climatological effective ozone temperature for a station at sea level for each month and different total ozone column amounts in DU as a function of latitude.

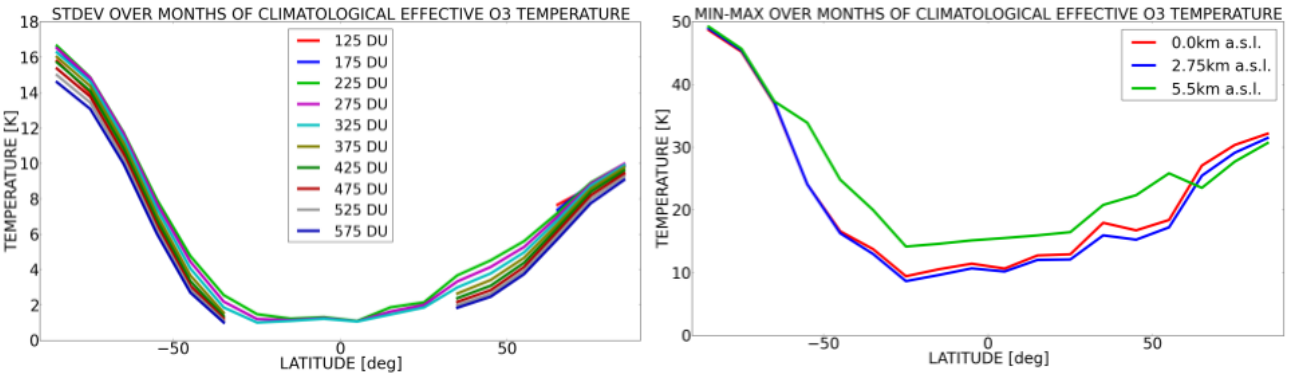


Figure 38: Standard deviation over all months for a station at sea level and different total ozone columns amounts (left panel) and minimum-maximum-range over all months and total column amounts at different station heights (right panel) of the climatological effective ozone temperature as a function of latitude.

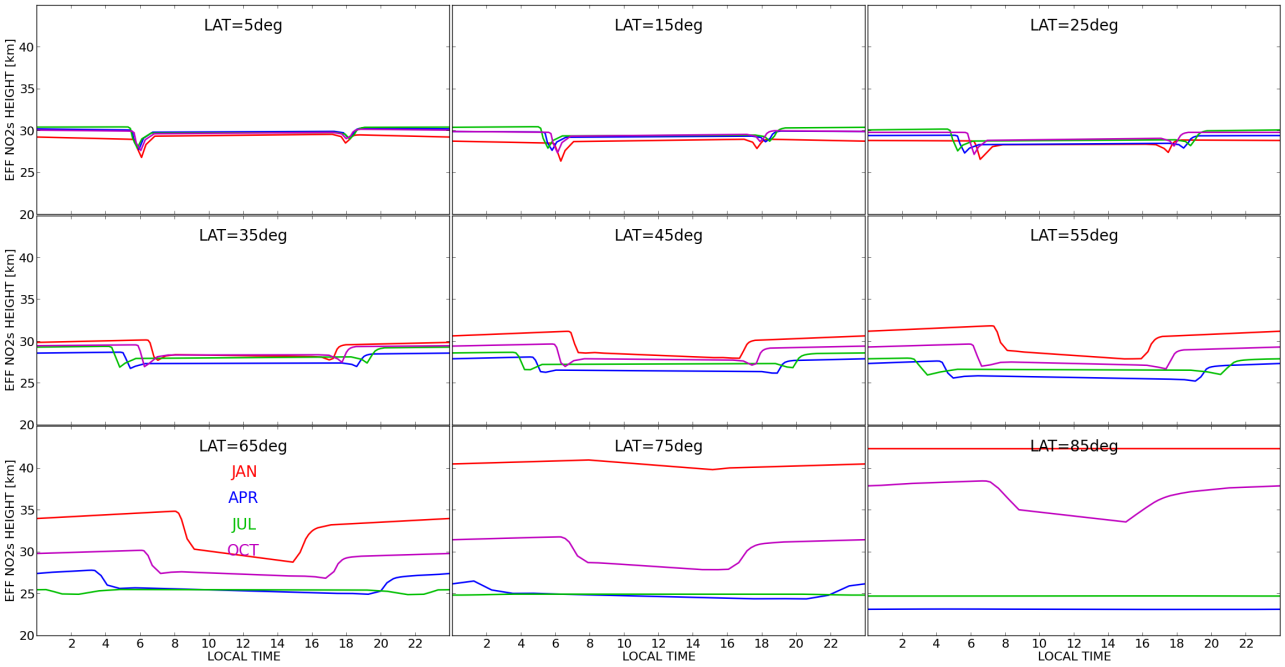


Figure 39: Climatological effective stratospheric NO_2 height for different latitudes for January, April, July and October as a function of the local time.

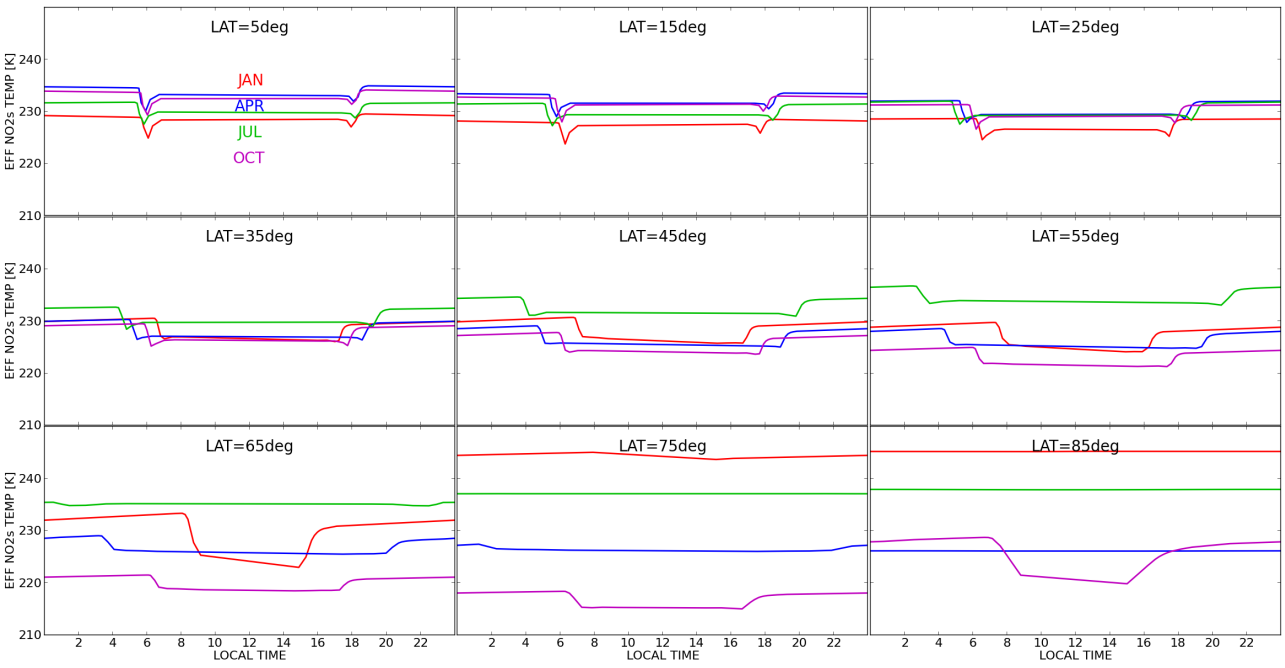


Figure 40: Climatological effective stratospheric NO_2 temperature for different latitudes for January, April, July and October as a function of the local time.

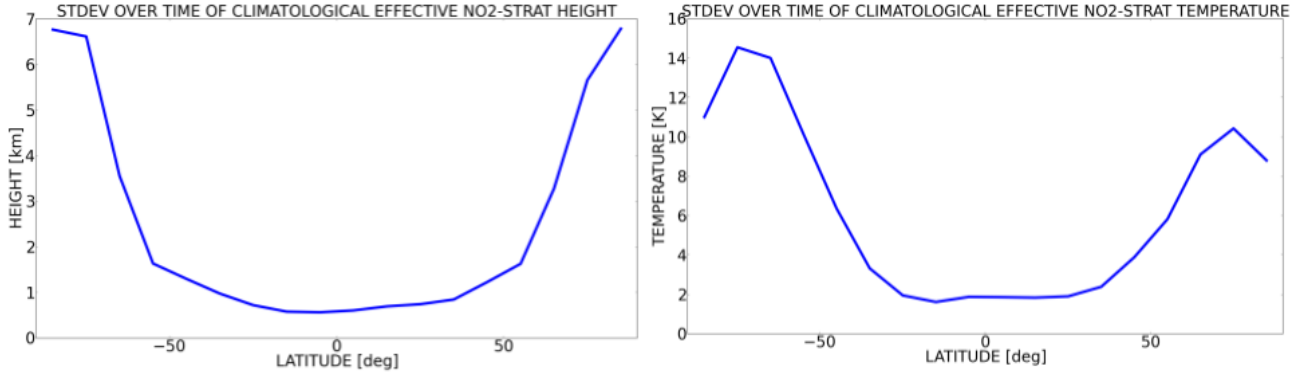


Figure 41: Standard deviation over all months and times of day of the climatological effective stratospheric NO_2 height (left panel) and temperature (right panel) as a function of latitude.

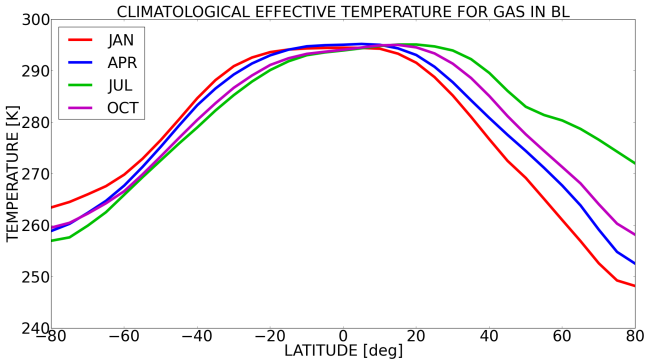


Figure 42: Climatological effective "boundary layer" (0 to 2 km) temperature for a station at sea level for the months of January, April, July and October as a function of latitude.

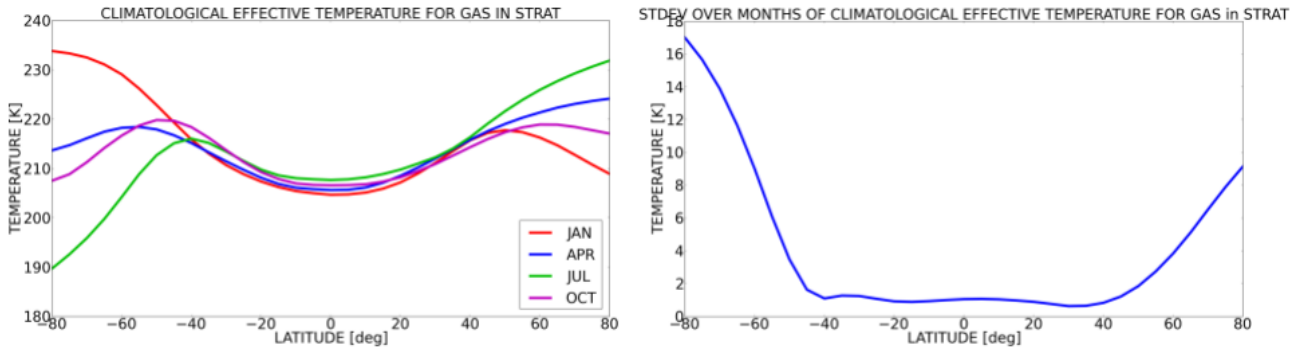


Figure 43: Climatological effective "stratospheric" (13 to 30 km) temperature for the months of January, April, July and October (left panel) and the standard deviation over all months (right panel) as a function of latitude.

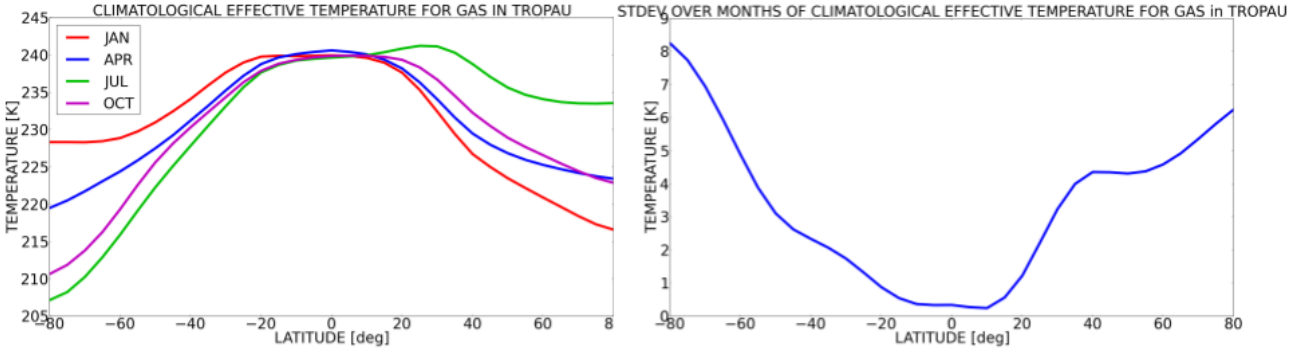


Figure 44: Climatological effective "tropopause" (6 to 15 km) temperature for the months of January, April, July and October (left panel) and the standard deviation over all months (right panel) as a function of latitude.

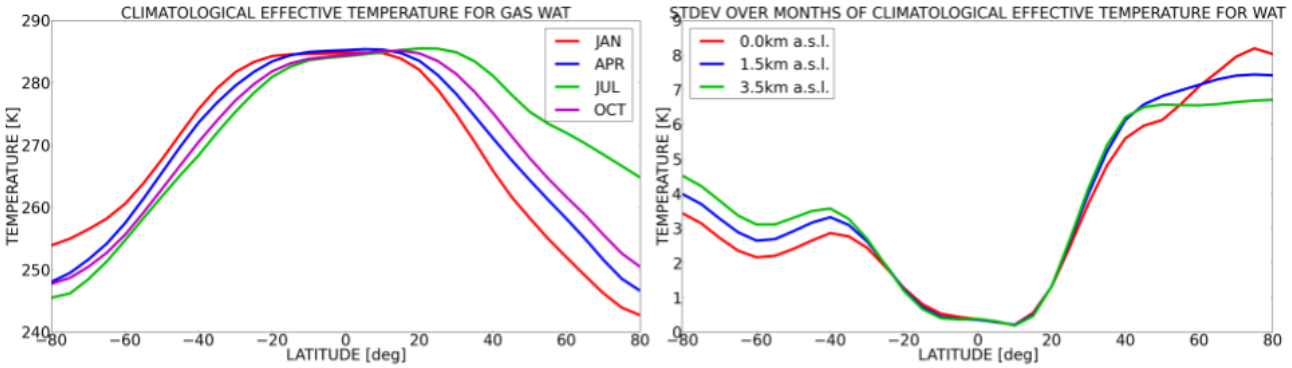


Figure 45: Climatological effective "water cloud" (0 to 6 km) temperature for a station at sea level for the months of January, April, July and October (left panel) and the standard deviation over all months for different station heights (right panel) as a function of latitude.

6.8.3 Stratospheric column

The Blick Software Suite includes a climatology for stratospheric NO_2 columns. It is based on the work of *Brohede et al.* [12] and depends on the latitude, season, and time of day (figure 46). The uncertainty of the climatological data is estimated a fifth of the standard deviation over all months and times of day (figure 47).

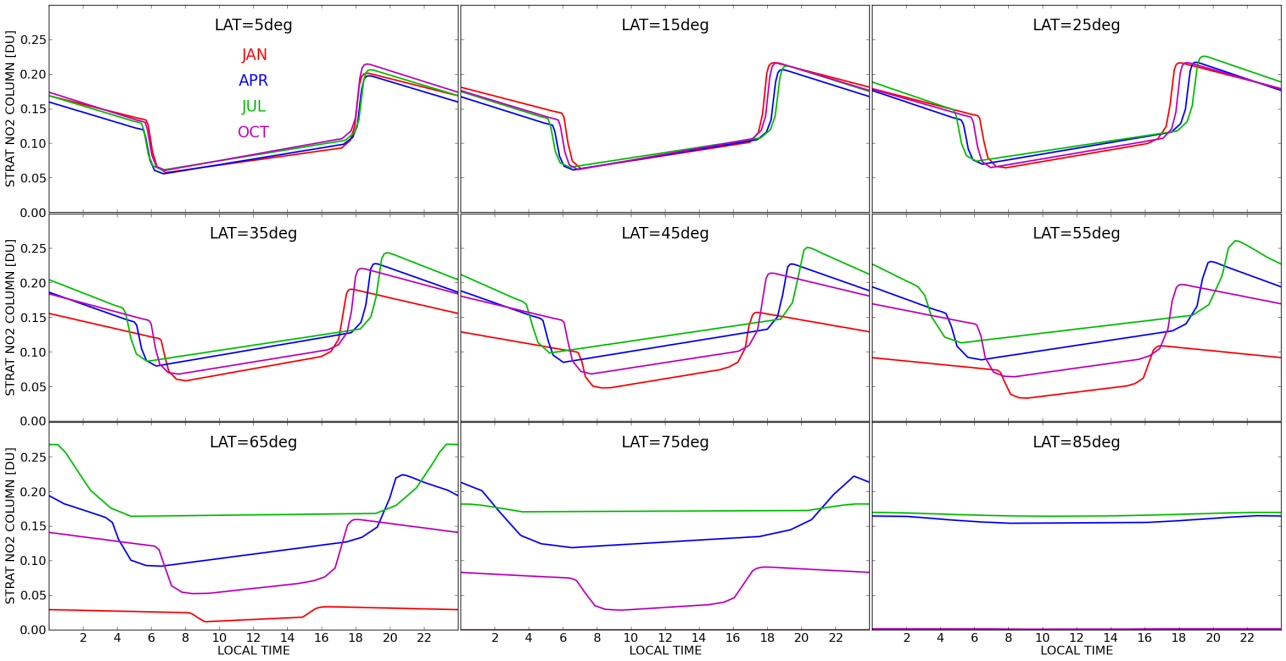


Figure 46: Climatological stratospheric NO_2 column amount in DU for different latitudes for January, April, July and October as a function of the local time.

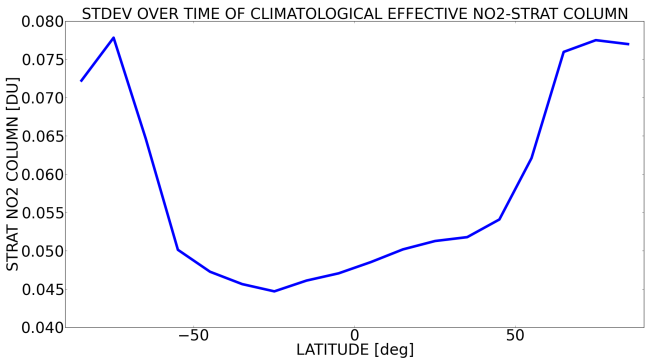


Figure 47: Standard deviation over all months and times of day of the climatological stratospheric NO_2 column amount in DU as a function of latitude.

7 References

[1] Cospar international reference atmosphere: 1986 (0 km to 120 km). URL `http://ccmc.gsfc.nasa.gov/modelweb/atmos/cospar1.html`.

[2] Absorption cross sections of bromine dioxide obro. URL `http://joseba.mpch-mainz.mpg.de/spectral_atlas_data/cross_sections/Halogen%20oxides/Br%20oxides/OBrO_FleischmannBurrows(2002)_298K_384-616nm(5cm-1).txt`.

[3] N. Abuhassan, A. Cede, and M. Kowalewski. *Pandora spectrometer system Installation and Maintenance Manual Version 4*, 2014. URL `http://sciglob.com`.

[4] A. M. Bass and R. J. Paur. The ultraviolet cross-sections of ozone. I. The measurements. II - Results and temperature dependence. In C. S. Zerefos and A. Ghazi, editors, *Atmospheric ozone; Proceedings of the Quadrennial Ozone Symposium, Halkidiki, Greece, September 3-7, 1984 (A86-48601 24-46).*, pages 606–616, 1985.

[5] S Beirle, H Sihler, and T Wagner. Linearisation of the effects of spectral shift and stretch in doas analysis. *Atmospheric Measurement Techniques*, 6(3):661–675, 2013.

[6] G. Bernhard, C. R. Booth, and J. C. Ehramjian. Version 2 data of the National Science Foundation's ultraviolet radiation monitoring network: South Pole. *Journal of Geophysical Research (Atmospheres)*, 109(D21), 2004.

[7] G Bernhard, RD Evans, GJ Labow, and SJ Oltmans. Bias in dobson total ozone measurements at high latitudes due to approximations in calculations of ozone absorption coefficients and air mass. *Journal of Geophysical Research: Atmospheres*, 110(D10), 2005.

[8] P. K. Bhartia and C. Wellemeyer. *TOMS-V8 total O3 algorithm ATBD*, 2002.

[9] B. A. Bodhaine, N. B. Wood, E. G. Dutton, and J. R. Slusser. On Rayleigh Optical Depth Calculations. *Journal of Atmospheric and Oceanic Technology*, 16:1854, November 1999. doi: 10.1175/1520-0426(1999)016<1854:ORODC>2.0.CO;2.

[10] Konstanze Bogumil, J Orphal, T Homann, S Voigt, P Spietz, OC Fleischmann, A Vogel, M Hartmann, H Kromminga, H Bovensmann, et al. Measurements of molecular absorption spectra with the sciamachy pre-flight model: instrument characterization and reference data for atmospheric remote-sensing in the 230–2380 nm region. *Journal of Photochemistry and Photobiology A: Chemistry*, 157(2):167–184, 2003.

[11] A Bongartz, J Kames, F Welter, and U Schurath. Near-uv absorption cross sections and trans/cis equilibrium of nitrous acid. *The Journal of Physical Chemistry*, 95(3):1076–1082, 1991.

[12] Samuel M Brohede, Craig S Haley, Chris A Mclinden, Christopher E Sioris, Donal P Murtagh, Svetlana V Petelina, Edward J Llewellyn, Ariane Bazureau, Florence Goutail, Cora E Randall, et al. Validation of odin/osiris stratospheric no2 profiles. *Journal of Geophysical Research: Atmospheres*, 112(D7), 2007.

[13] H Buiteveld, JHM Hakvoort, and M Donze. The optical properties of pure water. *Proc. SPIE in Ocean Optics XII*, 2258.

[14] JP Burrows, A Richter, A Dehn, B Deters, S Himmelmann, S Voigt, and J Orphal. Atmospheric remote-sensing reference data from gome-2. temperature-dependent absorption cross sections of o_3 in the 231–794nm range. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 61(4):509–517, 1999.

[15] Oliver C Fleischmann, Matthias Hartmann, John P Burrows, and Johannes Orphal. New ultraviolet absorption cross-sections of bro at atmospheric temperatures measured by time-windowing fourier transform spectroscopy. *Journal of Photochemistry and Photobiology A: Chemistry*, 168(1):117–132, 2004.

[16] J. F. Grainger and J. Ring. Anomalous Fraunhofer line profiles. *Nature*, 193:762, 1962.

[17] Christian A Gueymard. The sun's total and spectral irradiance for solar energy applications and solar radiation models. *Solar energy*, 76(4):423–453, 2004.

[18] C Hermans, AC Vandaele, S Fally, M Carleer, R Colin, B Coquart, A Jenouvrier, and M-F Merienne. Absorption cross-section of the collision-induced bands of oxygen from the uv to the nir. In *Weakly interacting molecular pairs: unconventional absorbers of radiation in the atmosphere*, pages 193–202. Springer, 2003.

[19] Abraham Horowitz, Richard Meller, and Geert K Moortgat. The uv–vis absorption cross sections of the α-dicarbonyl compounds: pyruvic acid, biacetyl and glyoxal. *Journal of Photochemistry and Photobiology A: Chemistry*, 146(1-2):19–27, 2001.

[20] Henrik Wann Jensen, Frédo Durand, Julie Dorsey, Michael M Stark, Peter Shirley, and Simon Premože. A physically-based night sky model. In *Proceedings of the 28th annual conference on Computer graphics and interactive techniques*, pages 399–408. ACM, 2001.

[21] JB Kerr, CT McElroy, DI Wardle, RA Olafson, and WFJ Evans. The automated brewer spectrophotometer. In *Atmospheric Ozone*, pages 396–401. Springer, 1985.

[22] Gary Knight, AR Ravishankara, and James B Burkholder. Laboratory studies of obro. *The Journal of Physical Chemistry A*, 104(47):11121–11125, 2000.

[23] Robert L Kurucz. New atlases for solar flux, irradiance, central intensity, and limb intensity. *Memorie della Societa Astronomica Italiana Supplementi*, 8:189, 2005.

[24] J Malicet, D Daumont, J Charbonnier, C Parisse, A Chakir, and J Brion. Ozone uv spectroscopy. ii. absorption cross-sections and temperature dependence. *Journal of atmospheric chemistry*, 21(3):263–273, 1995.

[25] R Meller, W Raber, JN Crowley, ME Jenkin, and GK Moortgat. The uv-visible absorption spectrum of methylglyoxal. *Journal of Photochemistry and Photobiology A: Chemistry*, 62(2):163–171, 1991.

[26] Richard Meller and Geert K Moortgat. Temperature dependence of the absorption cross sections of formaldehyde between 223 and 323 k in the wavelength range 225–375 nm. *Journal of Geophysical Research: Atmospheres (1984–2012)*, 105(D6):7089–7101, 2000.

[27] Jonathan Mittaz, Christopher J Merchant, and Emma R Woolliams. Applying principles of metrology to historical earth observations from satellites. *Metrologia*, 56(3):032002, 2019.

[28] David A Newnham and John Ballard. Visible absorption cross sections and integrated absorption intensities of molecular oxygen (o2 and o4). *Journal of Geophysical Research: Atmospheres (1984–2012)*, 103 (D22):28801–28815, 1998.

[29] James C Owens. Optical refractive index of air: dependence on pressure, temperature and composition. *Applied Optics*, 6(1):51–59, 1967.

[30] Kent F Palmer and Dudley Williams. Optical properties of water in the near infrared. *JOSA*, 64(8): 1107–1110, 1974.

[31] E Peters, F Wittrock, A Richter, LMA Alvarado, VV Rozanov, and JP Burrows. Liquid water absorption and scattering effects in doas retrievals over oceans. *Atmospheric Measurement Techniques*, 7(12):4203–4221, 2014.

[32] Ulrich Platt and Jochen Stutz. *Differential absorption spectroscopy*. Springer, 2008.

[33] Robin M Pope and Edward S Fry. Absorption spectrum (380–700 nm) of pure water. ii. integrating cavity measurements. *Applied optics*, 36(33):8710–8723, 1997.

[34] William H Press, Saul A Teukolsky, William T Vetterling, and Brian P Flannery. Numerical recipes in c: the art of scientific computing, 1992. *Cité en*, page 92, 1992.

[35] TI Quickenden and JA Irvin. The ultraviolet absorption spectrum of liquid water. *The Journal of Chemical Physics*, 72(8):4416–4428, 1980.

[36] Laurence S Rothman, D Jacquemart, Aetal Barbe, D Chris Benner, M Birk, LR Brown, MR Carleer, C Chackerian Jr, K Chance, LH et al Coudert, et al. The< i> hitran</i> 2004 molecular spectroscopic database. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 96(2):139–204, 2005.

[37] Laurence S Rothman, Iouli E Gordon, Alain Barbe, D Chris Benner, Peter F Bernath, Manfred Birk, Vincent Boudon, Linda R Brown, Alain Campargue, J-P Champion, et al. The< i> hitran</i> 2008 molecular spectroscopic database. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 110(9): 533–572, 2009.

[38] Laurence S Rothman, Iouli E Gordon, Yury Babikov, Alain Barbe, D Chris Benner, Peter F Bernath, Manfred Birk, Luca Bizzocchi, Vincent Boudon, Linda R Brown, et al. The hitran2012 molecular spectroscopic database. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 130:4–50, 2013.

[39] A Saiz-Lopez, RW Saunders, DM Joseph, SH Ashworth, and JMC Plane. Absolute absorption cross-section and photolysis rate of i 2. *Atmospheric Chemistry and Physics*, 4(5):1443–1450, 2004.

[40] Stanley P Sander. Temperature dependence of the nitrogen trioxide absorption spectrum. *The Journal of Physical Chemistry*, 90(17):4135–4142, 1986.

[41] Stanley P Sander and Randall R Friedl. Kinetics and product studies of the reaction chlorine monoxide+ bromine monoxide using flash photolysis-ultraviolet absorption. *The Journal of Physical Chemistry*, 93 (12):4764–4771, 1989.

[42] Beat Schmid, Joseph J Michalsky, Donald W Slater, James C Barnard, Rangasayi N Halthore, James C Liljegren, Brent N Holben, Thomas F Eck, John M Livingston, Philip B Russell, et al. Comparison of columnar water-vapor measurements from solar transmittance methods. *Applied Optics*, 40(12):1886–1896, 2001.

[43] A. Serdyuchenko, V. Gorshelev, M. Weber, W. Chehade, and J. P. Burrows. High spectral resolution ozone absorption cross-sections - Part 2: Temperature dependence. *Atmospheric Measurement Techniques Discussions*, 6:6613–6643, July 2013. doi: 10.5194/amtd-6-6613-2013.

[44] Peter Spietz. *Absorption Cross Sections for Iodine Species of Relevance to the Photolysis of Mixtures of I2 and O3 and for the Atmosphere*. PhD thesis, University of Bremen, 2005.

[45] Peter Spietz, Juan Carlos Gomez Martin, and John P Burrows. Spectroscopic studies of the i2/o3 photochemistry: Part 2. improved spectra of iodine oxides and analysis of the io absorption spectrum. *Journal of Photochemistry and Photobiology A: Chemistry*, 176(1):50–67, 2005.

[46] J Stutz, ES Kim, U Platt, P Bruno, C Perrino, and A Febo. Uv-visible absorption cross sections of nitrous acid. *Journal of Geophysical Research: Atmospheres (1984–2012)*, 105(D11):14585–14592, 2000.

[47] Ryan Thalman and Rainer Volkamer. Temperature dependent absorption cross-sections of o 2–o 2 collision pairs between 340 and 630 nm and at atmospherically relevant pressure. *Physical chemistry chemical physics*, 15(37):15371–15381, 2013.

[48] G Thuillier, L Floyd, TN Woods, R Cebula, E Hilsenrath, M Hersé, and D Labs. Solar irradiance reference spectra for two solar active levels. *Advances in Space Research*, 34(2):256–261, 2004.

[49] A. C. Vandaele, C. Hermans, P. C. Simon, M. Carleer, R. Colin, S. Fally, M. F. Mérienne, A. Jenouvrier, and B. Coquart. Measurements of the NO_2 absorption cross-section from 42,000 cm^{-1} to 10,000 cm^{-1} (238-1000 nm) at 220 K and 294 K. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 59: 171–184, May 1998. doi: 10.1016/S0022-4073(97)00168-4.

[50] Ann Carine Vandaele, Paul C Simon, Jean Michel Guilmot, Michel Carleer, and Réginald Colin. So2 absorption cross section measurement in the uv using a fourier transform spectrometer. *Journal of Geophysical Research: Atmospheres (1984–2012)*, 99(D12):25599–25605, 1994.

[51] Ann Carine Vandaele, Christian Hermans, and Sophie Fally. Fourier transform measurements of so2 absorption cross sections: Ii.: Temperature dependence in the 29 000–44 000 cm- 1 (227–345 nm) region. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 110(18):2115–2126, 2009.

[52] Michael E VanHoosier. Solar ultraviolet spectral irradiance data with increased wavelength and irradiance accuracy. In *SPIE's 1996 International Symposium on Optical Science, Engineering, and Instrumentation*, pages 57–64. International Society for Optics and Photonics, 1996.

[53] Rainer Volkamer, Peter Spietz, John Burrows, and Ulrich Platt. High-resolution absorption cross-section of glyoxal in the uv–vis and ir spectral ranges. *Journal of Photochemistry and Photobiology A: Chemistry*, 172(1):35–46, 2005.

[54] Andreas Wahner, Geoffrey S Tyndall, and ANDA R Ravishankara. Absorption cross sections for symmetric chlorine dioxide as a function of temperature in the wavelength range 240-480nm. *Journal of Physical Chemistry*, 91(11):2734–2738, 1987.

[55] Stephen G Warren. Optical constants of ice from the ultraviolet to the microwave. *Applied optics*, 23(8): 1206–1225, 1984.

[56] David M Wilmouth, Thomas F Hanisco, Neil M Donahue, and James G Anderson. Fourier transform ultraviolet spectroscopy of the a $2\pi 3/2$? x $2\pi 3/2$ transition of bro. *The Journal of Physical Chemistry A*, 103(45):8935–8945, 1999.

[57] Y. Zong, S. W. Brown, B. C. Johnson, K. R. Lykke, and Y. Ohno. Simple spectral stray light correction method for array spectroradiometers. *Applied Optics*, 45(6):1111–1119, 2006.