



# **Manual for Blick Software Suite 1.7**

Manual version 1.7, 24 Oct 2019

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## 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

## Acronyms and Abbreviations

2D	Two dimensional
LuftBlick	LuftBlick OG
AC	Alternating Current
AD	Analog-to-digital
AMF	Air mass factor
ASCII	American Standard Code for Information Interchange
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
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
ESA	European Space Agency
FEL lamp	ANSI standard 1000 watt quartz halogen lamp
FOV	Field of View
FSE	Fitting Setup Entry
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
L2Fit	Level 2 spectral fitting results file

L2H	Level 2 files other than L2Fit
L2Tot	Level 2 total columns file
L2Trop	Level 2 tropospheric information file
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
RAM	Random-access memory
rms	Root Mean Square
ROE	Readout electronics
RTC	Radiative Transfer Calculations
SkyFOV	Field of view for sky observations
SNR	Signal to noise ratio
SunFOV	Field of view for direct sun observations
SZA	Solar Zenith Angle
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 <http://pandonia.net/docs/>. 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.

The Blick Software Suite runs under the following open source license:

"Only under the following conditions you are free to share, copy, distribute, transmit the work or adapt it for your purpose:

- You may not use this work or modified versions of it for commercial purposes.
- If you alter, transform or build upon this work, you may distribute the resulting work only under the same license to this one."

For questions contact LuftBlick OG (LuftBlick) under [office@luftblick.at](mailto:office@luftblick.at).

## 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 1.7.

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

- Nader Abuhassan, main responsible for instrument hardware
- Martin Tiefengraber, instrument and algorithm research
- Matt Kowalewski, calibration and hardware
- Christian Retscher, special software support, data processing
- Elena Spinei, algorithm development
- Moritz Müller, operation, calibration and instrument research



- Daniel Santana, network operator, calibration and instrument research
- Christian Posch, software and network support
- Axel Kreuter, algorithm development

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-1.7.*_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 5.15.

### **/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**

Python consists of a basic software package and additional modules for specific purposes. These step-by-step instructions show how to download and install all modules needed in the Blick Software Suite. The files listed for the download are the Windows versions currently used in the Blick Software Suite version 1.7. Other platforms require different files, which should also be found in the same internet links. There is a good chance, that newer versions for each module are available. These newer versions should in principle also work fine, but it is not guaranteed. In general we recommend staying away from versions with subversions number 0 or 1 (e.g. version 3.5.1), since we have previously encountered simple bugs in these versions, which are typically quickly corrected in sub-version number 2. It is best to stay with the original version of Python until newer versions are tested. Note that it does not matter whether the Python modules are installed before or after the Blick Software Suite installation.

### **Program language "Python"**

<https://www.python.org/downloads/release/python-2710/>  
Save <python-2.7.10.msi> (from Windows x86 MSI installer)  
Execute msi-file, use default directory C:/Python27/

### **Module for numerical functions "NumPy"**

<http://sourceforge.net/projects/numpy/files/NumPy/1.7.1/>  
Save <numpy-1.7.1-win32-superpack-python2.7.exe>  
Execute msi-file, use default directory C:/Python27/Lib/Site-packages/

### **Module for mathematical functions "SciPy"**

<http://sourceforge.net/projects/scipy/files/scipy/0.12.0/>  
Save <scipy-0.12.0-win32-superpack-python2.7.exe>  
Execute exe-file, use default directory C:/Python27/Lib/Site-packages/

#### Module for GUI functions "wxpython"

<http://sourceforge.net/projects/wxpython/files/wxPython/2.8.12.1/>  
Save <wxPython2.8-win32-unicode-2.8.12.1-py27.exe>  
Execute file, use default directory C:/Python27/Lib/Site-packages/

#### Module for serial interface "pyserial"

<https://pypi.python.org/pypi/pyserial/2.6>  
Save <pyserial-2.6.tar.gz>  
Unpack <pyserial-2.6.tar.gz> to get <pyserial-2.6.tar>  
Unpack <pyserial-2.6.tar>  
In a command window change to the directory of the unpacked .../pyserial-2.6/  
Type "C:/Python27/python.exe setup.py install"  
Type "exit" to quit the command window

#### Module to use HDF "h5py"

<https://pypi.python.org/pypi/h5py/2.7.1>  
Save <h5py-2.7.1.win32-py2.7.msi>  
Execute file, use default directory C:/Python27/Lib/Site-packages/

#### Module for Java access "JPytype"

(only needed for instruments with "Spectrometer read out type -> OcOpt1", see section 5.3)

<http://sourceforge.net/projects/jpytype/files/JPytype/0.5.4/>  
Save <JPytype-0.5.4.2.win32-py2.7.exe>  
Execute file, use default directory C:/Python27/Lib/Site-packages/

(This module also needs the Java Development Kit, which can be obtained from <http://www.oracle.com/technetwork/java/javase/downloads/jdk7-downloads-1637583.html> for windows<jdk-7u5-windows-i586-p.exe>)

#### Imaging Library "PIL"

<http://www.pythonware.com/products/pil/>  
Save <PIL-1.1.7.win32-py2.7.exe>  
Execute file, use default directory C:/Python27/Lib/Site-packages/

#### System and process utilities "psutil"

<https://pypi.org/project/psutil/4.4.2/#files>  
Save <psutil-4.4.2.win32-py2.7.exe>  
Execute file, use default directory C:/Python27/Lib/Site-packages/

#### Camera module "OpenCV"

(only needed for instruments with "Camera read module -> OpenCV", see section 5.3)

<http://opencv.org/downloads.html>  
Save <OpenCV-2.4.6.0.exe>  
Execute file and extract files into a temporary directory  
Copy file <.../opencv/build/python/2.7/cv2.pyd> in directory C:/Python27/Lib/Site-packages/

### Camera module "VideoCapture"

(only needed for instruments with "Camera read module -> DirectX", see section 5.3)

<http://videocapture.sourceforge.net/>

Save <VideoCapture-0.9-4.zip> and unzip it

Copy content of /Python27/DLLs/ in directory C:/Python27/DLLs/

Copy content of /Python27/Lib/ in directory C:/Python27/Lib/

In file C:/Python27/Lib/VideoCapture.py replace lines

```
self.normalfont = ImageFont.load_path('helvetica-10.pil')
```

```
self.boldfont = ImageFont.load_path('helvB08.pil')
```

with these lines

```
self.normalfont = []
```

```
self.boldfont = []
```

### An optional free editor

<http://sourceforge.net/projects/spe/>

Save <SPE-0.8.2.a-wx2.6.1.0-py24.exe>

Execute file, use default directory C:/Python27/Lib/Site-packages/

As a shortcut you can pull "SPE.pyw" from C:/Python27/Lib/Site-packages/ onto the desktop

## 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. Basically, these settings 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.

### 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

In order to increase the update interval frequency (one week by default) do the following:

- 1) Use regedit.exe by writing "regedit" in Start - Run or where it says "Start Search"
- 2) Go to HKEY\_LOCAL\_MACHINE/SYSTEM/CurrentControlSet/Services/W32Time/TimeProviders/NtpClient
- 3) Double click on "SpecialPollInterval" in the right hand panel - default is 604800 (7 days) in seconds (Decimal). Change it to 40000 (<12 Hours).

Note: the computer time zone does not have to be set to UT. It can be the preferred local time of the operator.

### **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 appear 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.

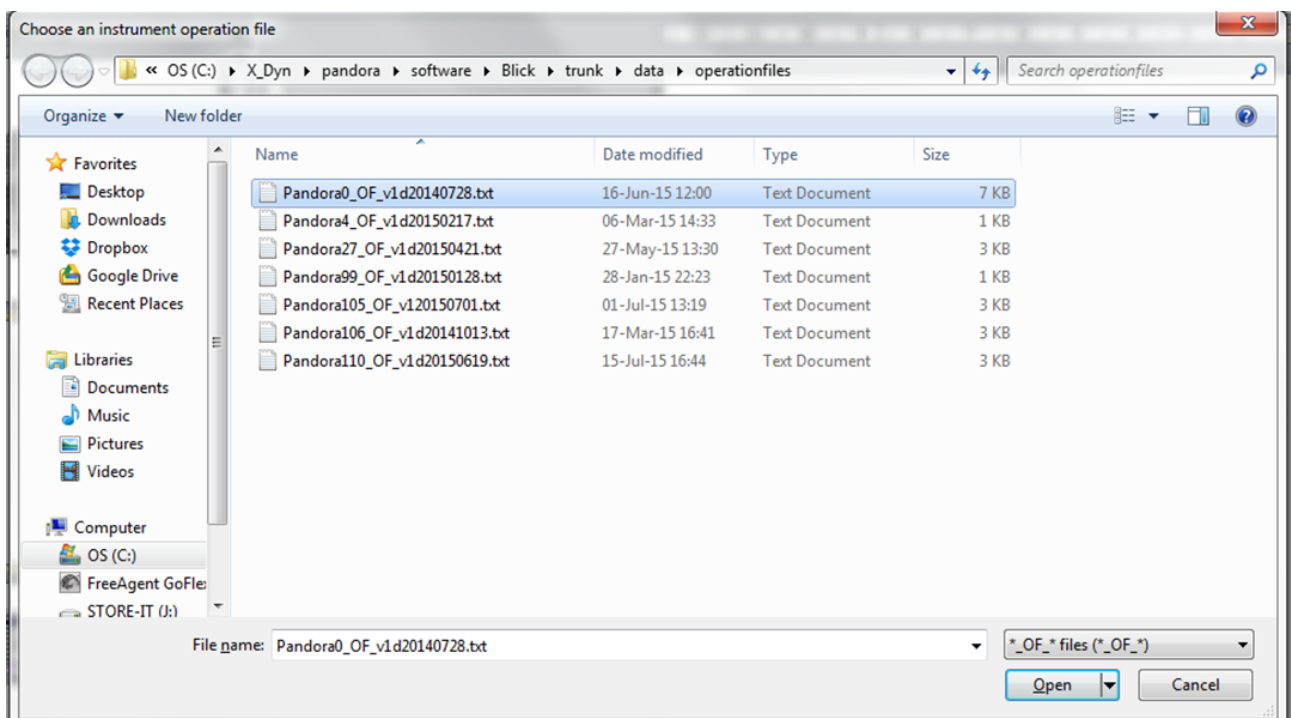


Figure 1: File dialog to select an IOF.



### 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 and solar/lunar angles
3. Connection status labels
4. Connection buttons for all interfaces
5. Auxiliary data 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
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

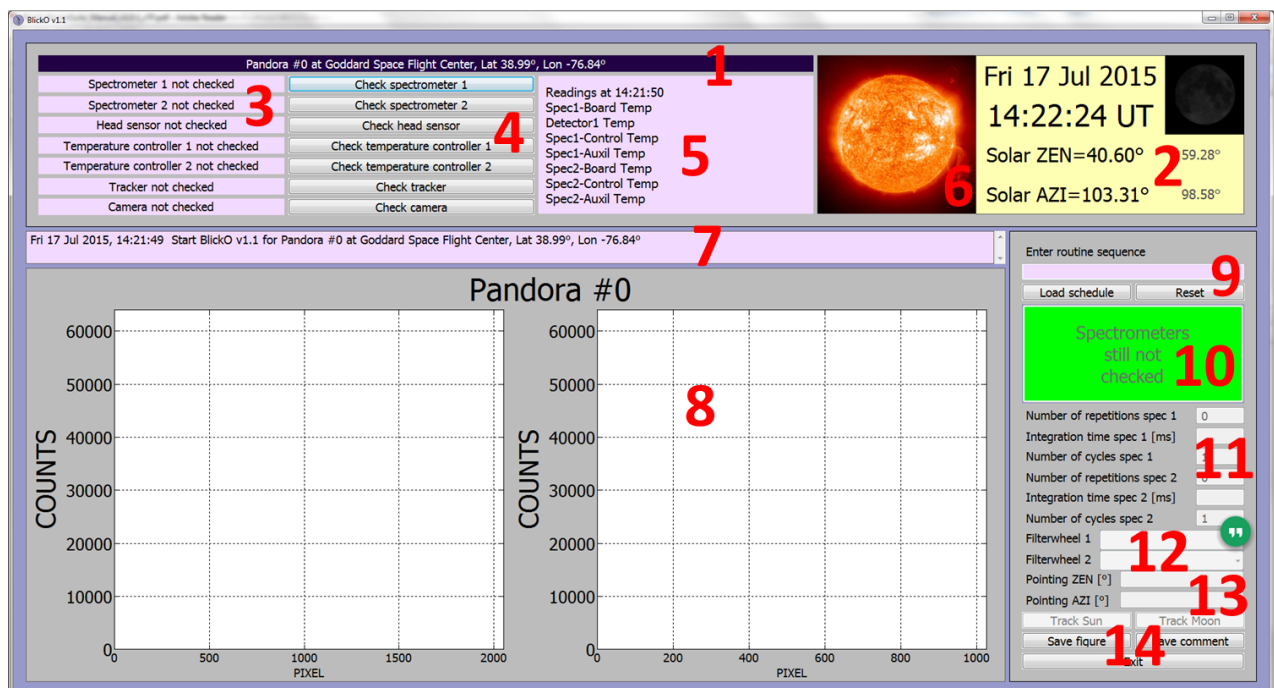


Figure 2: GUI of BlickO in real mode

### 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 specific 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.

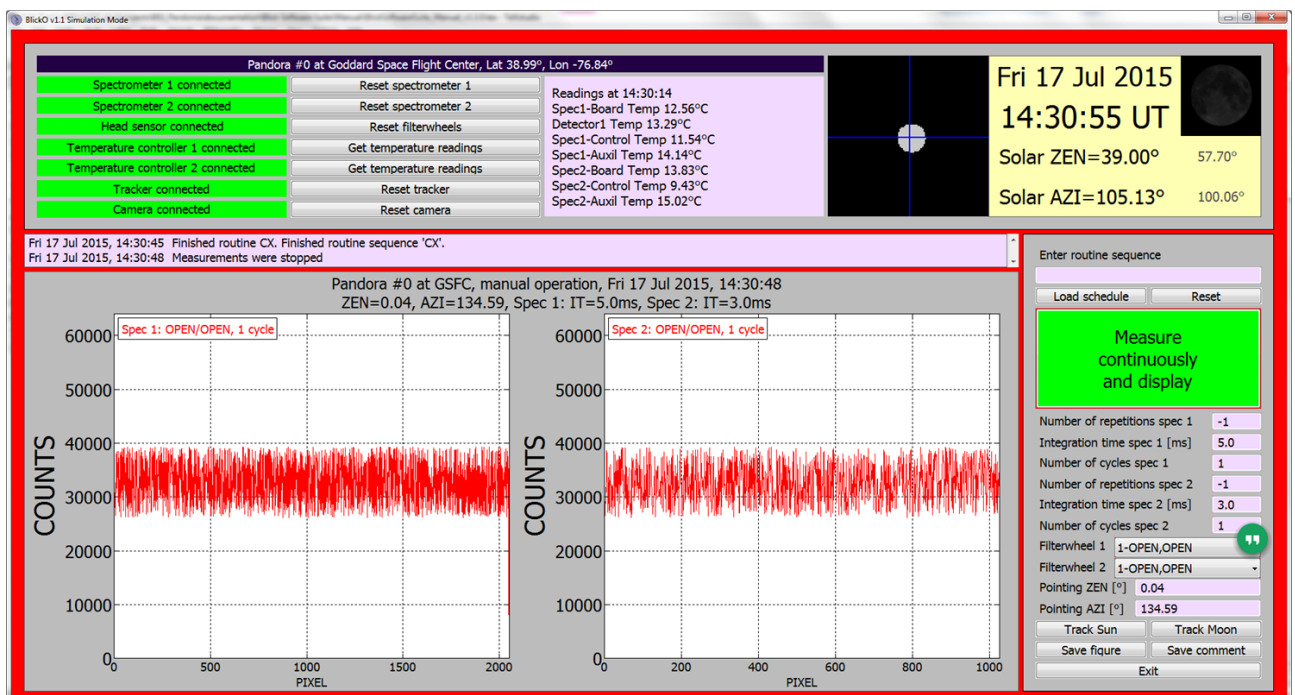


Figure 3: GUI of BlickO in simulation mode

### 3.1.4 Debug mode

One can also run the instrument in "Debug mode". For this purpose entry "Instrument operation mode" in the BlickO specific 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 5.14). 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  $\pm 10$  s, preferably within  $\pm 1$  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 specific 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 are 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, 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.

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.

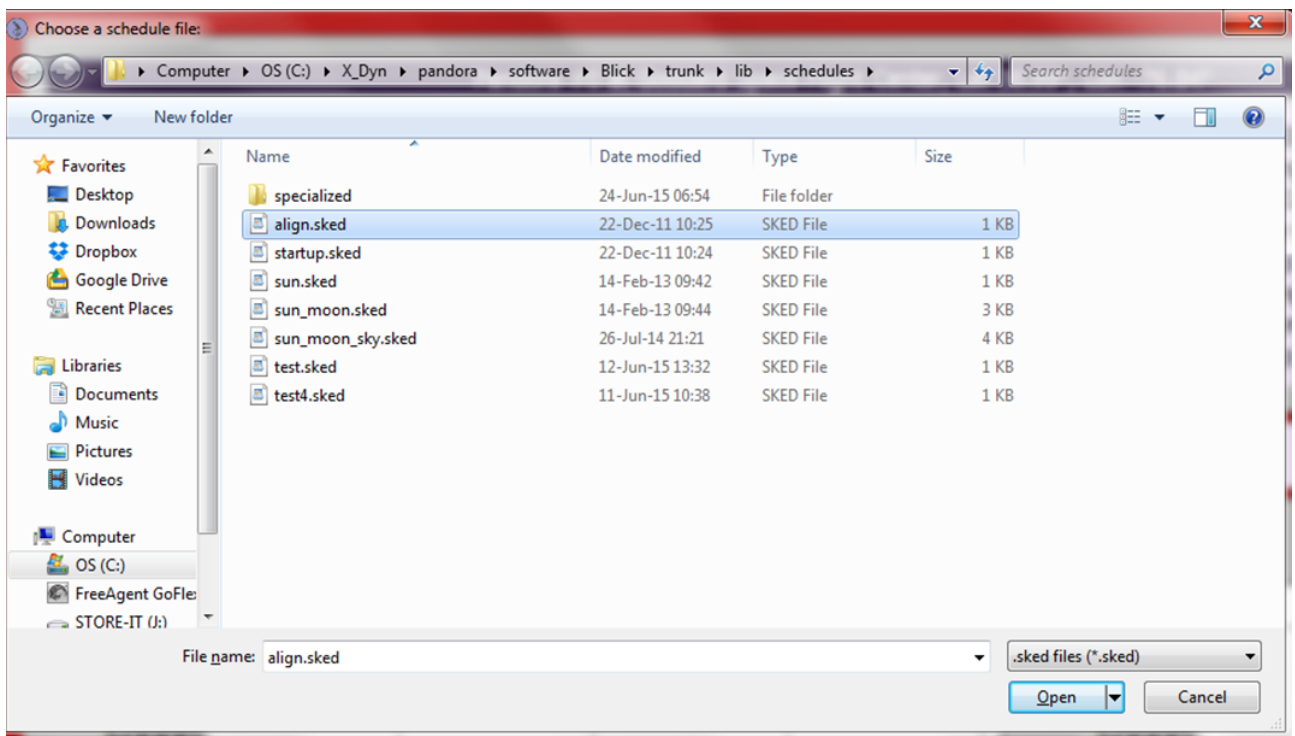


Figure 4: File dialog to select a schedule.

## 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=31)`, where the first number is the OMessage (in this case 3) and the second number the FMessage (in this case 1).

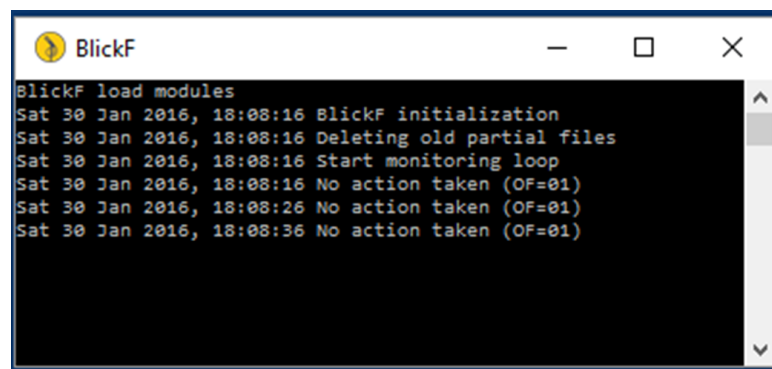


Figure 5: BlickF screenshot.

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).

**IMPORTANT:** To make a clean exit for BlickF, 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 described 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 used and is described in section 5.9.

When starting BlickP it 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 5.14).

## 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 [17]. 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 with open hole
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 with open hole; the standard azimuth is the one given in the BlickO Specific 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 with open hole
EU	Quick sky scan (5 zenith angles) at standard azimuth with open U340

#### Find routines F\*

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
FS	Find Sun; long sun search for all spectrometers, saves final figure and averaged data, but not spectral data
F1	=FS, but only doing the search for spectrometer 1
F2	=FS, but only doing the search for spectrometer 2
FA	=FS, but also saving the spectral data
FD	=FS, but with diffuser in the optical path
FU	=FS, but with U340 plus diffuser combination in the optical path
FN	=FA, but without doing a reset in the case the difference is too large
FM	=FS, but searching moon instead of the sun
FV	Quick sun search
FQ	Quick sun search (system-optimized)
FW	=FA, but showing the results in 4 wavelength regions
FF	Search routine with all "search options" listed

#### Help routines H\*

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

#### Camera routines K\*

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

MO	Direct-Moon with open hole
MU	Direct-Moon with U340
MD	Direct moon measurements during daytime with open hole
MT	Direct moon measurements during daytime with 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\*

SO	Direct-Sun with open hole
SU	Direct-Sun with U340
SB	Direct-Sun with BP300 (BP300 is a UVB bandpass filter with maximum transmission at 300nm)
SQ	Quick direct-Sun with open hole
SS	Quick direct-Sun with U340

### Target, tracker or test routines T\*

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

### 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\*

ZO	Zenith-Sky with open hole
ZU	Zenith-Sky with U340
ZB	Zenith-Sky with BP300

### 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 lose 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 'self-standing' (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 $\geq 0$	0
TIMEMODE	TOTAL, ADDED	ADDED
IT	CURRENT, CHANGE, MIN, MAX, min(IT) $\leq$ float $\leq$ max(IT), x+float $\geq 0$	CURRENT
DURATION	AUTO, float $\geq 0$ , x+float $\geq 0$	AUTO
NCYCLES	AUTO, CURRENT, integer $\geq 1$	AUTO
NREPETITIONS	AUTO, CURRENT, integer $\geq 0$ , x+integer $\geq 0$ , MAX1	AUTO
DARKRATIO	OPTIMIZED, OPT1, OPT2, 0 $\leq$ float $\leq 0.5$	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 $\leq$ float $\leq 10000$ , SATPERC	80
DARKESTIMATION	NEGLECT, THEORY	THEORY
ITLIMIT	ITMAX, min(IT) $\leq$ float $\leq$ max(IT), xITMAX, x+min(IT) $\leq$ float $\leq$ max(IT)	ITMAX
DELTA	MIDDLE, CONT, CAMERA, float $\geq 0$	MIDDLE
AZI	RESET, POWER, CURRENT, STANDARD, DAZI, - 360 $\leq$ float $\leq 360$	CURRENT
ZEN	CURRENT, DZEN, PARK, MAX, -180 $\leq$ float $\leq 180$	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 $\leq$ integer $\leq 9$ , any valid filter name	CURRENT
FW2	RESET, CURRENT, MOVE, 1 $\leq$ integer $\leq 9$ , any valid filter name	CURRENT
TYPE	ONLYL1, NOL1, SUN, MOON, SKY, TARGET, PROFILE, ALMUCANTAR, LAMP, SPECIAL	ONLYL1
DISTANCE	NO, float $\geq 0$	NO
XIJ	→ see description	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 placed 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 "Diagnostic 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  $46^\circ$  and ZENMODE=RELSUN and ZEN=-1.5, then the tracker will point to zenith angle  $46^\circ - 1.5^\circ = 44.5^\circ$ . 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 ANG SUN or ANG MOON. 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  $30^\circ$ , the solar azimuth  $105^\circ$ , AZIMODE=RELSUN and AZI=2, then the tracker will point to azimuth  $105^\circ + 2^\circ = 107^\circ$ . Differently, if AZIMODE=ANG SUN, the tracker will point to azimuth  $105^\circ + 2^\circ / \sin(30^\circ) = 109^\circ$ .

Keyword AZI can also be STANDARD. In this case the azimuth angle given in the BlickO Specific 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 Specific 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  $1^\circ$  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  $2^{n_{\text{bits}}}-1$ , with  $n_{\text{bits}}$  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 of 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 [17]. 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. Not counting the comment lines, a schedule file consists of several line-pairs, i.e. always an even number of lines. The second line of each line-pair, the "routine-line", contains a routine sequence just as it could also be written in the routine control (GUI-section 9). The first line of each line-pair, the "time-line", indicates the time of the routine sequence and its importance. This is an example of such a line-pair in the schedule file.

```
SOLARZEN75AM-0:05.2 FS e 2 x5  
FS (SO4)
```

We will refer to this example in the detailed description of the syntax. The "routine-line" is "FS(SO4)", which by itself entered in the routine control would cause the execution of routine FS followed by 4 times routine SO. The first line of the line-pair, the time-line, consists of 4 or 5 space separated expressions:

1. Time stamp (in our example "SOLARZEN75AM-0:05.2")
2. Reference routine ("FS")
3. Reference time of reference routine ("e")
4. Relative importance ("2")
5. Repetition information ("x5")

The 1st part of the time-line, the time stamp, is an expression, which defines a specific point of time. These are the options:

- "HH:MM": This is the time in hours and minutes (UT). The minutes can have decimals. E.g. "16:40.5" means UT 16:40:30.
- "SOLARNOON": This is the time of local solar noon, i.e. the time of smallest SZA.
- "LUNARNOON": This is the time of local lunar noon, i.e. the time of smallest lunar zenith angle (which of course can also be during the night).
- "SOLARMIDNIGHT": This is the time of local solar midnight, i.e. the time of largest SZA.
- "LUNARMIDNIGHT": This is the time of local lunar midnight, i.e. the time of largest lunar zenith angle.
- "SOLARAZIxxx": This is the time corresponding to solar azimuth xxx ( $-180 \leq xxx \leq 180$ ).
- "LUNARAZIxxx": This is the time corresponding to lunar azimuth xxx ( $-180 \leq xxx \leq 180$ ).
- "SOLARZENxxAM": This is the time corresponding to SZA xx before local solar noon ( $-90 \leq xx \leq 90$ ).
- "SOLARZENxxPM": This is the time corresponding to SZA xx after local solar noon ( $-90 \leq xx \leq 90$ ).
- "LUNARZENxxAM": This is the time corresponding to lunar zenith angle xx before local lunar noon ( $-90 \leq xx \leq 90$ ).
- "LUNARZENxxPM": This is the time corresponding to lunar zenith angle xx after local lunar noon ( $-90 \leq xx \leq 90$ ).

- "THEN": This is the time immediately after the end of the previously executed routine in the schedule.

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

Any of the time stamps listed above can have an optional additional "-HH:MM" or "+HH:MM". In this case the time is corrected for this value. So "SOLARZEN75AM-0:05.2" means 5 min and 12 sec before SZA 75° in the morning.

The 2nd part of the time-line is the reference routine. It must be set to the 2-character-identifier of one of the routines listed in the routine-line. The time-stamp will be applied to the first occurrence of this reference routine. In our example the time "SOLARZEN75AM-0:05.2" refers to routine "FS". If the time-stamp is "THEN", the reference routine has no importance.

The 3rd part of the time-line is the reference time of the reference routine. It can be a "b", an "m" or an "e" meaning the beginning, the middle or the end of the reference routine. In our example "SOLARZEN75AM-0:05.2 FS e" means the routine sequence "FS(SO4)" has to be started so that routine "FS" is finished 5 min and 12 sec before SZA 75° in the morning. If the time-stamp is "THEN", the reference time of the reference routine has no importance.

The 4th part of the time-line is the relative importance. This is an integer and is only needed for the case, where two line-pairs in the schedule file "compete" for the same time. If this happens, then the line-pair of higher relative importance (=higher number) is executed, while the other one is skipped. Here an example:

```
SOLARZEN75AM FS e 2 x5
FS(SO4)
10:30 SO b 10
SOSU3
```

It is possible that for a given day and latitude the SZA of 75° in the morning is just around 10:30 UT. Then BlickO would look at the relative importance of each line-pair and based on this it will execute the "SOSU3" at 10:30 UT (relative importance is 10) and will skip the "FO(SO4)" (relative importance is 2).

The 5th part of the time-line is the repetition information (optional). If it is not given, the routine line "FS(SO4)" is executed exactly once. If it is an "x" followed by an integer number, the routine line is repeated that many times. So in our example "x5" means the routine sequence "FS(SO4)" is repeated 5 times. The repetition information can also be a time stamp of the same format as the 1st part of the time-line. In this case the routine sequence is repeated until this time is reached. E.g.

```
SOLARZEN75AM FS e 2 SOLARZEN60PM
FS(SO4)
```

This means that "FS(SO4)" is started at SZA 75° in the morning and repeated until the SZA is 60° in the afternoon. Note that the number of repetitions will be reduced if another routine sequence of higher relative importance is scheduled to start.

If BlickO can successfully read through the schedule file, it will first create a "protocol file" of name /lib/schedules/XYZ.prot. This is a text file with the "translated" schedule for the day and the location. E.g. a schedule called "simple" is repeating "FS(SO4)" from sunrise to sunset:

```
#simple schedule
SOLARZEN90AM FS b 2 SOLARZEN90PM
FS(SO4)
```

This is the protocol file for this schedule for 17 Dec 2014, at Goddard Space Flight Center (it is truncated in the middle):

```
Predicted Pandora #0 measurements based on schedule 'simple'
for day 2014-12-17 at
Goddard Space Flight Center, USA, Lat 38.99°, Long -76.84°, 90m a.s.l.
File created on Wed 17 Dec 2014, 20:08:52 UT
```

```
-----
Time stamp 'SOLARZEN90AM FS b 2 SOLARZEN90PM' Command 'FS(SO4)'
FS 12:25:20-12:26:10 (SolarZEN 90.04-89.90) Wed 17 Dec 2014
SO 12:26:10-12:27:01 (SolarZEN 89.90-89.76) Wed 17 Dec 2014
SO 12:27:01-12:27:52 (SolarZEN 89.76-89.62) Wed 17 Dec 2014
SO 12:27:52-12:28:43 (SolarZEN 89.62-89.48) Wed 17 Dec 2014
SO 12:28:43-12:29:34 (SolarZEN 89.48-89.34) Wed 17 Dec 2014
FS 12:29:34-12:30:24 (SolarZEN 89.34-89.20) Wed 17 Dec 2014
SO 12:30:24-12:31:15 (SolarZEN 89.20-89.06) Wed 17 Dec 2014
SO 12:31:15-12:32:06 (SolarZEN 89.06-88.92) Wed 17 Dec 2014
SO 12:32:06-12:32:57 (SolarZEN 88.92-88.78) Wed 17 Dec 2014
SO 12:32:57-12:33:48 (SolarZEN 88.78-88.64) Wed 17 Dec 2014
FS 12:33:48-12:34:38 (SolarZEN 88.64-88.50) Wed 17 Dec 2014
SO 17:48:47-17:49:38 (SolarZEN 63.26-63.29) Wed 17 Dec 2014
SO 17:49:38-17:50:29 (SolarZEN 63.29-63.33) Wed 17 Dec 2014
SO 17:50:29-17:51:20 (SolarZEN 63.33-63.36) Wed 17 Dec 2014
FS 17:51:20-17:52:10 (SolarZEN 63.36-63.40) Wed 17 Dec 2014
...
SO 21:34:52-21:35:43 (SolarZEN 88.84-88.98) Wed 17 Dec 2014
FS 21:35:43-21:36:33 (SolarZEN 88.98-89.12) Wed 17 Dec 2014
SO 21:36:33-21:37:24 (SolarZEN 89.12-89.26) Wed 17 Dec 2014
SO 21:37:24-21:38:15 (SolarZEN 89.26-89.40) Wed 17 Dec 2014
SO 21:38:15-21:39:06 (SolarZEN 89.40-89.54) Wed 17 Dec 2014
SO 21:39:06-21:39:57 (SolarZEN 89.54-89.68) Wed 17 Dec 2014
FS 21:39:57-21:40:47 (SolarZEN 89.68-89.82) Wed 17 Dec 2014
SO 21:40:47-21:41:38 (SolarZEN 89.82-89.96) Wed 17 Dec 2014
SO 21:41:38-21:42:29 (SolarZEN 89.96-90.11) Wed 17 Dec 2014
-> last routine probably not executed due to time restriction
```

```
-----
Estimated number of occurrences for each routine
FS 132
SO 525
-----
```

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, overwrites the 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 Specific Configuration File (section 5.5), entry "Tracker parking

zenith angle and azimuth".

## 4.2.2 Standard schedules

The "standard schedules" listed in table 8 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 should 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 8). 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 gives more time resolution, but also increases the size of the raw data significantly and should therefore only be used in system with good internet connection.

Table 8: 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 9 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 9: 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 Specific 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	5.13	L2 data
Log Files	O	O,F,P	ASCII	5.14	Logger lines
Alignment Files	IO	O	ASCII	5.15	Sun/Moon search results

## 5.1 Meta Data

Table 10 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
L2H	All other Level 2 files, i.e. L2Tot (Total columns file) and L2Trop (Tropospheric information file)
All	All of the above files
Align	Alignment file

Table 10: Meta Data Overview

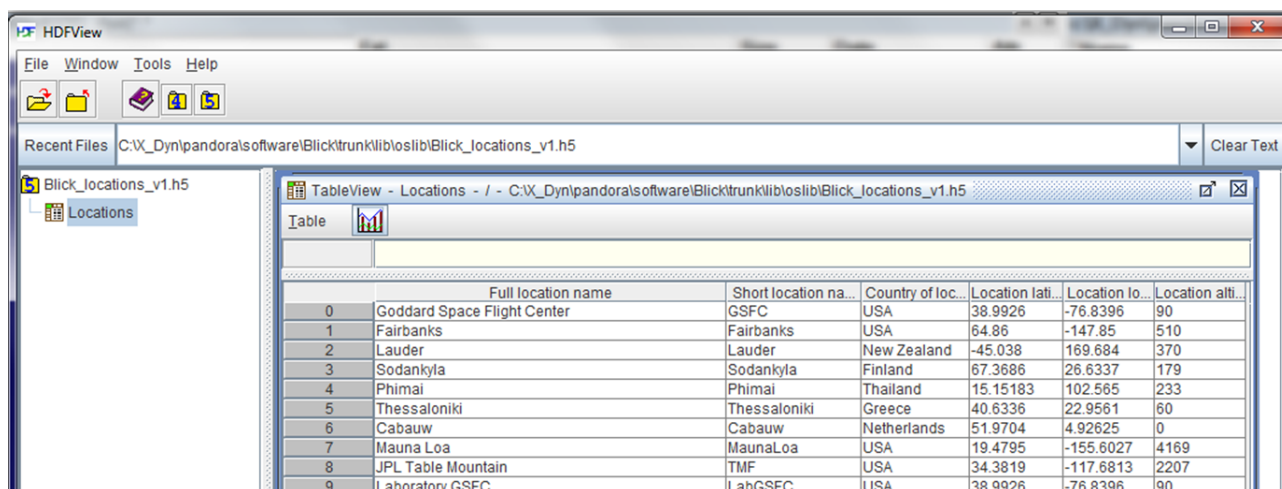
Name	Used by	Description
File name	All	Name of file
File generation date	All	File generation date as ISO 8601 string
Data description	All	Description of file type, e.g. "Instrument operation file"
Data file version	All but L0	typically a combination of characters and numbers, e.g. "c2p1s4"
Data originator name	IOF, ICF	Name of person that created the file
Data product status	L2H	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, L2Fit, 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, L2Fit, 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, L2Fit, 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)!
Nominal wavelengths [nm]	L1	Given for all regular pixels
Nominal wavelengths inside fitting window [nm]	L2Fit	Given for all pixels inside the fitting window

## 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 [http://pandonia.net/docs/software/Blick\\_Locations.h5](http://pandonia.net/docs/software/Blick_Locations.h5). The file includes one table called "Locations". Every row of the table contains the information of one instrument location (see figure 6).



	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 6: 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  $[-90^{\circ}, 90^{\circ}]$  (Minus=South of equator, Plus=North of equator)
6. Location longitude in degrees  $[-180^{\circ}, 180^{\circ}]$  (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 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 at 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](mailto: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 to follow 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 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 11 lists all possible IOF entries and their allowed settings, which are not already listed in the meta data table 10.

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:

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

`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 11: 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 $0 < \text{float} \leq 0.5$ , optimized split between dark and bright measurements based on detector properties (equation 58); the first number is for the case no dark map is given (equation 59), the optional second number is for the case a dark map is given (equation 61)
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 [%]	$0 < \text{float} \leq 100$
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
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 12

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 12: 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 13. 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 13: 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 Specific Configuration File

The BlickO Specific 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 Specific Configuration File is updated. The parameters of the BlickO Specific Configuration File are described in table 14. 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 14: Entries of BlickO Specific 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 <code>/lib/oslib/</code> . 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 <code>rd_cur.cur</code> 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
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)	
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	



## 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 15). 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 15: 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 up to 100 MB.

Table 16 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 16).

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 5.14), results from sun search routines, etc. An example of a L0 file header is shown in figure 7.

Table 16: 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, <code>yyyymmddThhmmssZ</code> (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	
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	

```

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_vld20160916.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, yyyyymmddThhmmssZ (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, positive=North
Column 7: Longitude at the beginning of the measurement [deg], negative=West of Greenwich, positive=East
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 retrieved
Column 10: North-South inclination angle at the beginning of the measurement [deg], -999=angle not retrieved
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 measurement
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 to target
Column 19: Pointing azimuth in degree, increases clockwise, absolute (0=north) or relative (see next column)
Column 20: Azimuth pointing mode: like zenith angle mode but also fixed scattering angles relative to target
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 factor)
Column 33: Uncertainty indicator: uncertainty is... 0=not given, 1=standard deviation, 2=rms to standard deviation
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 raw counts
-----

```

Figure 7: 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 17). This is an example of the beginning of a status line:

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



Table 17: 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 $\geq 0$
CURRTIME	Current time; 16-characters string ISO8601 format "YYYYMMDDTHH-MMSSZ"
OMESSAGE	Current OMessage as in table 2
MODE	Current measurement mode; "MANUAL" for manual operation, "ROUT-SEQU(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 $\geq 0$
NTRACKRESET	Number of tracker resets needed so far; integer $\geq 0$
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 $\geq 0$ 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 $\geq 0$ 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-ConfigParser>) 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 5.13) 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 18. Examples are given in the next section 5.9.3.

Table 18: 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 19). 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 19: 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 is provided in the software distribution and can also be downloaded under [http://pandonia.net/docs/software/Blick\\_ProcessingSetups.h5](http://pandonia.net/docs/software/Blick_ProcessingSetups.h5). 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'. For all the code-tables 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 6.4.3). The "standard unit" for a gas is  $\text{molc}/\text{cm}^2$  unless the standard amount of the gas is also given in parenthesis in another unit in table 20, in which case the unit in parenthesis is the standard unit. E.g. the standard unit is DU for ozone, cm for water vapor and  $\text{molc}^2/\text{cm}^5$  for oxygen dimer.

From the profile information the effective height  $h_{\text{EFF}j}$  and effective temperature  $T_{\text{EFF}j}$  for extinction process  $j$  (or trace gas  $j$ ) are calculated (also listed in table 20). 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  $h_{\text{EFF}j}$  is given by:

$$h_{\text{EFF}j} = \frac{\int_{\text{SURF}}^{ToA} n_j(h) \cdot h \cdot dh}{\int_{\text{SURF}}^{ToA} n_j(h) \cdot dh} \quad (2)$$

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:

$$T_{\text{EFF}j} = \frac{\int_{\text{SURF}}^{ToA} n_j(h) \cdot T_{\text{AIR}}(h) \cdot dh}{\int_{\text{SURF}}^{ToA} n_j(h) \cdot dh} \quad (3)$$

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

Table 20: Table "Trace Gases" in the fitting setups file

Short name	Symbol	Full name	Standard amount [molc/cm <sup>2</sup> ]	h <sub>EFF</sub> [km]	T <sub>EFF</sub> [K]
BrO	BrO	Bromine oxide	4e13	22.4	221.0
CH4	CH <sub>4</sub>	Methane	4.0302e19 (=1500 DU)	22.4	249.9
ClO	ClO	Chloride oxide	1e14	22.4	221.0
CO2	CO <sub>2</sub>	Carbon dioxide	8.1825e21 (=380 ppm of 1 std at-mosphere)	7.3	249.9
GLY	CHOCHO	Glyoxal	6e14	4.3	256.9
HCHO	HCHO	Formaldehyde	1.3434e16 (=0.5 DU)	4.3	256.9
HONO	HONO	Nitrous acid	2.6868e15 (=0.1 DU)	4.3	256.9
H2O	H <sub>2</sub> O	Water vapor	3.3428e22 (=1 cm precipitable water)	1.8	273.1
ICE	H <sub>2</sub> O	Ice	3.3428e22 (=1 cm)	8.0	245.0
IO	IO	Iodine monoxide	2e12	22.4	221.0
I2	I <sub>2</sub>	Molecular iodine	1e15	3.4	262.9
NO2	NO <sub>2</sub>	Nitrogen dioxide	1.3434e16 (=0.5 DU)	7.2	254.5
NO3	NO <sub>3</sub>	Nitrate	2e14	3.4	262.9
OBRO	OBRO	Bromine dioxide	1e13	22.4	221.0
OCIO	OCIO	Chloride dioxide	1e13	22.4	221.0
OH	OH	Hydroxyl radical	5e13	22.4	221.0
OIO	OIO	Iodine dioxide	1e14	3.4	262.9
O2	O <sub>2</sub>	Oxygen	4.5103e24 (=20.95 % of 1 std at-mosphere)	7.3	249.9
O2O2	O <sub>2</sub> O <sub>2</sub>	Oxygen dimer	1.2691e43 molc <sup>2</sup> /cm <sup>5</sup> (amount in 1 std atmosphere)	4.2	262.0
O3	O <sub>3</sub>	Ozone	8.0603e18 (=300 DU)	20.4	225.0
SO2	SO <sub>2</sub>	Sulfur dioxide	1.3434e16 (=0.5 DU)	4.0	259.2
WAT	H <sub>2</sub> O	Liquid water	3.3428e22 (=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 6.3). Each L1 configuration consists of a series of parameters, which make up one row of the L1 configuration table (see table 21). 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 6.3.1).
- 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 6.3.7).
- 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 6.3.8).
- Forth digit: This has no special meaning and often just has a number between 0 and 9.

Table 21: Columns of table "s-codes" in the Processing Setups File. The last column shows in parenthesis as an example the value of this parameters 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	S5	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 6.3.7), '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 22) [st00]
Creation date	S11	Date when this s-code was added [6-Oct-2015]
Author info	S50	Information about author of s-code [Alexander Cede]

Entry "qs-code" indicates, which set of parameters is used to determine the data quality flag (DQF) for the L1 data. Each line of table qs-codes lists a quality setup (see table 22). 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. Many of the entries in the table are comma separated strings of two numbers (e.g. "WLshift limits"). The first number is the limit to change from data quality 0 (DQ0) to data quality 1 (DQ1) and the second number to change from DQ1 to data quality 2 (DQ2). This is the meaning of DQ0, DQ1 and DQ2:

- DQ0 "High quality": no data quality indicator exceeds the DQ1 limit and therefore there are no indications that the data might not be of the highest possible quality. Those data can be used with high confidence.
- DQ1 "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 origin from instrumental sources (e.g. too large wavelength shift) or atmospheric sources (e.g. clouds increasing the uncertainty in direct sun measurements).

- DQ2 "Low quality": at least one data quality indicator exceeds the DQ2 limit and therefore the quality of the data is strongly reduced. For most purposes, the user should not use these data. As for DQ1, the low quality can origin from instrumental or atmospheric sources.

The syntax for the standard qs-codes is simply the combination of 'st' plus a number between 00 and 99.



Table 22: Columns of table "qs-codes" in the processing setups file. The last column shows in parenthesis as an example the value of this parameters 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 [Original 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,NO]
dc cycles needed	S11	Number of measured dark cycles needed; e.g. 2 means the quality is reduced if less than 2 dark cycles were measured [2,1]
Eff temp diff limits	S11	Effective temperature difference limits in °; e.g. 3.0 means the quality is reduced if the effective temperature differs more than 3.0° from the reference temperature [3.,10.]
nsig dc difference	S11	Limits for number of sigmas in dark count difference; e.g. 5.0 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 metho 'MAP' was requested AND if the ICF contains the dark map parameters [YES,NO]
Stray light level limits	S11	Limits for estimated average residual stray light level in percent; e.g. 2.0 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	S11	Wavelength shift limits in nm; e.g. 0.3 means the quality is reduced if the retrieved wavelength shift differs more than 0.3 nm from the nominal wavelength [0.3,1.0]
Pred WLshift limits	S11	Limits for wavelength shift difference from predicted shift in nm; e.g. 0.5 means the quality is reduced if the retrieved wavelength shift differs more than 0.5 nm from the expected shift based on the temperature [0.5,1.2]
Creation date	S11	Date when this qs-code was added [25-Jul-2016]
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 5.13.1 and 6.4). Each fitting setup consists of a series of parameters, which make up one row of the f-codes table (see table 23). 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 to 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 24). 't' stands for the theoretical extraterrestrial reference ("ExtRef" in table 24), 's' for the synthetic reference ("SyntXXX"), 'n' or 'f' for the spectrum of the same routine at the nearest or farthest 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 23 as \*f-code. In particular this means:

- npol, noffs, nwlc: if any of these parameters is set to an 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.
- 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='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.

Table 23: Columns of table "f-codes" in the processing setups file. The last column shows in parenthesis as an example the value of this parameters for f-code 'out0'.

Column name	Format	Description [Value for fitting setup out0]
f-code	S4	f-code [out0]
f-name	S300	f-code descriptive name [Original ozone setup using extraterrestrial reference]
Process types	S50	Comma separated string of process types, for which retrieval is applied (see table 7) [SUN]
Filter types	S50	Comma separated string of functional filters, for which retrieval is applied [U340]
Reference	S50	Reference spectrum used; for options see table 24 [ExtRef]
WL-starts	S50	Comma separated string with starting wavelengths of the fitting window [nm]. They must be monotonically increasing. [310]
WL-ends	S50	Comma separated string with ending wavelengths of the fitting window [nm]. They must be monotonically increasing, 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. [330]
npol	S4	Order of fitting polynomial or *f-code (see section 6.4) [4]
noffs	S4	Order of offset polynomial or *f-code (see section 6.4) [0]
nwlc	S4	Order of wavelength change polynomial or *f-code (see section 6.4) [1]
nresc	S4	Order of resolution change polynomial (see section 6.4) [-1]
Fitted gases	S100	Comma separated string with short names of gases to be fitted (see table 25) [O3,NO2,SO2,HCHO]
Gas sources	S500	Comma separated string with cross section source for each gas in column "Fitted Gases" (see table 25). 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. [Daumont4TGOME,Vandaele,Vandaele,MellMoort2000]
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 6.4.3). In this version only one optical depth fitting method per gas is given in the ICF. Therefore the processing can only be done, if the selected ICF matches the optical depth fitting methods listed in this entry. This may change in a future software version. [1,1,1,1]
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 a value in Kelvin or "CLIM" for climatology (option "CLIM" is not implemented yet in the current version). 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. [225,254.5,259.2,256.9]
Fitted temps	S50	Comma separated string with temperature treatment for each gas in column "Fitted Gases". NO=temperature not fitted, YES=temperature is fitted. [NO,NO,NO,NO]

Column name	Format	Description [Value for fitting setup 1]
Ring	S4	Is the Ring spectrum fitted (see section 6.4)? YES/NO/*f-code [NO]
Mol scatt	S4	Optical depth fitting method used for molecular scattering optical depth to be subtracted before the spectral fitting (see section 6.4)? 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 6.4)? YES/NO [NO]
Uncertainty	S5	Which uncertainty is used for the spectral fitting (see section 6.4)? NO means no uncertainty is included. MEAS means the measured (instrumental and atmospheric) uncertainty is used. INSTR means only the instrumental uncertainty is used. [MEAS]
s-code	S4	s-code for the L1 data that are used in the spectral fitting [mcal]
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 [NO]
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 26) [out0]
Creation date	S11	Date when this f-code was added [6-Oct-2015]
Author info	S50	Information about author of f-code [Alexander Cede]

Table 24: Options for "Reference"

Reference	Description
ExtRef	"ExtRef" refers to an extraterrestrial spectrum from another source (i.e. not measured by the Pandora unit), convoluted with the Pandora filter function; 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 <i>Bernhard et al.</i> [6]; the sources are: #1: <i>Kurucz</i> [19] spectrum normalized to <i>Thuillier et al.</i> [42], #2: SUSIM/Atlas 3 spectrum [45], #3: <i>Gueymard</i> [14] spectrum; the merged spectrum is #2 for $\lambda \leq 299.8$ nm; #1 corrected with smoothed #2 (triangular 0.7 nm FWHM slit) for $299.8 \text{ nm} < \lambda \leq 338.5$ nm; #1 corrected with smoothed #2 (triangular 4 nm FWHM slit) for $338.5 \text{ nm} < \lambda \leq 419.9$ nm; #1 corrected with smoothed #3 (triangular 20 nm FWHM slit) for $419.9 \text{ nm} < \lambda \leq 946.5$ nm; and #1 for $\lambda > 946.5$ nm
SyntXXX	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; XXX is the functional filter, for which it was made (e.g. "SyntOPEN", "SyntU340")
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 farthest 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 fourth column the instrumental uncertainty of the reference spectrum.

Table 25: Options for "Gas Sources"; column "Gas" corresponds to column "Short Name" of table 20

Gas	Name	Description
BrO	Wilmouth	<i>Wilmouth et al.</i> [50]
BrO	Fleischmann	<i>Fleischmann et al.</i> [12]
CH <sub>4</sub>	H2007	HITRAN 2008 <i>Rothman et al.</i> [31]
CH <sub>4</sub>	H2012	HITRAN 2012 <i>Rothman et al.</i> [32]
ClO	Sander	<i>Sander and Friedl</i> [35]
CO <sub>2</sub>	HITRAN	HITRAN 2004 <i>Rothman et al.</i> [30]
CO <sub>2</sub>	H2007	HITRAN 2008 <i>Rothman et al.</i> [31]
CO <sub>2</sub>	H2012	HITRAN 2012 <i>Rothman et al.</i> [32]
GLY	Volkamer	<i>Volkamer et al.</i> [47]
HCHO	MellMoort2000	<i>Meller and Moortgat</i> [21]
HONO	Bongartz	<i>Bongartz et al.</i> [9]
HONO	Stutz	<i>Stutz et al.</i> [40]
H <sub>2</sub> O	HITRAN	HITRAN 2004 <i>Rothman et al.</i> [30]
H <sub>2</sub> O	H2012	HITRAN 2012 <i>Rothman et al.</i> [32]
ICE	Warren	<i>Warren</i> [49]
IO	Spietz	<i>Spietz et al.</i> [39]
I <sub>2</sub>	Saiz-Lopez	<i>Saiz-Lopez et al.</i> [33]
NO <sub>2</sub>	Vandaele	<i>Vandaele et al.</i> [43]
NO <sub>3</sub>	Sander	<i>Sander</i> [34]
OB <sub>2</sub> O	Fleischmann	<i>Fle</i> [2]
OB <sub>2</sub> O	Knight	<i>Knight et al.</i> [18]
OCIO	Wahner	<i>Wahner et al.</i> [48]
OH	H2012	HITRAN 2012 <i>Rothman et al.</i> [32]
OIO	Spietz	<i>Spietz</i> [38]
O <sub>2</sub>	H2012	HITRAN 2012 <i>Rothman et al.</i> [32]
O <sub>2</sub> O <sub>2</sub>	Hermans	<i>Hermans et al.</i> [15]
O <sub>2</sub> O <sub>2</sub>	Thalman	<i>Thalman and Volkamer</i> [41]
O <sub>2</sub> O <sub>2</sub>	HermansNewnham	<i>Hermans et al.</i> [15] for $\lambda \leq 454.42$ nm combined with <i>Newnham and Ballard</i> [22] for $\lambda > 454.42$ nm
O <sub>2</sub> O <sub>2</sub>	ThalmanNewnhamQPol	<i>Thalman and Volkamer</i> [41] for $\lambda \leq 596$ nm combined with <i>Newnham and Ballard</i> [22] for $\lambda > 596$ nm

Gas	Name	Description
O3	GOME	<i>Burrows et al.</i> [11]
O3	Daumont	<i>Malicet et al.</i> [20]
O3	Harmonics2013	<i>Serdyuchenko et al.</i> [37]
O3	IBassPaur	<i>Bass and Paur</i> [4] taken from <a href="http://igaco-o3.fmi.fi/ACSO/cross_sections.html">http://igaco-o3.fmi.fi/ACSO/cross_sections.html</a>
O3	H2012	HITRAN 2012 <i>Rothman et al.</i> [32]
O3	BassPaurGOME	<i>Bass and Paur</i> [4] for $\lambda \leq 332.69$ nm combined with <i>Burrows et al.</i> [11] for $\lambda > 332.69$ nm
O3	Harmonics_H2012	<i>Serdyuchenko et al.</i> [37] for $\lambda \leq 1100$ nm combined with HITRAN 2012 <i>Rothman et al.</i> [32] for $\lambda > 1100$ nm
O3	IDaumont5T	<i>Malicet et al.</i> [20] taken from <a href="http://igaco-o3.fmi.fi/ACSO/cross_sections.html">http://igaco-o3.fmi.fi/ACSO/cross_sections.html</a>
O3	IDaumont4T	IDaumont5T without using 273 K
O3	Daumont4TGOME	IDaumont4T for $\lambda \leq 522$ nm plus IGOME for $\lambda > 522$ nm
O3	IGOME	<i>Burrows et al.</i> [11] taken from <a href="http://igaco-o3.fmi.fi/ACSO/cross_sections.html">http://igaco-o3.fmi.fi/ACSO/cross_sections.html</a>
O3	IVoigtH	<i>Voigt et al.</i> [46] for 1000 mbar
O3	IVoigtL	<i>Voigt et al.</i> [46] for 100 mbar
O3	ISCIAMACHY	<i>Bogumil et al.</i> [8] taken from <a href="http://igaco-o3.fmi.fi/ACSO/cross_sections.html">http://igaco-o3.fmi.fi/ACSO/cross_sections.html</a>
SO2	Vandaele	<i>Vandaele et al.</i> [44]
WAT	QBPP	Combination of <i>Quickenden and Irvin</i> [29] for $\lambda < 280$ nm, <i>Buiteveld et al.</i> [10] for $\lambda < 402$ nm, <i>Pope and Fry</i> [27] for $\lambda < 730$ nm and <i>Palmer and Williams</i> [24] for $\lambda > 730$ nm
WAT	QBPPcP	QBPP corrected with <i>Peters et al.</i> [25] between 402 nm and 507 nm

Entry "qf-code" indicates, which set of parameters is used to determine the DQ for the L2Fit data. The principle is the same as for the qs-codes.

The parameters are listed in table 26. The syntax for the standard qf-codes is usually the same as for the f-code, for which it is primarily used.

Table 26: Columns of table "qf-codes" in the processing setups file. The last column shows in parenthesis as an example the value of this parameters for qf-code 'out0'.

Column name	Format	Description [ <i>Value for quality setup out0</i> ]
qf-cumber	S4	qf-code [ <i>out0</i> ]
qf-Name	S100	qf-code descriptive name [ <i>Standard ozone fitting quality limits</i> ]
Fitting result	S5	Limits for fitting result index (see table 36) [ <i>0,3</i> ]
wrms limits	S15	Normalized weighted rms limits [ <i>1e-2,2e-2</i> ]
WL shift limits	S11	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 [ <i>0.2,0.5</i> ]
Creation date	S11	Date when this qf-code was added [ <i>26-Jul-2016</i> ]
Author info	S50	Information about author of qf-code [ <i>Alexander Cede</i> ]



### 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 such as L2Tot and L2Trop (see sections 5.13.2 and 6.5). Each retrieval setup consists of a series of parameters, which make up one row of the r-codes table (see table 27). 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.

Table 27: Columns of table "r-codes" in the processing setups file. The last column shows in parenthesis as an example the value of this parameters for r-code 'out0'.

Column name	Format	Description [Value for retrieval setup out0]
r-code	S4	r-code [out0]
r-Name	S100	r-code descriptive name [Standard direct ozone and SO2 retrieval]
L2 type	S6	Level 2 data type produced: L2Tot or L2Trop [L2Tot]
Algorithm type	S50	Algorithm type used: 'Direct-Version1', 'O4RatioSky-Version1' [Direct-Version1]
Output gases	S50	Comma separated string of gases to be written in output file [O3,SO2]
Product status	S50	Comma separated string of product status for each output gas (see table 28); same length as "Output gases" [official,unusable]
qr-codes	S30	Comma separated string of qr-codes used for each output gas (see table 29); same length as "Output gases" [out0,sut0]
f-codes	S30	Comma separated string of f-codes used in the retrieval; note that some L2 algorithms only allow one f-code to be used, while others allow more than one (see section 6.5) [out0]
Creation date	S11	Date when this r-code was added [20-May-2016]
Author info	S50	Information about author of r-code [Alexander Cede]

Table 28: 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.
unevaluated	Data are in research stage, not yet evaluated 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.

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 29. The syntax for the standard qr-codes is usually the same as for the r-code, for which it is primarily used.

Table 29: Columns of table "qr-codes" in the processing setups file. The last column shows in parenthesis as an example the value of this parameters for qr-code 'out0'.

Column name	Format	Description [Value for quality setup out0]
qr-code	S4	qr-code [out0]
qr-Name	S100	qr-code descriptive name [Standard ozone data quality limits]
Uncertainty limits	S15	Uncertainty limits in the standard unit of the gas (see table 20); negative value means this parameter is not used [3,5]
SNR limits	S15	Signal to noise limits; negative value means this parameter is not used [-1,-1]
AMF limits	S11	AMF limits; negative value means this parameter is not used [5,7]
Creation date	S11	Date when this qr-code was added [27-Jul-2016]
Author info	S50	Information about author of qr-code [Alexander Cede]

### 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](mailto: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.

$$x_s = 3.46 \cdot \left( \frac{x - x_{\text{MIN}}}{x_{\text{MAX}} - x_{\text{MIN}}} - 0.5 \right) \quad (4)$$

x is an unscaled data-point,  $x_s$  is a scaled data-point and  $x_{\text{MIN}}$  and  $x_{\text{MAX}}$  are estimates of the minimum and the maximum of the distribution of the unscaled data. So the  $x_s$  are distributed approximately between -1.73 and +1.73. The values for  $x_{\text{MIN}}$  and  $x_{\text{MAX}}$  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  $x_{\text{MIN}}=0$  and  $x_{\text{MAX}}=\text{npix}$ .

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

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

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

Details for every line of the ICF, which is not already given in the meta data table 10, 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.

$$VD = V_0 + V_1 \cdot IT^{V_2} \quad (6)$$

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  $A_{SLi}$  in equation 66) 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  $B_{SLi}$  in equation 66) 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  $A_{ICi}$  in equation 66) 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  $B_{ICi}$  in equation 66) 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  $2^{n_{\text{bits}}}-1$ ;  $n_{\text{bits}}$ =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 6.3.3).

### **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  $C_{\text{CORR}}$ .

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

$C$  are the counts before correction,  $T_{\text{RE}}$  is the radiometric effective temperature (measured and stored in the data files),  $T_{\text{RR}}$  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 11), 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 30. 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 30. Formulas for some of the slit functions are given in equations 8 to 12, where  $\lambda$  is the wavelength and  $S(\lambda)$  is the slit function. Typical fitting methods used are "Symmetric modified Lorentzian" and "Symmetric modified Gaussian".

Table 30: Slit function fitting methods

Name	Parameters
Symmetric triangle	A <sub>2</sub> : half of base width [nm]
Asymmetric triangle	A <sub>2</sub> : from center to left edge at base [nm] A <sub>3</sub> : from center to right edge at base [nm]
Symmetric trapezoid	A <sub>2</sub> : half of base width [nm] A <sub>3</sub> : half of top width [nm]
Trapezoid asymmetric on bottom	A <sub>2</sub> : half of base width left [nm] A <sub>3</sub> : half of base width right [nm] A <sub>4</sub> : half of top width [nm]
Symmetric double-trapezoid	A <sub>2</sub> : half of base width [nm] A <sub>3</sub> : half of top width [nm] A <sub>4</sub> : height of flexion point A <sub>5</sub> : half of middle width [nm]
Double-trapezoid both sides free	A <sub>2</sub> : half of base width left [nm] A <sub>3</sub> : half of base width right [nm] A <sub>4</sub> : half of top width [nm] A <sub>5</sub> : height of left flexion point A <sub>6</sub> : height of right flexion point A <sub>7</sub> : half of left middle width [nm] A <sub>8</sub> : half of right middle width [nm]
Double-trapezoid left side free	A <sub>2</sub> : half of base width left [nm] A <sub>3</sub> : half of base width right [nm] A <sub>4</sub> : half of top width [nm] A <sub>5</sub> : height of left flexion point A <sub>6</sub> : half of left middle width [nm]
Double-trapezoid right side free	A <sub>2</sub> : half of base width left [nm] A <sub>3</sub> : half of base width right [nm] A <sub>4</sub> : half of top width [nm] A <sub>5</sub> : height of right flexion point A <sub>6</sub> : half of right middle width [nm]
Symmetric modified Lorentzian (Equation 8 with A <sub>6</sub> =1)	A <sub>2</sub> : half width [nm] A <sub>3</sub> : steepness

Name	Parameters
Asymmetric modified Lorentzian (Equation 9)	A <sub>2</sub> : half width [nm] A <sub>3</sub> : steepness A <sub>4</sub> : asymmetry
Symmetric modified Gaussian (Equation 10 with A <sub>6</sub> =1)	A <sub>2</sub> : half width [nm] A <sub>3</sub> : steepness
Symmetric modified double Lorentzian (Equation 8)	A <sub>2</sub> : half width of mode 1 [nm] A <sub>3</sub> : steepness of mode 1 A <sub>4</sub> : half width of mode 2 [nm] A <sub>5</sub> : steepness of mode 2 A <sub>6</sub> : fractional strength of mode 1
Symmetric modified double Gaussian (Equation 10)	A <sub>2</sub> : half width of mode 1 [nm] A <sub>3</sub> : steepness of mode 1 A <sub>4</sub> : half width of mode 2 [nm] A <sub>5</sub> : steepness of mode 2 A <sub>6</sub> : fractional strength of mode 1
Symmetric modified Lorentz-Gauss combo (Equation 11)	A <sub>2</sub> : half width of Lorentz mode [nm] A <sub>3</sub> : steepness of Lorentz mode A <sub>4</sub> : half width of Gauss mode [nm] A <sub>5</sub> : steepness of Gauss mode A <sub>6</sub> : fractional strength of Lorentz mode
Truncated symmetric modified Gaussian (Equation 12)	A <sub>2</sub> : reduced half width [nm] A <sub>3</sub> : steepness A <sub>4</sub> : cut-off position
Symmetric trapezoid with inclined top-part	A <sub>2</sub> : half of base width [nm] A <sub>3</sub> : half of top width [nm] A <sub>4</sub> : angle of top part [degrees]
Asymmetric modified Gaussian (Equation 10 with A <sub>6</sub> =1 for $\lambda \leq A_0$ and equation 10 with A <sub>6</sub> =0 for $\lambda > A_0$ )	A <sub>2</sub> : half width left [nm] A <sub>3</sub> : steepness left A <sub>4</sub> : half width right [nm] A <sub>5</sub> : steepness right [nm]

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



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

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

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

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

### 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 11).

### 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  $\mu\text{m}$ . 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 $A_x$ polynomial

This polynomial is evaluated at the air-wavelengths for the center of each pixel in  $\mu\text{m}$ . The evaluated data are the slit function parameter  $A_x$  ( $x=2, 3, \dots$ ) for each pixel (see table 30).

### Slit function parameter $A_x$ 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 11), 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 list of values resulting from a linear fit of the wavelength temperature sensitivity  $k$  [nm/K] in the scaled pixels. If the last element of the list equals 0, then  $k$  equals the first element of the list and is constant for all

pixels. If the last element of the list equals 1, then  $k$  is linearly dependent on the scaled pixels with slope and intercept being the first and second element of the list respectively. For a given  $k$ , one can estimate the "best" wavelength  $\lambda$  of a pixel-center using equation 13.

$$\lambda = \lambda_{\text{NOM}} - k \cdot (T_{\text{WE}} - T_{\text{WR}}) \quad (13)$$

$\lambda_{\text{NOM}}$  is the nominal center-wavelength (from the dispersion),  $T_{\text{WE}}$  is the wavelength effective temperature,  $T_{\text{WR}}$  is the wavelength reference temperature and  $k$  is the wavelength temperature sensitivity.

## Resolution temperature dependence

This is analogous to "Dispersion temperature dependence", but refers to the resolution (FWHM of slit function). Equation 13 applies when replacing  $\lambda$  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 31. 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 31. 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  $B_5$ .

Table 31: Stray light function fitting methods

Name	Parameters
Symmetric power decay (Equation 14)	$B_1$ : power parameter $B_2 > 0$ : merge level $B_3 > 0$ : far field stray light level
Asymmetric power decay (Equation 14 for $\lambda \leq B_0$ and equation 14 with $B_4$ , $B_5$ and $B_6$ instead of $B_1$ , $B_2$ and $B_3$ for $\lambda > B_0$ )	$B_1$ : power parameter left $B_2 > 0$ : merge level left $B_3 > 0$ : far field stray light level left $B_4$ : power parameter right $B_5 > 0$ : merge level right $B_6 > 0$ : far field stray light level right

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

## Slit function parameter $B_x$ polynomial

This polynomial is evaluated at the air-wavelengths for the center of each pixel in  $\mu\text{m}$ . The evaluated data are the slit function parameter  $B_x$  ( $x=1, 2, \dots$ ) for each pixel (see table 31).

## Slit function parameter $B_x$ rms

This is the rms of slit function parameter  $B_x$  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 6.3.7). The options for the transition method are given in table 32. Parameter  $C_0$ , the air-wavelength of the pixel-center is common to each transition function and therefore not listed in table 32.

Table 32: Inband outband transition methods

Name	Parameters
Symmetric linear wavelength transition The inband equals $S(\lambda)$ 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 $S(\lambda)$ for $\lambda - C_0 > -C_1$ and for $\lambda - C_0 < C_3$ , 0 for $\lambda - C_0 < -C_1 - C_2$ and for $\lambda - C_0 > C_3 + C_2$ 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 $S(\lambda)$ for $\Delta\lambda < C_1$ , 0 for $\lambda - C_0 < -C_1 - C_2$ and for $\lambda - C_0 > C_1 + C_3$ 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 $S(\lambda)$ for $\lambda - C_0 > -C_1$ and for $\lambda - C_0 < C_3$ , 0 for $\lambda - C_0 < -C_1 - C_2$ and for $\lambda - C_0 > C_3 + C_4$ 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 $C_x$ polynomial

This polynomial is evaluated at the air-wavelengths for the center of each pixel in  $\mu\text{m}$ . The evaluated data are the slit function parameter  $C_x$  ( $x=1, 2, \dots$ ) for each pixel (see table 32).

## Slit function parameter $C_x$ rms

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

## 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  $\text{W/m}^2/\text{nm}$ .

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 corresponding 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  $\text{W/m}^2/\text{nm}$ .

### **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 ( $x_{\text{MIN}}$ =entry "Wavelength minima for sensitivities",  $x_{\text{MAX}}$ =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  $\text{W/m}^2/\text{nm}$ , 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 24). The next strings give the cross section source and the reference temperature used, e.g. "O3:Daumont(225.0K)" (see table 25). The last string gives the extraterrestrial spectrum used to calculate the Ring cross sections, e.g. "RING:XThoullier" (see table 24).

### **Spectra wavelength grid; first, last and step [nm]**

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

### **Spectra scale [to $\text{W/m}^2/\text{nm}$ ]**

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

### **Reference spectrum**

This is the scaled convoluted extraterrestrial spectrum using the data source, wavelength grid and scale as given in the ICF-entries above (see also table 24).

## Standard spectrum

This is the scaled convoluted "standard" spectrum 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 20.

## Ring spectrum scale

This is the scale factor for the "Ring spectrum". 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<sub>2</sub> and N<sub>2</sub> [13]. Roughly speaking, it manifests itself by a broadening of the solar and atmospheric spectral features present in measured spectra.

## Ring spectrum

This is the scaled convoluted Ring spectrum using the data source, wavelength grid and scale as given in the ICF entries above. The convoluted Ring spectrum is calculated using equation 83, 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 25 (name starts with "RING").

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

This is the air-wavelength grid used for the OD-fitting parameters A, B and C (see section 6.4.3).

## Temperature scale [K]

This is the temperature scale factor (see section 6.4.3).

## Optical depth scale

This is the scale factor for OD-fitting parameters A, B and C (see section 6.4.3). 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.

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

This is the constant (or linear, quadratic) term in temperature of the scaled convoluted OD-fitting parameter Ax (or Bx, Cx) (see section 6.4.3) for absorber with name GAS (see table 25) using the data source, wavelength grid and scale as given in the ICF-entries above. 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)

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 6.4.5).

## Reference wavelength for wavelength change retrieval [nm]

This is the reference wavelength  $\lambda_{REF}$  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:

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

$\lambda_{iNOM}$  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 6.3.9.

$$\lambda_{iBEST} = \lambda_{iNOM} + \Delta\lambda_i \quad (16)$$

## Wavelength change retrieval parameters for FUNCFILT

This entry lists five parameters needed to retrieve the wavelength change polynomial (see equation 15) for a measurement using "functional filter" FUNCFILT. A functional filter is basically any filter listed in entries 19 or 20 of the IOF (see table 11), which is not a neutral density filter (e.g. U340, BP300). Note that OPEN is also considered a functional filter. The second of the five parameters is the order of the wavelength change polynomial (nWLC in equation 15).

## 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 and are 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  $W/m^2/nm$ .

## 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. If this entry is not given, then it is assumed that the synthetic reference spectrum does not contain any trace gas absorption features. Each string starts with the short name of the trace gas as given in table 20 and followed by a colon. After this there are three comma separated numbers. The first one is the estimated slant column of the gas in its standard units (see section 5.10.1). The second one is the estimated effective temperature of the gas absorption included in the synthetic reference spectrum. The third one is the optical depth fitting method used to estimate the gas absorption included in the synthetic reference spectrum (see section 6.4). E.g. the string "O3:533.4,258.1K,OD3" means that an estimated 533.4 DU of ozone absorption at an effective temperature of 258.1 K is included in the synthetic reference spectrum and was determined using optical depth fitting method 3. At the end of the string (after the entries for all the trace gases) is the approximate AMF for the synthetic reference spectrum after "AMF:", i.e. "AMF:1.234" means the AMF was 1.234.

## 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

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

## Relative reference spectrum change with resolution

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

## Standard total optical depth change with resolution

This is the change of the ICF-entry "Standard total optical depth" 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 the all instrumental corrections to the raw data (see section 6.3). 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_sSSSScCpP.txt`. X, Y, LLL, YYYYMMDD are as for the L0 file (section 5.7). The segment "sSSSScCpP" 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). 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 measurement have been included in the data correction, but the data lines are longer since the instrumental uncertainty is listed in addition to the total uncertainty.

Table 33 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 33).

For entry "Level 1 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 16) 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 11). 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 33: 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, <code>yyyymmddThhmmssZ</code> (ISO 8601)	
Fractional days since 2000-1-1 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 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	
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 6.3
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	
Level 1 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 22
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 22
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 uncertainty or dark count uncertainty measured	
Number of pixels, where DQ2 sigma ranges of dark count and bright count do not overlap, -9=no bright count uncertainty or dark count uncertainty measured	
Index of (not dead, blind, warm or saturated) pixel with the highest corrected counts	
Uncertainty [%] of data from pixel with the highest counts based on measured bright count uncertainty and measured dark count uncertainty in the case the uncertainty indicator is 9 or 10; -9 otherwise	See also section 6.2
Uncertainty [%] of data from pixel with the highest counts based on measured bright count uncertainty and theoretical dark count uncertainty in the case the uncertainty indicator is >=7; -9 otherwise	See also section 6.2
Uncertainty [%] of data from pixel with the highest counts based on theoretical bright count uncertainty and measured dark count uncertainty in the case the uncertainty indicator is 4, 9 or 10; -9 otherwise	See also section 6.2
Uncertainty [%] of data from pixel with the highest counts based on theoretical bright count uncertainty and theoretical dark count uncertainty in the case the uncertainty indicator is 3 or 4 or >=7; -9 otherwise	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
Uncertainty of mean over blind and oversampled pixels in the bright counts, -9 if there is no bright count uncertainty	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
Uncertainty of mean over blind and oversampled pixels in the dark counts, -9 if there is no dark count uncertainty	See also section 6.2
Number of function evaluations used for dark background fitting, -9 if no background fitting was done	See also section 6.3
rms of unweighted fitting residuals for dark background fitting, -9 if no background fitting was done	See also section 6.3
Normalized rms of weighted fitting residuals for dark background fitting, -9 if no background fitting was done	See also section 6.3
Mean difference dark map to measured dark count, -9 if no background fitting was done	See also section 6.3
rms of difference dark map to measured dark count, -9 if no background fitting was done	See also section 6.3
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 6.3
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 6.3
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 6.3
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 6.3
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 6.3
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 6.3
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 measured uncertainty was given	X=1 until the value of ICF entry "Dark background fitting settings" plus two

Column name	Remark
Stray light correction method: 0=no stray light correction, 1=simple method, 2=uncorrected matrix method, 3=corrected matrix method	See also section 6.3.7
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 6.3.7
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 6.3
Last cost function at wavelength change determination [nm], -9=no wavelength change determination	See also section 6.3
rms of final radiometric difference at wavelength change determination, -9=no wavelength change determination	See also section 6.3
Number of pixels not included in the wavelength change retrieval, -9=no wavelength change determination	See also section 6.3
Number of pixels not included in the wavelength correction, -9=no wavelength correction	See also section 6.3
Mean wavelength correction applied [%], -9=no wavelength correction	See also section 6.3
Standard deviation of wavelength correction applied [%], -9=no wavelength correction	See also section 6.3
Minimum wavelength correction applied [%], -9=no wavelength correction	See also section 6.3
Maximum wavelength correction applied [%], -9=no wavelength correction	See also section 6.3
Expected wavelength shift based on effective temperature [nm], -9=no effective temperature given	See also section 6.3
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 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
Scale factor for data (to obtain unscaled data and uncertainty divide then by this number)	
Uncertainty indicator (see manual for exact meaning)	See table 34
Level 1 data type, data are... 1=corrected count rate [s <sup>-1</sup> ], 2=radiance [W/m <sup>2</sup> /nm/sr], 3=irradiance [W/m <sup>2</sup> /nm]	
Level 1 data for each pixel, 0 is NOT a 'true' zero if the corresponding value in the uncertainty is -2, -3, -4 or -5	
Uncertainty of level 1 data for each pixel, -1=no uncertainty was measured and pixel is inside the range of the filter, -2=no uncertainty was measured and pixel is outside the range of the filter, -3=uncertainty was measured, but pixel is outside the range of the filter, -4=saturated data, -5=the wavelength is inside the valid range, but the sensitivity at this wavelength equals 0, -9=no uncertainty was determined since no dark correction was attempted	
Instrumental uncertainty of level 1 data for each pixel, -2=pixel is outside the range of the filter, -4=saturated data	

Table 34: Meaning of column 'Uncertainty indicator'

Number	Description
0	No bright count was measured and dark count was measured for one cycle only. Uncertainty is not valid. Instrumental uncertainty is based on theoretical dark count uncertainty.
1	No bright count was measured and dark count was measured with uncertainty based on the measured standard deviation of the data. Uncertainty is based on the measured dark count uncertainty. Instrumental uncertainty is based on the theoretical dark count uncertainty.
2	Bright count was measured for one cycle only and no dark count was measured. Uncertainty is not valid. Instrumental uncertainty is based on the theoretical bright count uncertainty.
3	Both bright and dark count were measured for one cycle only. Uncertainty is not valid. Instrumental uncertainty is based on the theoretical uncertainties of bright and dark count.
4	Bright count was measured for one cycle only and dark count was measured with uncertainty based on the measured standard deviation of the data. Uncertainty is not valid. Instrumental uncertainty is based on the theoretical uncertainties of bright and dark count.
5	Bright count was measured with uncertainty based on the measured standard deviation of the data and no dark count was measured. Uncertainty is based on the measured bright count uncertainty. Instrumental uncertainty is based on the theoretical bright count uncertainty.
6	Bright count was measured with uncertainty based on the measured standard error to a straight line fitted in the data and no dark count was measured. Uncertainty is based on the measured bright count uncertainty. Instrumental uncertainty is based on the theoretical bright count uncertainty.
7	Bright count was measured with uncertainty based on the measured standard deviation of the data and dark count was measured for one cycle only. Uncertainty is based on the measured bright count uncertainty and theoretical dark count uncertainty. Instrumental uncertainty is based on the theoretical uncertainties of bright and dark count.
8	Bright count was measured with uncertainty based on the measured standard error to a straight line fitted in the data and dark count was measured for one cycle only. Uncertainty is based on the measured bright count uncertainty and theoretical dark count uncertainty. Instrumental uncertainty is based on the theoretical uncertainties of bright and dark count.
9	Both bright and dark count were measured with uncertainty based on the measured standard deviation of the data. Uncertainty is based on the measured uncertainties of bright and dark count. Instrumental uncertainty is based on the theoretical uncertainties of bright and dark count.
10	Bright count was measured with uncertainty based on the measured standard error to a straight line fitted in the data and dark count was measured with uncertainty based on the measured standard deviation of the data. Uncertainty is based on the measured uncertainties of bright and dark count. Instrumental uncertainty is based on the theoretical uncertainties of bright and dark count.

## 5.13 L2 Files

### 5.13.1 L2Fit Files

BlickP converts the L1 data into L2Fit data by applying the L2Fit algorithm (see section 6.4). 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_fFFFFcCpP.txt`. X, Y, LLL, YYYYMMDD are as for the L0 file (section 5.7). The segment "fFFFFcCpP" is the "Data file version". C and P are as for the L1 file (section 5.12). FFFF is the "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 35 lists the maximum possible data columns in the L2Fit file. The real number of columns varies with the instrument, s-code and f-code. 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:

$$\lambda_{\text{EFFj}} = \frac{\sum_i \lambda_i \cdot \tau_{ji} / \sigma_i^2}{\sum_i \tau_{ji} / \sigma_i^2} \quad (17)$$

$\lambda_{\text{EFFj}}$  is the effective fitting wavelength for trace gas j, the  $\lambda_i$  are the wavelength centers for each pixel i inside the fitting window,  $\tau_{ji}$  are the absorption cross sections for gas j at pixel i and  $\sigma_i$  are the measurement uncertainties (in log-space) at pixel i.

As for L1 data, the "Level 2 Fit data quality flag" can have values DQ0, DQ1 and DQ2 for QA data and DQ10, DQ11 and DQ12 otherwise.

Table 35: Columns in L2Fit file

Column name	Remark
Two letter code of measurement routine	See section 4.1
UT date and time at center of measurement, yyymmddThhmmssZ (ISO 8601)	
Fractional days since 2000-1-1 UT midnight for center 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 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	
Data processing type index	See table 7
Solar zenith angle at the center-time of the measurement in degree	
Solar azimuth at the center-time of the measurement in degree, 0=north, increases clockwise	
Lunar zenith angle at the center-time of the measurement in degree	
Lunar azimuth at the center-time of the 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: 0,1,2=no error or warning, 3,4=warning, >4=error	See table 36
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 or no fitting done	Equation 109
Normalized rms of fitting residuals weighted with measured uncertainty, -9=fitting not successful or no fitting done	Equation 110
Normalized rms of fitting residuals weighted with instrumental uncertainty, -9=fitting not successful or no fitting done	Equation 110
Expected rms based on measured uncertainty, -9=fitting not successful or no fitting done or no uncertainty given	Equation 111
Expected normalized weighted rms based on measured uncertainty, -9=fitting not successful or no fitting done or no uncertainty given	Equation 112
Expected rms based on instrumental uncertainty, -9=fitting not successful or no fitting done or no uncertainty given	Equation 111
Expected normalized weighted rms based on instrumental uncertainty, -9=fitting not successful or no fitting done or no uncertainty given	Equation 112



Column name	Remark
GAS slant column amount [GASUNIT], -9e99=fitting not successful	Fitted slant column in unit GASUNIT for gas GAS
Uncertainty of GAS slant column amount [GASUNIT] based on measured uncertainty, -8=fitting not successful, -1=cross section is zero in this wavelength range, -3=spectral fitting was done, but no uncertainty could be retrieved	Equation 114
Uncertainty of GAS slant column amount [GASUNIT] based on instrumental uncertainty, -8=fitting not successful, -1=cross section is zero in this wavelength range, -3=spectral fitting was done, but no uncertainty could be retrieved	Equation 114
Uncertainty of GAS slant column amount [GASUNIT] based on rms, -8=fitting not successful, -1=cross section is zero in this wavelength range, -3=spectral fitting was done, but no uncertainty could be retrieved	Equation 115
GAS effective temperature [K], -9=no fitting done or fitting not successful, 0=cross section is zero in this wavelength range or differential optical depth is too small to retrieve the temperature	Fitted effective temperature for gas GAS
Uncertainty of GAS effective temperature [K] based on measured uncertainty, -8=fitting not successful, -1=cross section is zero in this wavelength range, -2=differential optical depth is too small to retrieve the temperature, -3=spectral fitting was done, but no uncertainty could be retrieved	Equation 114
Uncertainty of GAS effective temperature [K] based on instrumental uncertainty, -8=fitting not successful, -1=cross section is zero in this wavelength range, -2=differential optical depth is too small to retrieve the temperature, -3=spectral fitting was done, but no uncertainty could be retrieved	Equation 114
Uncertainty of GAS effective temperature [K] based on rms, -8=fitting not successful, -1=cross section is zero in this wavelength range, -2=differential optical depth is too small to retrieve the temperature, -3=spectral fitting was done, but no uncertainty could be retrieved	Equation 115
Direct GAS air mass factor	Direct moon air mass factor (AMF) for direct moon data, direct sun AMF otherwise, see equation 116
Effective GAS fitting wavelength [nm], -9=fitting not done or not successful	See equation 17
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
Climatological station pressure [hPa]	Possibly used to correct for molecular scattering OD
Molecular scattering air mass factor used for molecular scattering subtraction before the fitting	
Climatological station temperature [K]	Possibly used in the L2 algorithm
Climatological effective O2O2 height [km]	Possibly used in the L2 algorithm



Column name	Remark
Fitted Ring spectrum, -9e99=no fitting done or fitting not successful	Ring spectrum slant column
Uncertainty of fitted Ring spectrum based on measured uncertainty, -8=fitting not successful	Equation 114
Uncertainty of fitted Ring spectrum based on instrumental uncertainty, -8=fitting not successful	Equation 114
Uncertainty of fitted Ring spectrum based on rms, -8=fitting not successful	Equation 115
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
Fitting polynomial coefficient, order X	X=0 to maximum 10, see 6.4
Uncertainty of fitting polynomial coefficient based on measured uncertainty, order X, -8=fitting not successful	Equation 114
Uncertainty of fitting polynomial coefficient based on instrumental uncertainty, order X, -8=fitting not successful	Equation 114
Uncertainty of fitting polynomial coefficient based on rms, order X, -8=fitting not successful	Equation 115
Mean value of measured data inside fitting window [same units as measurements]	$\bar{F}$ from equation 90
Offset polynomial coefficient, order X	X=0 to maximum 5, see 6.4
Uncertainty of offset polynomial coefficient, order X, based on measured uncertainty, -8=fitting not successful	Equation 114
Uncertainty of offset polynomial coefficient, order X, based on instrumental uncertainty, -8=fitting not successful	Equation 114
Uncertainty of offset polynomial coefficient, order X, based on rms, -8=fitting not successful	Equation 115
Wavelength change polynomial coefficient, order X	X=0 to maximum 5, see 6.4
Uncertainty of wavelength change polynomial coefficient, order X, based on measured uncertainty, -8=fitting not successful	Equation 114
Uncertainty of wavelength change polynomial coefficient, order X, based on instrumental uncertainty, -8=fitting not successful	Equation 114
Uncertainty of wavelength change polynomial coefficient, order X, based on rms, -8=fitting not successful	Equation 115
Resolution change polynomial coefficient, order X	X=0 to maximum 5, see 6.4
Uncertainty of resolution change polynomial coefficient, order X, based on measured uncertainty, -8=fitting not successful	Equation 114
Uncertainty of resolution change polynomial coefficient, order X, based on instrumental uncertainty, -8=fitting not successful	Equation 114
Uncertainty of resolution change polynomial coefficient, order X, based on rms, -8=fitting not successful	Equation 115

Index	Description
Level 2 Fit 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 26
Sum over $2^i$ using those $i$ , for which the corresponding data quality parameter exceeds the DQ2 limit (same parameters as for DQ1)	
Level 1 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
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 level 1 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 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
Sum over $2^i$ , 0=spectra were interpolated in time, 1=spectra are corrected for off-target signal	See table 23
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
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 measured uncertainty for each pixel inside the fitting window multiplied by $1e5$ , 9e5=pixel was not used for fitting, 0=no measured uncertainty was given	
Normalized slant column residuals weighted with instrumental uncertainty for each pixel inside the fitting window multiplied by $1e5$ , 9e5=pixel was not used for fitting, 0=no measured uncertainty was given	

Table 36: Meaning fo fitting error indices

Index	Description
0	Successful fitting using measured uncertainty
1	Successful fitting using instrumental uncertainty
2	Successful fitting without including uncertainty
3	Warning: Some gases have not been fitted, since their optical depth was zero in the range of the valid data; otherwise successful fitting
4	Warning: No fitting was done since the measurements equal the reference; all differential slant columns are set to zero
5	Error: The reference data do not fully include the wavelength range of the fitting
6	Error: No fitting done since number of measured data or reference data is smaller than number of fitting parameters
7	Error: No fitting because of rank deficiency in design matrix
8	Error: lstsq raised LinAlgError
9	Error: Negative values were in the covariance matrix
10	Error: Encountered singular covariance matrix in non-linear fitting
>10	Errors in leastsq (see description of scipy.optimize.leastsq function), e.g. 11=maximum number of function evaluations reached

### 5.13.2 L2Tot and L2Trop Files

BlickP converts the L2Fit data into L2Tot and L2Trop data by applying an L2 algorithm (see section 6.5). L2Tot files contain total vertical column trace gas amounts retrieved from direct sun or moon observations. L2Trop files contain trace gas information in the troposphere such as surface concentration, tropospheric vertical column amount and layer height. These "higher order L2 files" (L2H) are ASCII-text files with a header, which includes meta data (see section 5.1), a description of the data columns and the data. L2H files are not daily files anymore. They include the whole time series of measurements for a given instrument at a given location.

L2H files are called `PandoraXsY_LLL_L2H_rRRRRpP.txt`. X, Y and LLL are as for the L0 file (section 5.7). H can be "Tot" or "Trop". 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. Since the ICF version is "allowed" to vary over time, it is listed as a column in the data themselves (see table 37).

The size of the L2H 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 37 lists the maximum possible data columns in the L2H file. The real number of columns varies with the instrument and L2H type (see column "Remark"). The meaning of each column is described in the header after the meta data.

For some L2 algorithms, e.g. the "Five Angles O2O2-Ratio Algorithm" (section 6.5.2), L2Fit data from more than one f-code can be used. In this case some of the L2 data columns refer to one f-codes only, which is always the first of the f-codes listed in r-code entry "f-codes" (see table 27).

For L2Tot files the "type of uncertainty" reported depends on the setting of Fitting Setup Entry FSE "Uncertainty" as given in the f-code (see table 23). I.e. not "all uncertainties" as given in the L2Fit files are used for the L2H files as described in table 37.

Differently to L1 and L2Fit files, entry "Level 2 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 28). 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. This means f-code entry "Reference" starts with "Synt" (see table 24), 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 L2H files are not daily files, their content changes over time. Hence differently from L1 and L2Fit files, the content of a L2H file is not "fixed" with a given L2H 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 L2H 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 L2H file or move it in another directory, otherwise it will be overwritten. For official PGN data, previous versions of L2H 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_L2H_rRRRRpP_disusedYYYYMMDD.txt` ).

Table 37: Columns in L2H file

Column name	Remark
UT date and time for center of measurement, yyyyymmddThhmmssZ (ISO 8601)	For retrievals including more than one spectrum, the "Center of measurement" is the center-time of the spectrum, to which all other are interpolated
Fractional days since 2000-1-1 UT midnight for center of measurement	
Effective duration of measurement in seconds	This is for the 'effective' measurements set, i.e. the measurement at the highest PZA for L2Trop
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	
Solar zenith angle for center of measurement in degree	
Solar azimuth for center of measurement in degree, 0=north, increases clockwise	
Lunar zenith angle for center of measurement in degree	L2Tot only
Lunar azimuth for center of measurement in degree, 0=north, increases clockwise	L2Tot only
Pointing zenith angle for center of measurement in degree	L2Trop only
Pointing azimuth for center of measurement in degree, 0=north, increases clockwise	L2Trop only
GAS total vertical column amount [GASUNIT], -9e99=retrieval not successful	Retrieved total vertical column amount for gas GAS in unit GASUNIT, L2Tot only
Uncertainty of GAS total vertical column amount [GASUNIT] based on measured uncertainty, -8=retrieval not successful, -1=cross section is zero in this wavelength range, -3=spectral fitting was done, but no uncertainty could be retrieved	L2Tot only for FSE "Uncertainty"=MEAS, equation 114
Uncertainty of GAS total vertical column amount [GASUNIT] based on instrumental uncertainty, -8=retrieval not successful, -1=cross section is zero in this wavelength range, -3=spectral fitting was done, but no uncertainty could be retrieved	L2Tot only for FSE "Uncertainty"=INSTR, equation 114
Uncertainty of GAS total vertical column amount [GASUNIT] based on rms, -8=retrieval not successful, -1=cross section is zero in this wavelength range, -3=spectral fitting was done, but no uncertainty could be retrieved	L2Tot only for FSE "Uncertainty"=NO, equation 115
GAS effective temperature [K], -8=retrieval not successful, 0=cross section is zero in this wavelength range or differential optical depth is too small to retrieve the temperature	Retrieved effective temperature for gas GAS, L2Tot only

Column name	Remark
Uncertainty of GAS effective temperature [K] based on measured uncertainty, -8=retrieval not successful, -1=cross section is zero in this wavelength range, -2=differential optical depth is too small to retrieve the temperature, -3=spectral fitting was done, but no uncertainty could be retrieved	L2Tot only for FSE "Uncertainty"=MEAS, equation 114
Uncertainty of GAS effective temperature [K] based on instrumental uncertainty, -8=retrieval not successful, -1=cross section is zero in this wavelength range, -2=differential optical depth is too small to retrieve the temperature, -3=spectral fitting was done, but no uncertainty could be retrieved	L2Tot only for FSE "Uncertainty"=INSTR, equation 114
Uncertainty of GAS effective temperature [K] based on rms, -8=retrieval not successful, -1=cross section is zero in this wavelength range, -2=differential optical depth is too small to retrieve the temperature, -3=spectral fitting was done, but no uncertainty could be retrieved	L2Tot only for FSE "Uncertainty"=NO, equation 115
Direct GAS air mass factor	L2Tot only
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	L2Tot only
GAS surface concentration [ppb], -9e99=retrieval not successful	Retrieved surface concentration for gas GAS in ppb, L2Trop only
Uncertainty of GAS surface concentration [ppb], -8=retrieval not successful	L2Trop only
GAS tropospheric vertical column amount [GASUNIT], -9e99=retrieval not successful	Retrieved tropospheric vertical column amount for gas GAS in unit GASUNIT, L2Trop only
Uncertainty of GAS tropospheric vertical column amount [GASUNIT], -8=retrieval not successful	L2Trop only
GAS surface concentration index, integer >0 (see manual), -8=retrieval not successful	See section 6.5.2; L2Trop only
GAS heterogeneity flag, 0=well mixed conditions, 1=heterogeneous conditions, -8=retrieval not successful	See section 6.5.2; L2Trop only
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	
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 29
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 29
Direct GAS air mass factor	As in L2Fit
Fitting result index: 1,2=no error or warning, >2=error or warning	For L2Trop this is the maximum over all sets for the first f-code used

Column name	Remark
rms of unweighted spectral fitting residuals, -9=fitting not successful	Only for FSE "Uncertainty"=NO, equation 109, for L2Trop this is the mean, minimum and maximum over all sets for the first f-code used
Normalized rms of spectral fitting residuals weighted with measured uncertainty, -9=fitting not successful	Only for FSE "Uncertainty"=MEAS, equation 110, for L2Trop this is the mean, minimum and maximum over all sets for the first f-code used
Normalized rms of spectral fitting residuals weighted with instrumental uncertainty, -9=fitting not successful	Only for FSE "Uncertainty"=INSTR, equation 110, for L2Trop this is the mean, minimum and maximum over all sets for the first f-code used
Expected rms of unweighted spectral fitting residuals based on measured uncertainty, -9=fitting not successful or no uncertainty given	Only for FSE "Uncertainty"=NO, equation 111, for L2Trop this is the mean, minimum and maximum over all sets for the first f-code used
Expected normalized rms of weighted spectral fitting residuals based on measured uncertainty, -9=fitting not successful or no uncertainty given	Only for FSE "Uncertainty"=MEAS or INSTR, equation 112, for L2Trop this is the mean, minimum and maximum over all sets for the first f-code used
Expected rms of unweighted spectral fitting residuals based on instrumental uncertainty, -9=fitting not successful or no uncertainty given	Only for FSE "Uncertainty"=NO, equation 111, for L2Trop this is the mean, minimum and maximum over all sets for the first f-code used
Expected normalized rms of weighted spectral fitting residuals based on instrumental uncertainty, -9=fitting not successful or no uncertainty given	Only for FSE "Uncertainty"=MEAS or INSTR, equation 112, for L2Trop this is the mean, minimum and maximum over all sets for the first f-code used
Mean value of measured data inside fitting window [same units as measurements]	As in L2Fit, L2Tot only
Climatological station pressure [mbar]	
Climatological station temperature [K]	L2Trop only
Climatological effective O2O2 height [km]	L2Trop only
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
Level 2 Fit 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	For L2Trop this is the minimum and maximum over all sets for the first f-code used
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	As in L2Fit, for L2Trop this is the maximum over all sets for the first f-code used
Sum over $2^i$ using those i, for which the corresponding data quality parameter exceeds the DQ2 limit (same parameters as for DQ1)	For L2Trop this is the maximum over all sets for the first f-code used
Level 1 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, for L2Trop this is the minimum and maximum over all sets for the first f-code used



Column name	Remark
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, for L2Trop this is the maximum over all sets for the first f-code used
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, for L2Trop this is the maximum over all sets for the first f-code used
Wavelength effective temperature [°C], 999=no effective temperature given	As in L1, for L2Trop this is the mean over all sets for the first f-code used
Estimated average residual stray light level [%] (only valid for stray light correction methods 2 and higher)	As in L1, for L2Trop this is the mean, minimum and maximum over all sets for the first f-code used
Retrieved wavelength shift from level 1 data [nm], -9=no wavelength change determination	As in L1, for L2Trop this is the mean, minimum and maximum over all sets for the first f-code used
Retrieved wavelength shift from spectral fitting [nm], -9=no wavelength change fitting	As in L2Fit, for L2Trop this is the mean, minimum and maximum over all sets for the first f-code used
Integration time [ms]	As in L1, for L2Trop this is the minimum and maximum over all sets for the first f-code used
Number of dark count cycles	As in L1, for L2Trop this is the mean, minimum and maximum over all sets for the first f-code used
Effective position of filterwheel #1, 0=filterwheel not used, 1-9 are valid positions	As in L1, for L2Trop this is the minimum and maximum over all sets for the first f-code used
Effective position of filterwheel #2, 0=filterwheel not used, 1-9 are valid positions	As in L1, for L2Trop this is the minimum and maximum over all sets for the first f-code used

## 5.14 Log Files

BlickO, BlickP and BlickF create log-files, which report 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 error message. Note that most log-entries 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 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
```

## 5.15 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  $4 \cdot n_{\text{SPEC}} + 4$  lines, where  $n_{\text{SPEC}}$  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.* [16].

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

### 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 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 8.

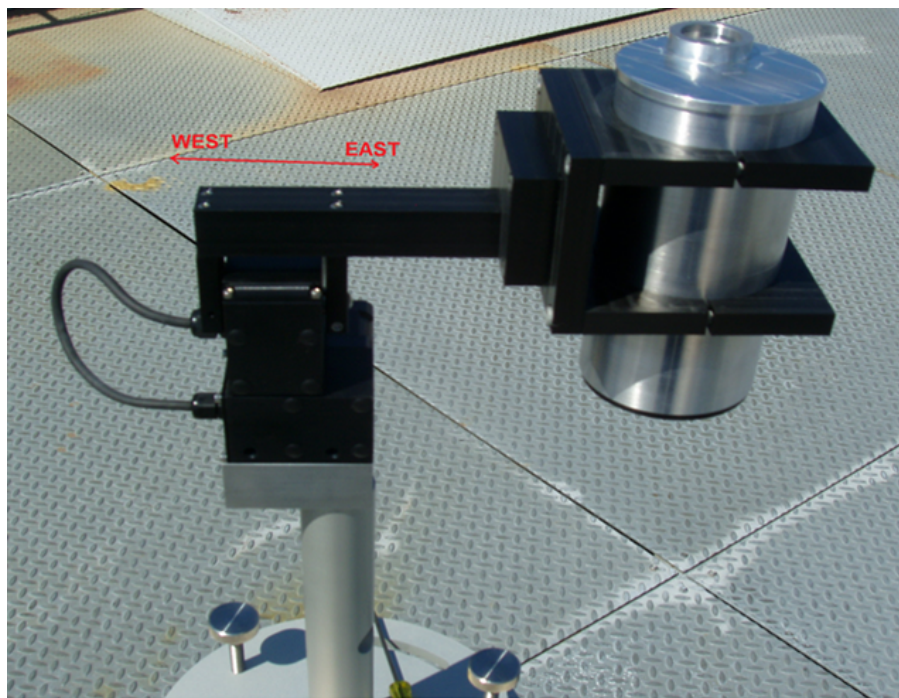


Figure 8: Head sensor position after tracker reset

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 9, 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 9, 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  $(\rho, \theta, \varphi)$ , where  $\rho$  is the distance from the origin,  $\theta$  is the zenith angle (between  $0^\circ$  and  $180^\circ$ ), measured from the positive z-axis, and  $\varphi$  is the azimuth (between  $0^\circ$  and  $360^\circ$ ), 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  $\varphi$  is different from the standard spherical coordinate convention, where  $\varphi$  is taken counterclockwise. So in our definition  $\varphi=0^\circ$  is North,  $\varphi=90^\circ$  East,  $\varphi=180^\circ$  South and  $\varphi=270^\circ$  West.

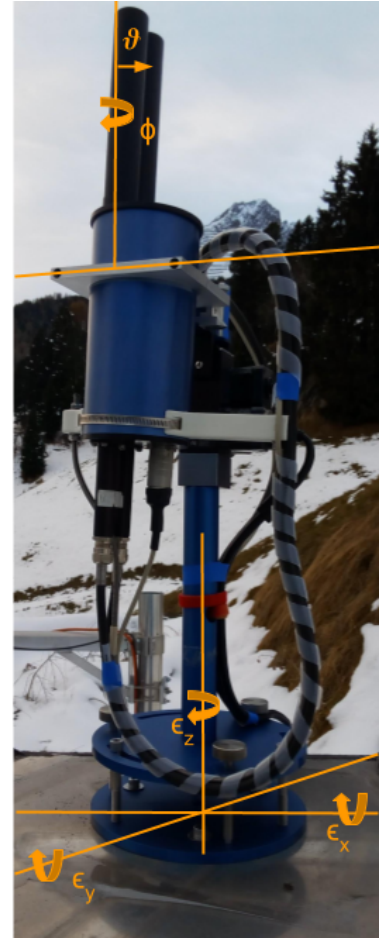
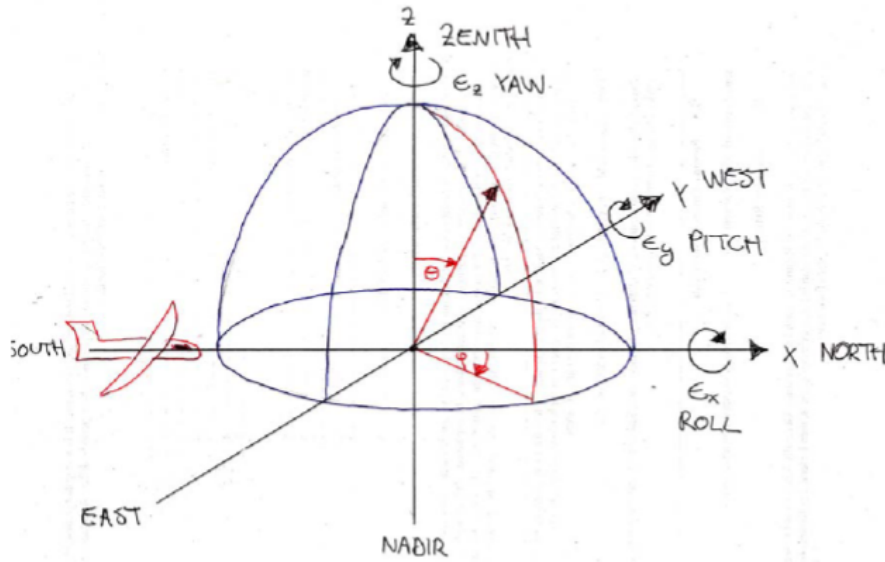


Figure 9: Horizontal frame and leveling angles

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

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

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

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

Since in this context we always deal with "directions" rather than "points",  $\rho$  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  $\epsilon_x$ ,  $\epsilon_y$  and  $\epsilon_z$  (see figure 9). 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  $\epsilon_x$ ,  $\epsilon_y$  and  $\epsilon_z$  correspond to roll, pitch and yaw of an airplane flying along the x-axis to increasing values (from South to North, see figure 9).  $\epsilon_x$  and  $\epsilon_y$  are also called West-East correction and North-South correction respectively and  $\epsilon_z$  is also called Azimuth correction. Equation 20 gives the relationship of  $P_T$  and  $P_H$ :

$$P_H = R_z(\epsilon_z) \cdot R_y(\epsilon_y) \cdot R_x(\epsilon_x) \cdot P_T = R(\epsilon_x, \epsilon_y, \epsilon_z) \cdot P_T \quad (20)$$

$P_H$  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.

$$\begin{aligned} R_x(\epsilon_x) &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\epsilon_x & \sin\epsilon_x \\ 0 & -\sin\epsilon_x & \cos\epsilon_x \end{pmatrix} \\ R_y(\epsilon_y) &= \begin{pmatrix} \cos\epsilon_y & 0 & -\sin\epsilon_y \\ 0 & 1 & 0 \\ \sin\epsilon_y & 0 & \cos\epsilon_y \end{pmatrix} \\ R_z(\epsilon_z) &= \begin{pmatrix} \cos\epsilon_z & \sin\epsilon_z & 0 \\ -\sin\epsilon_z & \cos\epsilon_z & 0 \\ 0 & 0 & 1 \end{pmatrix} \end{aligned} \quad (21)$$

$R$  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  $\epsilon_x$ ,  $\epsilon_y$  and  $\epsilon_z$  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.

$$P_T = R^{-1}(\epsilon_x, \epsilon_y, \epsilon_z) \cdot P_H = R_x(-\epsilon_x) \cdot R_y(-\epsilon_y) \cdot R_z(-\epsilon_z) \cdot P_H \quad (22)$$

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 8), then we can fully describe the alignment of the instrument by the 3 "leveling" angles  $\epsilon_x$ ,  $\epsilon_y$  and  $\epsilon_z$ .

However in practice the 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  $\vartheta$  and azimuth  $\phi$  (see figure 9). Then the position of the optical axis after a zenith motion of  $\theta$  and an azimuth motion of  $\varphi$  in the tracker reference frame is given by equation 23.

$$P_T = R_z(\varphi) \cdot R_y(-\theta) \cdot R_z(\phi) \cdot R_y(-\vartheta) \cdot e_z = R(0, -\theta, \varphi) \cdot R(0, -\vartheta, \phi) \cdot e_z = R(0, -\theta, \varphi) \cdot P_{0\text{AXT}} \quad (23)$$

$e_z$  is the 3x1-elements z-axis-unit-vector (0,0,1). Applying  $R(0, -\vartheta, \phi)$  on  $e_z$  gives the 3x1-elements vector  $P_{0\text{AXT}}$ , the direction of the optical axis after the tracker reset. Then applying  $R(0, -\theta, \varphi)$  on  $P_{0\text{AXT}}$  gives  $P_T$ , the direction of the optical axis after having moved the zenith motor for  $\theta$  and the azimuth motor for  $\varphi$ . So given



the zenith and azimuth motion angles  $\theta$  and  $\varphi$  and knowing the position of the optical axis after the tracker reset relative to the z-axes  $\vartheta$  and  $\phi$  we can calculate the coordinates of the optical axis in the tracker frame  $P_T$ . For the opposite, i.e. getting  $\theta$  and  $\varphi$  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  $\theta$ ,  $\varphi$ ,  $\epsilon_x$ ,  $\epsilon_y$ ,  $\epsilon_z$ ,  $\vartheta$  and  $\phi$ .

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

So once we have the full set of leveling angles  $\epsilon_x$ ,  $\epsilon_y$ ,  $\epsilon_z$ ,  $\vartheta$  and  $\phi$ , we can calculate the "true" pointing in the horizontal reference frame  $P_H$  for each pair of tracker motion angles  $\theta$  and  $\varphi$ . And, using the inversion of equation 24, we can calculate the motion angles  $\theta$  and  $\varphi$  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 given absolute position  $P_H$  is not exactly reached. E.g. if  $\epsilon_x = \epsilon_y = \epsilon_z = 0^\circ$ ,  $\vartheta = 1^\circ$  and  $\phi = 90^\circ$ , the instrument cannot point exactly to the zenith. 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  $\varphi$  will point the instrument in the same direction (zenith), if  $\theta = 0^\circ$ .

## 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 [16], 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 5.15). An example for such a sun search is shown in figure 10.

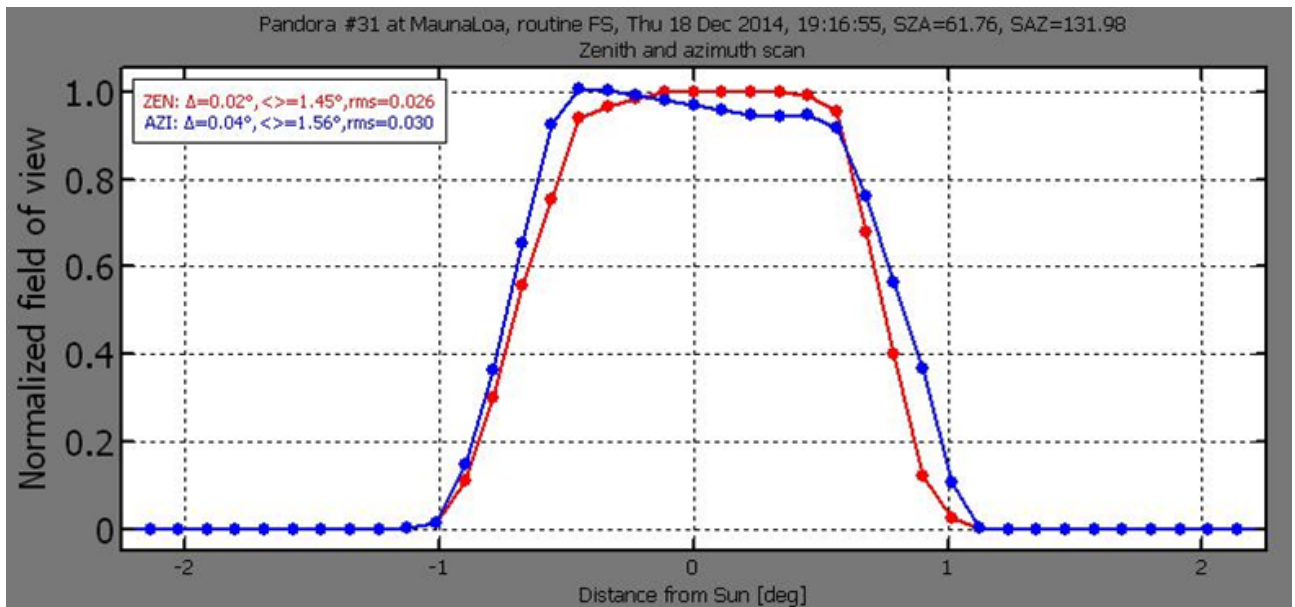


Figure 10: Sun search for Pandora #31 at Mauna Loa on 18 Dec 2014. Red line is the sun scan in zenith direction ("up-down") and blue line in azimuth direction ("left-right"). In this case the apparent angles differ from the true angles by  $0.02^\circ$  in zenith and  $0.04^\circ$  in azimuth.

After a successful sun-search we can calculate angles  $(\theta_H, \varphi_H)$ , which correspond to point  $P_H$ , the position of the sun in the horizontal reference frame, and we have measured angles  $(\theta_T, \varphi_T)$ , the tracker motion angles of

the maximum signal, which correspond to  $\theta$  and  $\varphi$  in equation 24. Now we try to solve equation 24 with given  $\theta_H$ ,  $\varphi_H$ ,  $\theta_T$  and  $\varphi_T$  to obtain the leveling angles. The technique BlickO uses is based on a linearization of equation 24 and iterations to find the solution. Equation 25 shows the first order approximations of the rotation matrices from equation 21 at position  $\epsilon + \Delta\epsilon$ :

$$\begin{aligned} R_x(\epsilon + \Delta\epsilon) &\approx \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\epsilon & \sin\epsilon \\ 0 & -\sin\epsilon & \cos\epsilon \end{pmatrix} + \Delta\epsilon \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & -\sin\epsilon & -\cos\epsilon \\ 0 & \cos\epsilon & -\sin\epsilon \end{pmatrix} = R_x(\epsilon) + \Delta\epsilon \cdot V_x(\epsilon) \\ R_y(\epsilon + \Delta\epsilon) &\approx \begin{pmatrix} \cos\epsilon & 0 & -\sin\epsilon \\ 0 & 1 & 0 \\ \sin\epsilon & 0 & \cos\epsilon \end{pmatrix} + \Delta\epsilon \cdot \begin{pmatrix} -\sin\epsilon & 0 & \cos\epsilon \\ 0 & 1 & 0 \\ -\cos\epsilon & 0 & -\sin\epsilon \end{pmatrix} = R_y(\epsilon) + \Delta\epsilon \cdot V_y(\epsilon) \\ R_z(\epsilon + \Delta\epsilon) &\approx \begin{pmatrix} \cos\epsilon & \sin\epsilon & 0 \\ -\sin\epsilon & \cos\epsilon & 0 \\ 0 & 0 & 1 \end{pmatrix} + \Delta\epsilon \cdot \begin{pmatrix} -\sin\epsilon & -\cos\epsilon & 0 \\ \cos\epsilon & -\sin\epsilon & 0 \\ 0 & 0 & 1 \end{pmatrix} = R_z(\epsilon) + \Delta\epsilon \cdot V_z(\epsilon) \end{aligned} \quad (25)$$

The 3-3-elements matrices  $V_x$ ,  $V_y$  and  $V_z$  are the first derivatives of the rotation matrices in  $\epsilon$ . Using equation 25 we can linearize equation 24 at position  $\theta$ ,  $\varphi$ ,  $\epsilon_x + \Delta\epsilon_x$ ,  $\epsilon_y + \Delta\epsilon_y$ ,  $\epsilon_z + \Delta\epsilon_z$ ,  $\vartheta + \Delta\vartheta$  and  $\phi + \Delta\phi$ .

$$\begin{aligned} P_H &\approx R_z(\epsilon_z) \cdot R_y(\epsilon_y) \cdot R_x(\epsilon_x) \cdot R(0, -\theta, \varphi) \cdot R_z(\phi) \cdot R_y(-\vartheta) \cdot e_z \\ &+ \Delta\epsilon_x \cdot R_z(\epsilon_z) \cdot R_y(\epsilon_y) \cdot V_x(\epsilon_x) \cdot R(0, -\theta, \varphi) \cdot R_z(\phi) \cdot R_y(-\vartheta) \cdot e_z \\ &+ \Delta\epsilon_y \cdot R_z(\epsilon_z) \cdot V_y(\epsilon_y) \cdot R_x(\epsilon_x) \cdot R(0, -\theta, \varphi) \cdot R_z(\phi) \cdot R_y(-\vartheta) \cdot e_z \\ &+ \Delta\epsilon_z \cdot V_z(\epsilon_z) \cdot R_y(\epsilon_y) \cdot R_x(\epsilon_x) \cdot R(0, -\theta, \varphi) \cdot R_z(\phi) \cdot R_y(-\vartheta) \cdot e_z \\ &+ \Delta\vartheta \cdot R_z(\epsilon_z) \cdot R_y(\epsilon_y) \cdot R_x(\epsilon_x) \cdot R(0, -\theta, \varphi) \cdot R_z(\phi) \cdot V_y(-\vartheta) \cdot e_z \\ &+ \Delta\phi \cdot R_z(\epsilon_z) \cdot R_y(\epsilon_y) \cdot R_x(\epsilon_x) \cdot R(0, -\theta, \varphi) \cdot V_z(\phi) \cdot R_y(-\vartheta) \cdot e_z \end{aligned} \quad (26)$$

$$P_H \approx P + \Delta\epsilon_x \cdot C_x + \Delta\epsilon_y \cdot C_y + \Delta\epsilon_z \cdot C_z + \Delta\vartheta \cdot C_\vartheta + \Delta\phi \cdot C_\phi$$

All  $C_x$ ,  $C_y$ , etc. in equation 26 are 3x1-element vectors. Rearranging 26 we obtain a system of linear equations:

$$P_H - P = \Delta P = \begin{pmatrix} C_{xx} & C_{yx} & C_{zx} & C_{\vartheta x} & C_{\phi x} \\ C_{xy} & C_{yy} & C_{zy} & C_{\vartheta y} & C_{\phi y} \\ C_{xz} & C_{yz} & C_{zz} & C_{\vartheta z} & C_{\phi z} \end{pmatrix} \cdot \begin{pmatrix} \Delta\epsilon_x \\ \Delta\epsilon_y \\ \Delta\epsilon_z \\ \Delta\vartheta \\ \Delta\phi \end{pmatrix} = C \cdot \Delta\epsilon \quad (27)$$

Equation 27 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 27. This makes sense, since we are trying to get 5 pieces of information out of equation 27, 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 28.

$$\Delta P = \begin{pmatrix} \Delta P_1 \\ \Delta P_2 \\ \dots \\ \Delta P_N \end{pmatrix} = \begin{pmatrix} C_1 \\ C_2 \\ \dots \\ C_N \end{pmatrix} \cdot \Delta\epsilon = C \cdot \Delta\epsilon \quad (28)$$

N is the number of sun searches used,  $\Delta P$  is a  $3N \times 1$ -elements vector and C is a  $3N \times 5$ -elements matrix. For  $N > 2$  equation 28 is an overdetermined system of linear equations, which we can solve in a least squares sense with the pseudo-inverse matrix.

$$\Delta \epsilon = [C^T \cdot C]^{-1} \cdot C^T \cdot \Delta P = \text{pinv}(C) \cdot \Delta P \quad (29)$$

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 5.15).
2. Take a first guess for the leveling angles. At the very beginning the first guess is  $\epsilon(i=0)=(0,0,0,0,0)$ . When a previous determination of the leveling had been done, then this is used as first guess.
3. Calculate  $\Delta P$  and C using  $\epsilon(i)$  and the sun search results as in equation 28.
4. Calculate the "cost-function", which is the sum-of-squares over  $\Delta P$ .
5. Get  $\Delta \epsilon(i)$  from equation 29.
6. Get the next guess for the leveling angles  $\epsilon(i+1)=\epsilon(i)+\Delta \epsilon(i)$ .
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 quite always that the instrument has been moved or the tracker has slipped. In such 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  $0.14^\circ$  and comparable to our tracking accuracy, while for the solar position it is  $0.02^\circ$  [16].
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 27). Then BlickO puts some constraints on the leveling angles. It sets  $\vartheta=0$  and  $\phi=0$  and fixes the relationship between  $\epsilon_x$  and  $\epsilon_y$ .

$$\frac{\epsilon_x}{\epsilon_y} = \tan(\varphi_H) \quad \text{with} \quad \left| \frac{\epsilon_x}{\epsilon_y} \right| < 1000 \quad (30)$$

So e.g. if the solar azimuth is  $180^\circ$  (=South), then  $\epsilon_x$  is set to zero or if the solar azimuth is  $225^\circ$  (=South-West), then  $\epsilon_x = \epsilon_y$ . With these constraints equation 27 reduces to equation 31, which can be solved with the iterative method described above.

$$\Delta P = \begin{pmatrix} C_{xx} + \tan(\varphi_H) \cdot C_{yx} & C_{zx} \\ C_{xy} + \tan(\varphi_H) \cdot C_{yy} & C_{zy} \\ C_{xz} + \tan(\varphi_H) \cdot C_{yz} & C_{zz} \end{pmatrix} \cdot \begin{pmatrix} \Delta \epsilon_y \\ \Delta \epsilon_z \end{pmatrix} \quad (31)$$



### 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  $2.5^\circ$  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 11). The FWHM of the SkyFOV is about  $1.5^\circ$  and is determined by the diameter of the fiber and the distance between lens and fiber (see figure 11).

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  $0.3^\circ$ . This means that the centers of the FOVs can vary by as much as this angle.

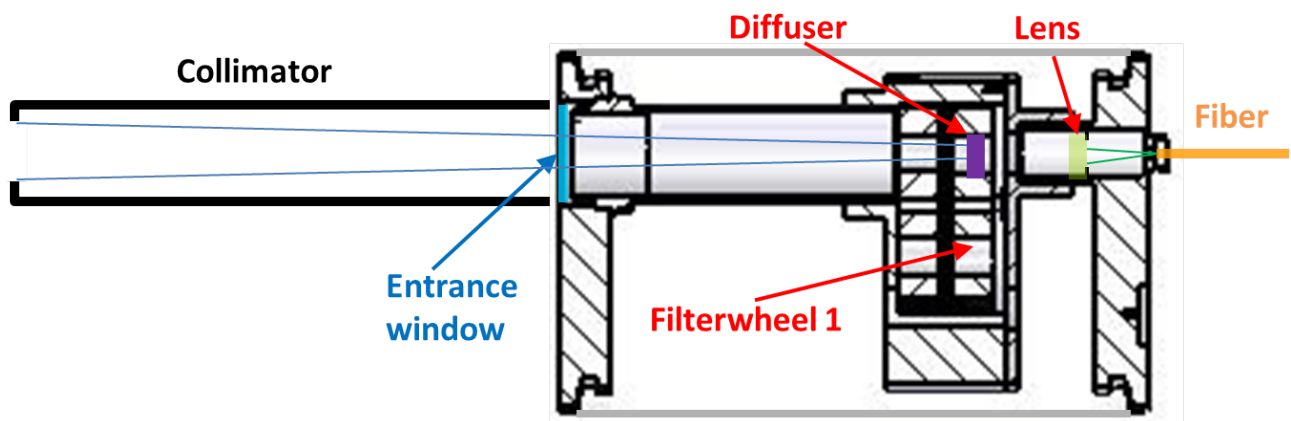


Figure 11: Schematics of the Pandora head sensor. The SunFOV is determined by the aperture on top of the collimator and the aperture behind the diffuser (thin blue lines). The SkyFOV is determined by the focal length of the lens and the diameter of the fiber (thin green lines).

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)  $80.0^\circ$  and pointing azimuth (PAZ)  $180.0^\circ$ , 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= $80.11^\circ$ , PAZ= $179.97^\circ$  for spectrometer 1 and PZA= $79.94^\circ$ , PAZ= $180.20^\circ$  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 6.3.1), 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

$$\begin{aligned} N_e &= N_{eT} + N_{e\gamma} \\ &= N_{eT} + N_\gamma \cdot QE \\ &= I_{eT} \cdot \Delta t + I_\gamma \cdot QE \cdot \Delta t \end{aligned} \tag{32}$$

$\Delta t$  Exposure time (or integration time) [s]

$N_e$  Total number of electrons accumulated within  $\Delta t$  [1]

$N_{eT}$  Number of thermal electrons accumulated within  $\Delta t$  [1]

$N_{e\gamma}$  Number of electrons produced by incident photons within  $\Delta t$  [1]

$N_\gamma$  Number of incident photons within  $\Delta t$  [1]

$QE$  Detector quantum efficiency for this wavelength, number of electrons per number of photons [1]

$I_{eT}$  Mean rate of thermal electrons during  $\Delta t$ , electrons per second [1/s]

$I_\gamma$  Mean rate of incident photons during  $\Delta t$ , 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.

$$\begin{aligned} V &= N_e \cdot q_e \cdot \frac{A}{C_0} + \text{OFFSET}_V \\ &= N_e \cdot \text{GAIN}_V + \text{OFFSET}_V \end{aligned} \quad (33)$$

V	Output voltage [V]
$q_e$	Electron charge [C]
$C_0$	Output node capacitance [ $F=C/V$ ]
A	Amplifier voltage gain [1]
$\text{OFFSET}_V$	Electrical offset added by the amplifier [V]
$\text{GAIN}_V$	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).

$$\begin{aligned} C &= V \cdot F \\ &= N_e \cdot \text{GAIN}_V \cdot F + \text{OFFSET}_V \cdot F \\ &= N_e \cdot \text{GAIN} + \text{OFFSET} \end{aligned} \quad (34)$$

C	Raw counts [DN]
F	Analog-digital conversion factor [DN/V]
OFFSET	(Count) offset ( $=\text{OFFSET}_V \cdot F$ ) [DN]
GAIN	(Count) gain ( $=\text{GAIN}_V \cdot F$ ) per electron [DN]

A single dark measurement  $\text{DC}_i$  and a single bright measurement  $\text{BC}_i$  are given by:

$$\begin{aligned} \text{DC}_i &= \text{OFFSET}_i + \text{GAIN}_i \cdot N_{eT_i} \\ &= \text{OFFSET}_i + \text{GAIN}_i \cdot I_{eT_i} \cdot \Delta t_i \\ \text{BC}_i &= \text{OFFSET}_i + \text{GAIN}_i \cdot [N_{eT_i} + N_{e\gamma_i}] \\ &= \text{OFFSET}_i + \text{GAIN}_i \cdot [I_{eT_i} + I_{\gamma_i} \cdot \text{QE}] \cdot \Delta t_i \end{aligned} \quad (35)$$

where  $i$  is the measurement index. In the following paragraphs each of the parameters in equation 35 is discussed separately:

### $\Delta t$

We assume the uncertainty in the exposure time  $\Delta t$  to be negligible and set the variance ( $\sigma^2$ ) to zero. There might be a systematic error (bias) in  $\Delta t$  (see section 6.3.5), but we do not assume this bias changing over time.

$$\sigma_{\Delta t}^2 = 0 \quad (36)$$

## 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 35 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](http://en.wikipedia.org/wiki/Electronic_noise)).

$$\sigma_{OFFSET}^2(\text{SHORT-TERM}) = \sigma_{READ}^2 \quad (37)$$

## 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.

$$\sigma_{GAIN}^2(\text{SHORT-TERM}) = 0 \quad (38)$$

## 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.

$$\sigma_{QE}^2(\text{SHORT-TERM}) = 0 \quad (39)$$

## $N_{eT}$

The number of thermal electrons is the product of  $I_{eT}$  times  $\Delta t$ . 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](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](http://en.wikipedia.org/wiki/Poisson_distribution)). For the (short-term) uncertainty of  $N_e$  follows

$$\sigma_{N_{eT}}^2(\text{SHORT-TERM}) = N_{eT} \quad (40)$$

## $N_{e\gamma}$

The number of electrons produced by incident photons is the product of  $I_\gamma$  times QE times  $\Delta t$ . The rate of incident photons  $I_\gamma$  depends on the light source. For a constant light source, e.g. a stable lamp,  $I_\gamma$  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](http://en.wikipedia.org/wiki/Shot_noise)).

$$\sigma_{N_{e\gamma}}^2(\text{SHORT-TERM,stable}) = N_{e\gamma} \quad (41)$$

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  $I_\gamma$  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  $I_\gamma$ . The total (short-term) uncertainty of  $N_{e\gamma}$  is therefore a combination of the photon noise and the input rate variation.

$$\begin{aligned} \sigma_{N_{e\gamma}}^2(\text{SHORT-TERM}) &= N_{e\gamma} + \sigma_{I_\gamma}^2 \cdot QE^2 \cdot \Delta t^2 \\ &= N_{e\gamma} + \sigma_{eINPUT}^2 \end{aligned} \quad (42)$$

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

From equations 33 to 42 we can compose the total short-term (<1 min) uncertainties of  $BC_i$  and  $DC_i$  respectively:

$$\begin{aligned}
 \sigma_{DCi}^2 &= \sigma_{READi}^2 + GAIN_i^2 \cdot N_{eTi} \\
 &= \sigma_{READi}^2 + GAIN_i^2 \cdot I_{eTi} \cdot \Delta t_i \\
 \sigma_{BCi}^2 &= \sigma_{READi}^2 + GAIN_i^2 \cdot [N_{eTi} + N_{e\gamma i} + \sigma_{eINPUTi}^2] \\
 &= \sigma_{READi}^2 + GAIN_i^2 \cdot [I_{eTi} + I_{\gamma i} \cdot QE_i] \cdot \Delta t_i + \sigma_{INPUTi}^2
 \end{aligned} \tag{43}$$

$\sigma_{INPUT}$  is the product of  $\sigma_{eINPUT}$  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  $n_{BC}$  repetitions of BC-measurements  $BC_i$  and  $n_{DC}$  repetitions of DC-measurements  $DC_i$ , all at the same integration time  $\Delta t$ . The total time of bright measurements  $n_{BC} \cdot \Delta t$  or dark measurements  $n_{DC} \cdot \Delta t$  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

$$\begin{aligned}
 DC &= \frac{1}{n_{DC}} \cdot \sum_{i=1}^{n_{DC}} DC_i = OFFSET + GAIN \cdot I_{eT} \cdot \Delta t \\
 BC &= \frac{1}{n_{BC}} \cdot \sum_{i=1}^{n_{BC}} BC_i = OFFSET + GAIN \cdot [I_{eT} + I_{\gamma} \cdot QE] \cdot \Delta t
 \end{aligned} \tag{44}$$

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

$$\sigma_{DCi}^2 = \frac{1}{n_{DC} - 1} \cdot \sum_{i=1}^{n_{DC}} (DC_i - DC)^2 \tag{45}$$

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  $\sigma_{BCi}$  (first line of equation 46). 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  $\sigma_{BCi}$  (second line of equation 46). In the latter case the points on the fitted straight line are called  $BC_{iFIT}$ .

$$\begin{aligned}
 \sigma_{BCi}^2 &= \frac{1}{n_{BC} - 1} \cdot \sum_{i=1}^{n_{BC}} (BC_i - BC)^2 \\
 \sigma_{BCi}^2 &= \frac{1}{n_{BC} - 2} \cdot \sum_{i=1}^{n_{BC}} (BC_i - BC_{iFIT})^2
 \end{aligned} \tag{46}$$

From equations 43 and 44 we can derive the noise in the averaged dark measurements  $\sigma_{DC}$ :

$$\sigma_{DC}^2 = \frac{\sigma_{DCi}^2}{n_{DC}} = \frac{1}{n_{DC}} \cdot [\sigma_{READ}^2 + GAIN^2 \cdot I_{eT} \cdot \Delta t] \quad (47)$$

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](http://en.wikipedia.org/wiki/Standard_error)).

For the uncertainty of the averaged bright measurements  $\sigma_{BC}$  we use the same equations and distinguish two cases. The first line in equation 48 is for the case that  $\sigma_{INPUT}$  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 48 is for the case that  $\sigma_{INPUT}$  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).

$$\begin{aligned} \sigma_{BC}^2(\text{STAT}) &= \frac{1}{n_{BC}} \cdot [\sigma_{READ}^2 + GAIN^2 \cdot (I_{eT} + I_{\gamma} \cdot QE) \cdot \Delta t + \sigma_{INPUT}^2] = \frac{\sigma_{BCi}^2}{n_{BC}} \\ \sigma_{BC}^2(\text{SYS}) &= \frac{1}{n_{BC}} \cdot [\sigma_{READ}^2 + GAIN^2 \cdot (I_{eT} + I_{\gamma} \cdot QE) \cdot \Delta t] + \sigma_{INPUT}^2 > \frac{\sigma_{BCi}^2}{n_{BC}} \end{aligned} \quad (48)$$

## 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 35:

$$CC_i = BC_i - DC_i = GAIN \cdot I_{\gamma i} \cdot QE \cdot \Delta t \quad (49)$$

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 43:

$$\begin{aligned} \sigma_{CCi}^2 &= \sigma_{DCi}^2 + \sigma_{BCi}^2 \\ &= 2 \cdot \sigma_{READ}^2 + GAIN^2 \cdot [2 \cdot I_{eT} + I_{\gamma} \cdot QE] \cdot \Delta t + \sigma_{INPUT}^2 \\ &= 2 \cdot \sigma_{READ}^2 + 2 \cdot GAIN^2 \cdot I_{eT} \cdot \Delta t + GAIN \cdot CC_i + \sigma_{INPUT}^2 \\ &= 2 \cdot \sigma_{DCi}^2 + GAIN \cdot CC_i + \sigma_{INPUT}^2 \\ &= \sigma_{INSTR}^2 + \sigma_{INPUT}^2 \end{aligned} \quad (50)$$

In this equation we have split the uncertainty of the corrected counts in the "instrumental noise"  $\sigma_{INSTR}$  and the "input variation"  $\sigma_{INPUT}$ . If we assume no input variation ( $\sigma_{INPUT}=0$ ) and furthermore neglect  $I_{eT}$ , which can be done for low exposure times and/or low temperatures, then equation 50 reduces to:

$$\sigma_{CCi}^2 = 2 \cdot \sigma_{READ}^2 + GAIN \cdot CC_i \quad (51)$$

Figure 12 shows the estimated  $\sigma_{CCi}$  from equation 51 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.

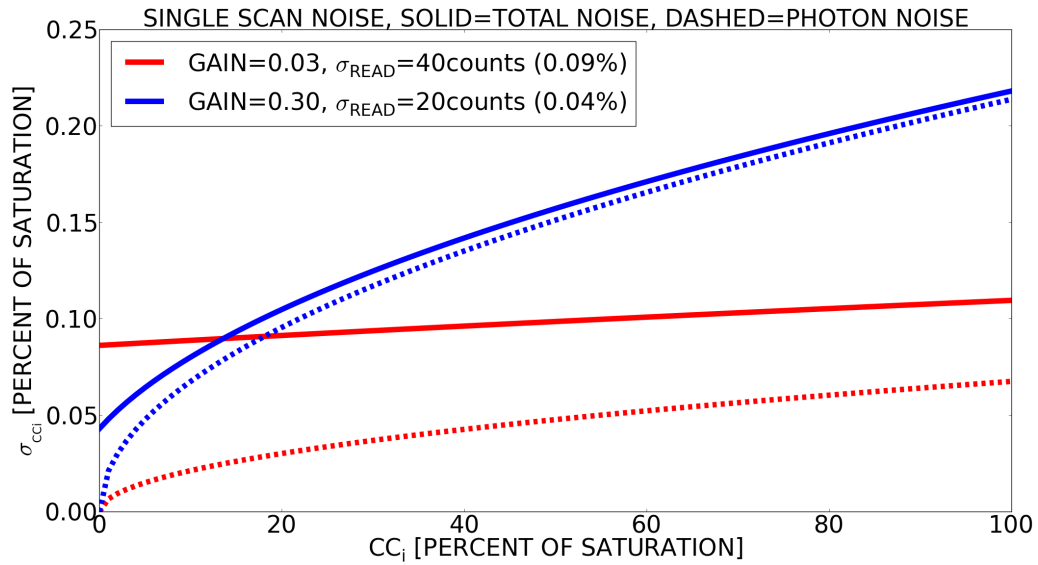


Figure 12: Noise of dark corrected counts for a single bright and dark measurement as a function of the corrected counts, expressed as a fraction of saturation.

The SNR of  $\text{CC}_i$  based on equation 51 is given by:

$$\text{SNR}_i = \frac{\text{CC}_i}{\sigma_{\text{CCI}}} = \frac{\text{CC}_i}{\sqrt{2 \cdot \sigma_{\text{READ}}^2 + \text{GAIN} \cdot \text{CC}_i}} \quad (52)$$

This is shown in figure 13. 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.

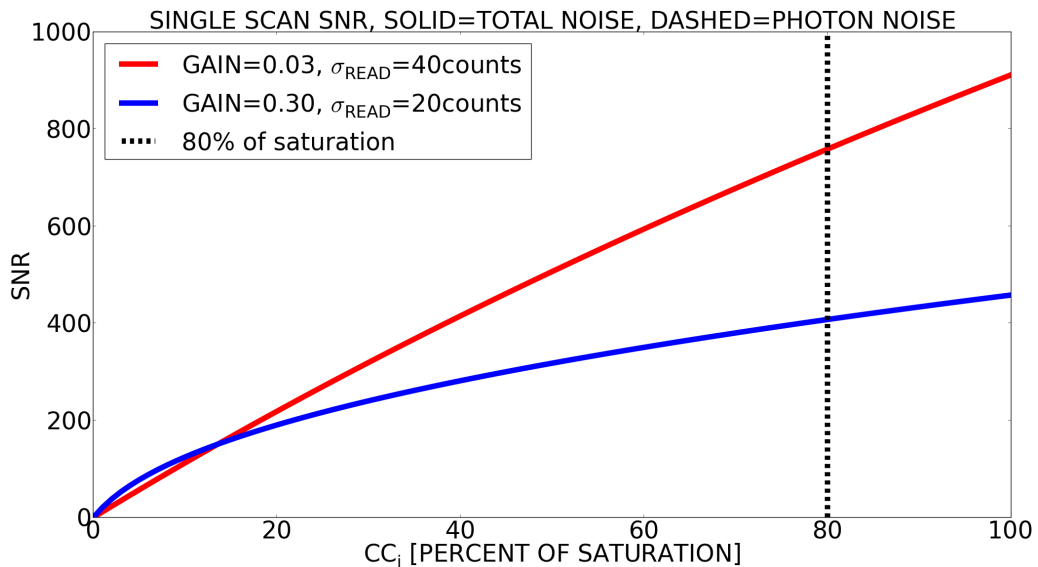


Figure 13: SNR of dark corrected counts for a single bright and dark measurement as a function of the corrected counts, expressed as a fraction of saturation.

### 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 44 we get for the corrected counts CC:

$$CC = BC - DC = GAIN \cdot I_\gamma \cdot QE \cdot \Delta t \quad (53)$$

For the uncertainty of CC follows from equations 47 and 48:

$$\begin{aligned} \sigma_{CC}^2 &= \sigma_{DC}^2 + \sigma_{BC}^2 \\ &= \left( \frac{1}{n_{DC}} + \frac{1}{n_{BC}} \right) \cdot [\sigma_{READ}^2 + GAIN^2 \cdot I_{eT} \cdot \Delta t] + \frac{1}{n_{BC}} \cdot [GAIN^2 \cdot I_\gamma \cdot QE \cdot \Delta t] \\ &= \left( \frac{1}{n_{DC}} + \frac{1}{n_{BC}} \right) \cdot \sigma_{DCi}^2 + \frac{1}{n_{BC}} \cdot GAIN \cdot CC \\ &= \sigma_{INSTR}^2 \end{aligned} \quad (54)$$

Here we assume no input variation ( $\sigma_{INPUT}=0$ ), 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 54 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).

$$\sigma_{INSTR}^2 = \frac{\sigma_{DCi}^2}{n \cdot f_{DC}} + \frac{\sigma_{DCi}^2 + GAIN \cdot CC}{n \cdot (1 - f_{DC})} \quad (55)$$

$n$  is the sum of  $n_{DC}$  and  $n_{BC}$ . Deriving equation 55 for  $f_{DC}$  yields:

$$\frac{\partial \sigma_{INSTR}^2}{\partial f_{DC}} = \frac{-\sigma_{DCi}^2}{n \cdot f_{DC}^2} + \frac{\sigma_{DCi}^2 + GAIN \cdot CC}{n \cdot (1 - f_{DC})^2} \quad (56)$$

For the extreme conditions, we obtain this solution:

$$f_{DCOPT} = \frac{-\sigma_{DCi}^2}{GAIN \cdot CC} \pm \sqrt{\left( \frac{\sigma_{DCi}^2}{GAIN \cdot CC} \right)^2 + \frac{\sigma_{DCi}^2}{GAIN \cdot CC}} \quad (57)$$

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

$$f_{DCOPT} = ODR = \sqrt{q^2 - q} - q \quad (58)$$

where  $q$  is given by

$$q = \frac{\sigma_{DCi}^2}{GAIN \cdot CC} \geq \frac{\sigma_{READ}^2}{GAIN \cdot CC} \quad (59)$$

If we neglect  $I_{eT}$ , which can be done for low exposure times and/or low temperatures, we can replace  $\sigma_{CCi}$  by  $\sigma_{READ}$ . ODR as a function of  $q$  is shown in figure 14.

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.

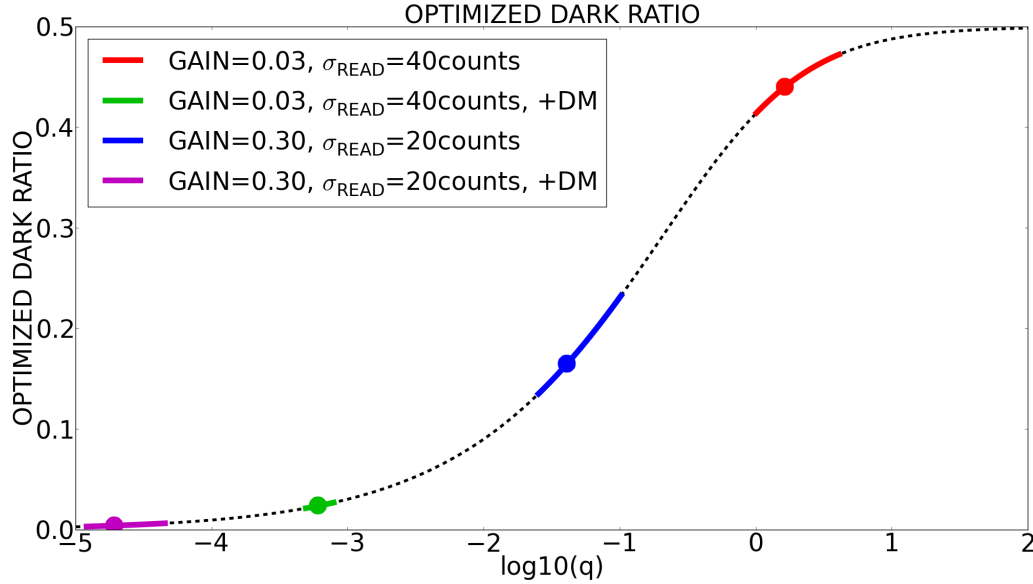


Figure 14: Optimized dark ratio as a function of  $q$  from equation 59 or 61 for  $q$ -values ranging from  $1e-5$  to  $1e2$ . The colored lines are for CC-values ranging from 20% to 80% of saturation for typical CMOS- and CCD-systems respectively. The colored dots are for CC-values at 50% of saturation. 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 6.3.1 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  $\sigma_{DCi}$  divided by square root of the number of pixels  $\sqrt{n_{\text{pix}}}$ . Including this reduction, equation 55 becomes

$$\sigma_{\text{INSTR}}^2 = \frac{\sigma_{DCi}^2}{n \cdot n_{\text{PIX}} \cdot f_{\text{DC}}} + \frac{\sigma_{DCi}^2 + \text{GAIN} \cdot \text{CC}}{n \cdot (1 - f_{\text{DC}})} \quad (60)$$

and consequently  $q$  changes to

$$q = \frac{\sigma_{DCi}^2}{\sigma_{DCi}^2 \cdot [n_{\text{PIX}} - 1] + n_{\text{PIX}} \cdot \text{GAIN} \cdot \text{CC}} \quad (61)$$

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 14).

Figure 15 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.

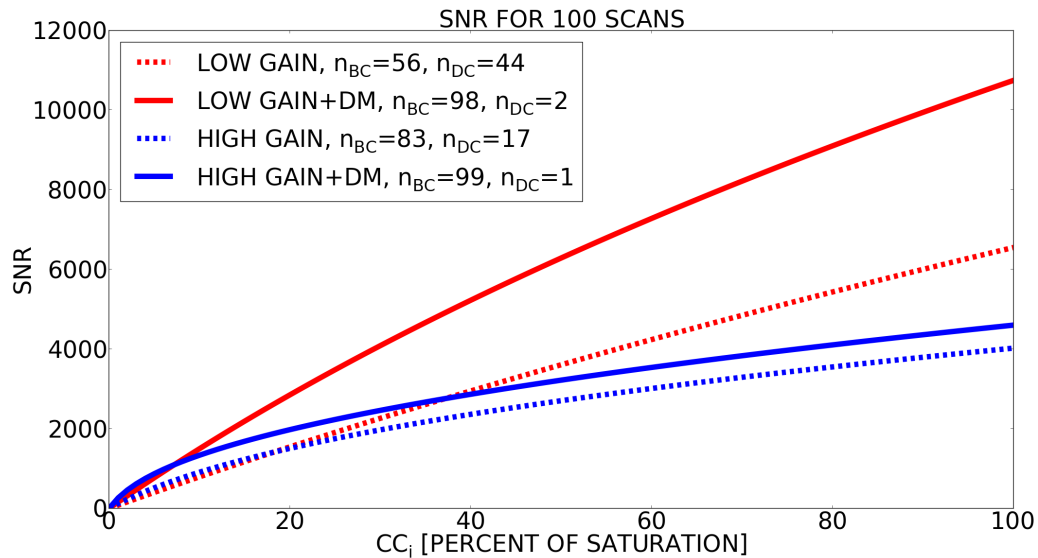


Figure 15: SNR of averaged dark corrected counts for a total number of 1000 single scans as a function of the corrected counts, expressed as fraction of saturation. Solid lines show dark mapping method, where all 1000 scans are spent taking BC data. Dashed lines refer to the immediate dark method, where 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 16, 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.

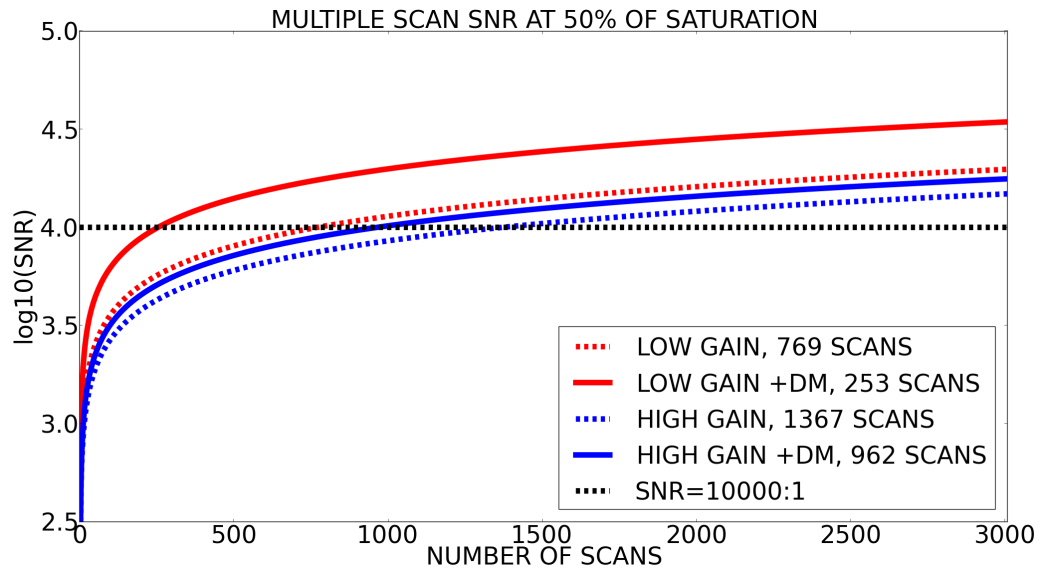


Figure 16: SNR of averaged dark corrected counts at 50% of saturation as a function of the number of scans averaged with (solid) and without (dashed) using a dark map. The black dashed line is for SNR=10000:1. Values listed in the legend give the number of scans needed to exceed an SNR of 10000:1.

## 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 35 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 6.3.1). 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 L1 Algorithm - Data Correction

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.

$$L1_i = L0_i \tag{62}$$

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).

### 6.3.1 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 17. 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.

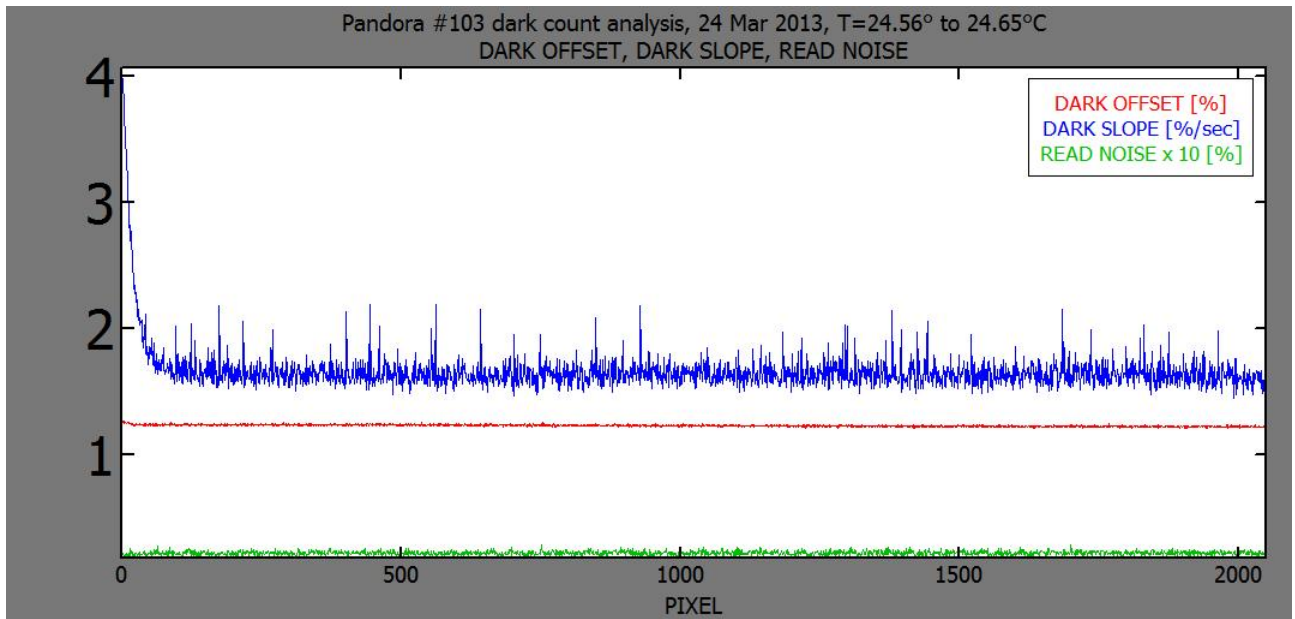


Figure 17: Dark offset (red), dark slope (blue) and read noise (green) of Pandora 103 as a function of pixel. Data are for a set temperature of 20 °C. The electronics board temperature is about 25 °C.

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  $DC_i$ :

$$DC_{Ei} = DC_i \quad (63)$$

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:

$$DC_{FINEi} = A_{ICi} \cdot \exp^{B_{ICi} \cdot (T_{RE} - T_{RR})} + A_{SLi} \cdot \exp^{B_{SLi} \cdot (T_{RE} - T_{RR})} \cdot IT \quad (64)$$

$T_{RE}$  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 65:

$$DC_{BGi} = E_0 \cdot \exp^{-E_1 \cdot pixind} + C_0 + C_1 \cdot pixind + \dots + C_{N+1} \cdot pixind^N \quad (65)$$

$pixind$  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.  $E_0$  and  $E_1$  are the parameters of the exponential part and  $C_0$ ,  $C_1$ , 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 17). 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  $DC_{Ei}$ :

$$DC_{Ei} = DC_{BGi} + DC_{FINEi} \quad (66)$$

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  $L1_i$  after dark correction are given by:

$$L1_i = \left( L1_i^* - \frac{1}{n_{BLIND}} \cdot \sum_{j=1}^{n_{BLIND}} L1_j^* \right) - \left( DC_{Ei} - \frac{1}{n_{BLIND}} \cdot \sum_{j=1}^{n_{BLIND}} DC_j \right) \quad (67)$$

$DC_{Ei}$  is from equation 63 or 66 and  $n_{BLIND}$  is the number of blind pixels in the detector (see section 6.2.6). The ' $n_{BLIND}$ -terms' in equation 67 are not included if the detector has no blind pixels or if no 'blind correction' is requested in the data processing.

### 6.3.2 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 18. 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:

$$NLC_i = E_0 \cdot \exp^{-E_1 \cdot (L1_i^*)^{E_2}} + C_0 + C_1 \cdot L1_i^* + \dots + C_{N+1} \cdot (L1_i^*)^N \quad (68)$$

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  $L1_i$  after non-linearity correction are given by:

$$L1_i = \frac{L1_i^*}{NLC_i} \quad (69)$$

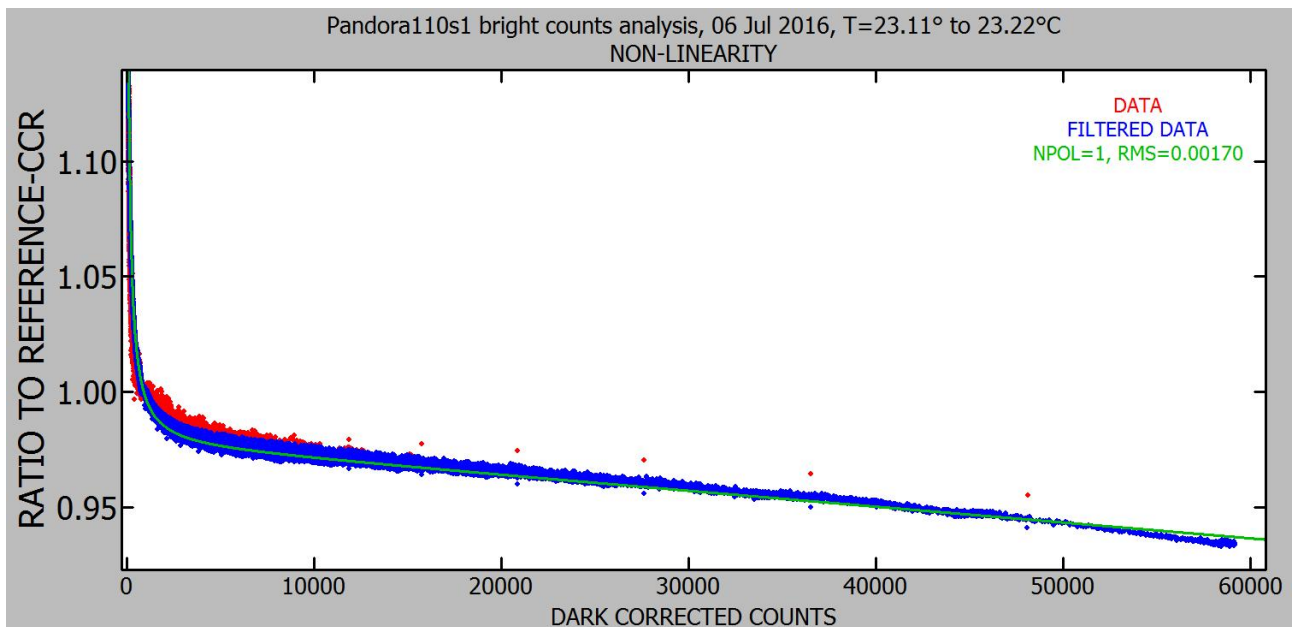


Figure 18: Non-linearity effect for Pandora 110. Data are in red, the data passing the filter criteria in blue and the fit in the blue data is in green.

### 6.3.3 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 19 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.

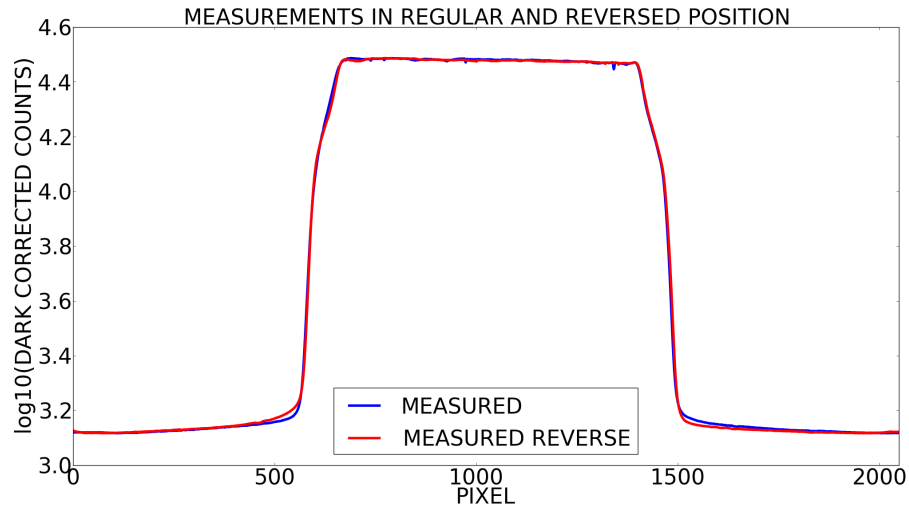


Figure 19: Logarithm of dark corrected counts as a function of the pixel number for measurements, where only the central part of the detector (pixels 600 to 1500) was illuminated and the left and right side blocked. Blue line is for the detector in regular orientation. Red line shows the same illumination 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:

$$L1_i = L1_i^* - \Delta LAT_i \quad (70)$$

$\Delta LAT_i$  is the latency correction vector. It is determined in a recursive way as shown in equation 71.

$$\begin{aligned} \Delta LAT_1 &= 0 \\ \Delta LAT_{i+1} &= \Delta LAT_i \cdot (1 - c_{DECAY}) + L1_i^* \cdot c_{GAIN} \end{aligned} \quad (71)$$

$c_{DECAY}$  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 second one, etc. For Pandora 106, these constants were determined to  $c_{DECAY}=6.3e-3$  and  $c_{GAIN}=1.8e-5$ . Figure 20 is a zoom of figure 19 in linear scale. The black line are the latency corrected counts.

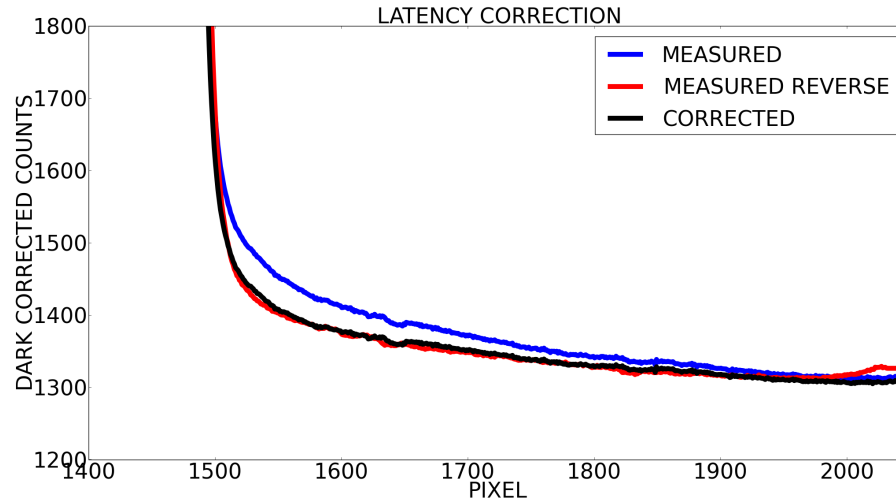


Figure 20: Zoom of figure 19 in linear scale. Blue line are the regular measurements, black line the regular measurements with the latency correction applied.

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  $c_{\text{DECAY}}$  and  $c_{\text{GAIN}}$  is extremely risky, difficult and time-consuming as the detector has to be removed from the spectrometer.

### 6.3.4 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 21). 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  $\pm 1\%$ . 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  $\pm 1\%$  to  $\pm 0.25\%$  (figure 21). During radiometric calibration we only determine the PRNU for the binned pixels.

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

$$L1_i = \frac{L1_i^*}{\text{PRNU}_i} \quad (72)$$

$\text{PRNU}_i$  is the  $1 + \text{PRNU}/100$  for pixel  $i$ .

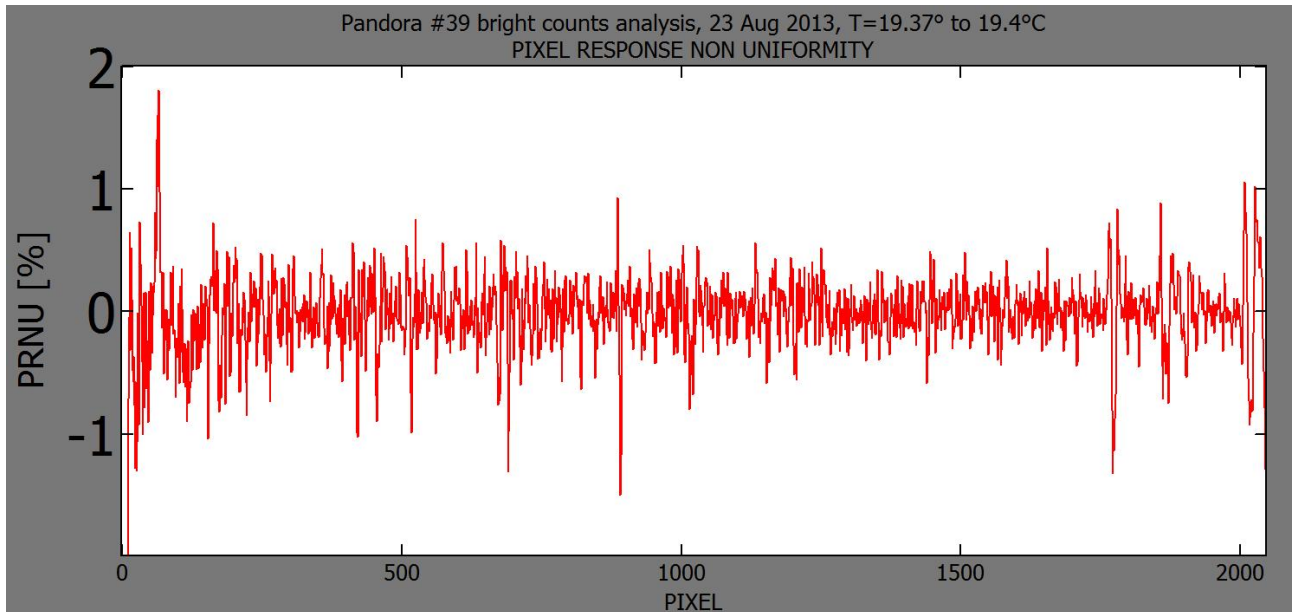


Figure 21: PRNU for Pandora 39 as a function of pixel. Note that the detector for this unit is binning 16 pixels at each scan, which reduces the "single pixel" PRNU by a factor of 4.

### 6.3.5 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 18 in section 6.3.2) 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:

$$L1_i = \frac{L1_i^*}{t - \Delta t} \quad (73)$$

$t$  is the nominal integration time and  $\Delta t$  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.

### 6.3.6 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:

$$L1_i = \frac{L1_i^*}{TC_i} \quad (74)$$

$TC_i$  is the temperature correction polynomial evaluated at pixel  $i$ .

### 6.3.7 Stray Light Correction

The different options for stray light correction are listed in table 21. 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  $L1_i$  are given by:

$$L1_i = L1_i^* - MEAN(L1_i^* \text{ for } \lambda_i < 290nm) \quad (75)$$

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 [51]. 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.

$$\vec{L1} = \mathbf{M} \cdot \vec{L1}^* \quad (76)$$

$\vec{L1}$  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 75 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.

### 6.3.8 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  $[W/m^2/nm]$  for direct sun or direct moon data and to  $[W/m^2/nm/sr]$  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 22 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.

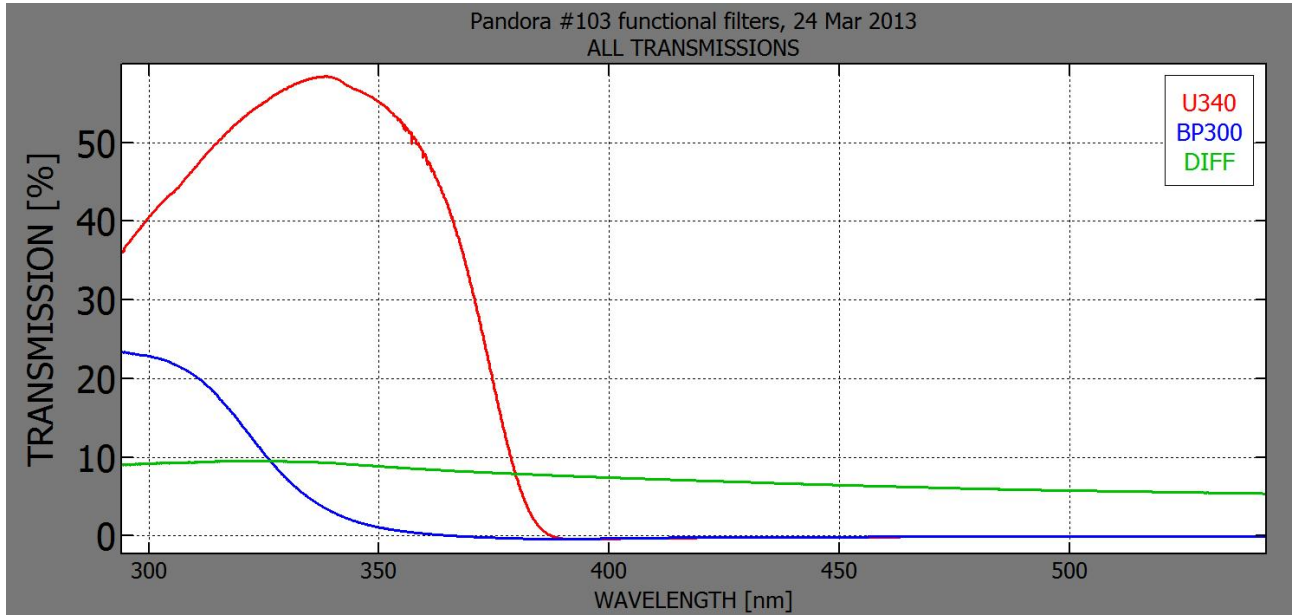


Figure 22: Measured transmissions for filters in Pandora 103 as a function for wavelength. U340 is a colored glass bandpass filter with peak transmission at 340 nm (red line). BP300 is an interference bandpass filter with peak transmission at 300 nm. DIFF is a ground quartz diffuser. Note that the fact 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 6.3.7).

Figure 23 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:

$$L1_i = \frac{L1_i^*}{\text{SENS}_i} \quad (77)$$

$\text{SENS}_i$  is the sensitivity (or calibration function) of the instrument at pixel  $i$ .

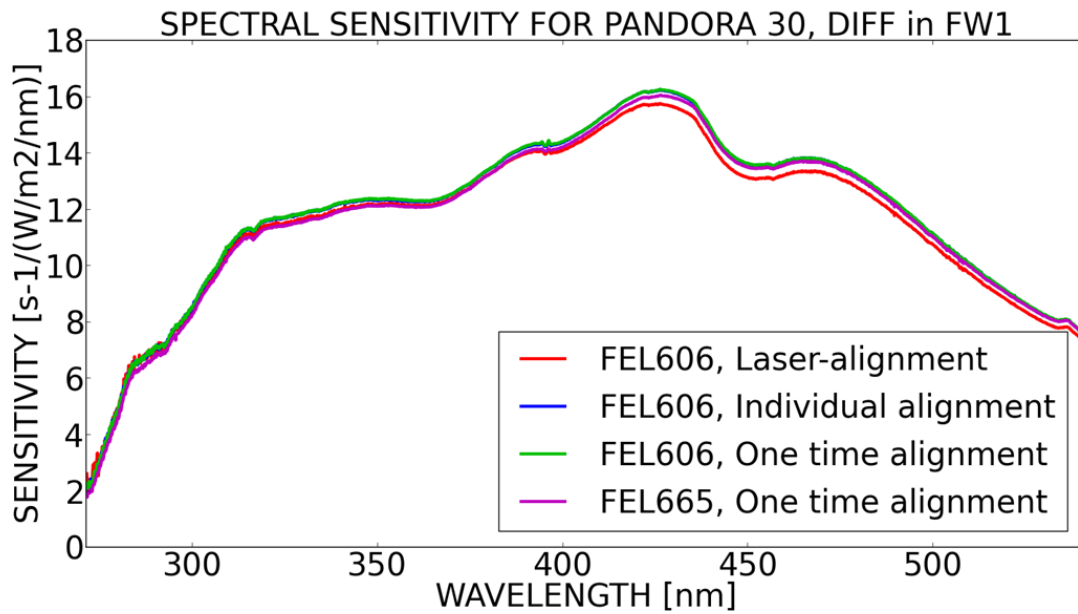


Figure 23: Absolute sensitivity of Pandora 30 for direct sun observations (i.e. with a diffuser in the filterwheels). Different lines refer to different alignment methods and different calibration lamps.

### 6.3.9 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 compared to a theoretical high resolution extraterrestrial spectrum [6] and shifted to the nominal wavelength grid.

Note that this wavelength change retrieval based on the measured spectra is less accurate than the one done during the spectral fitting (see section 6.4), since it does not properly take into account the instrument's sensitivity and the influence of strong and moderately strong absorbers. This is especially true for the visible region above 600 nm, where etaloning and strong absorbers such as water vapor and molecular oxygen are acting. Therefore the wavelength change retrieved from the spectra and from the spectral fitting may differ quite a lot.

## 6.4 L2Fit Algorithm - Spectral Fitting

The L2Fit data are the result of applying the Blick spectral fitting algorithm (BlickSFA) on the L1 data, which is described in this section.

### 6.4.1 Lambert-Beer's law

BlickSFA is based on Lambert-Beer's law.

$$F(\lambda) = F_0(\lambda) \cdot \exp \left( - \sum_{j=1}^{n_{EX}} \tau_{Sj}(\lambda) \right) \quad (78)$$

$\lambda$	Wavelength
$F_0(\lambda)$	Spectrum at wavelength $\lambda$ reaching the top of the atmosphere; that is the "Extraterrestrial spectrum" adjusted for the Sun-Earth distance
$F(\lambda)$	Spectrum at wavelength $\lambda$ reaching the instrument's entrance window
$n_{EX}$	Number of extinction processes in the atmosphere
$\tau_{Sj}(\lambda)$	Slant optical depth at wavelength $\lambda$ for extinction process $j$

The slant optical depth  $\tau_{Sj}(\lambda)$  is given by:

$$\begin{aligned} \tau_{Sj}(\lambda) &= qs_j^*(\lambda) \cdot \sigma_j(\lambda, T_j) \\ &= qs_j(\lambda) \cdot \tau_{STDj}(\lambda, T_j) \\ &= m_j(\lambda) \cdot q_j \cdot \tau_{STDj}(\lambda, T_j) \end{aligned} \quad (79)$$

$qs_j^*(\lambda)$	Absolute slant column amount for extinction process $j$ at wavelength $\lambda$ (units e.g. molecules per $cm^2$ )
$T_j$	Effective temperature of extinction process $j$ (see equation 3)
$\sigma_j(\lambda, T_j)$	Cross section for extinction process $j$ at wavelength $\lambda$ and effective temperature $T_j$ (units e.g. $cm^2$ per molecule)
$\tau_{STDj}(\lambda, T_j)$	"Standard vertical optical depth" for extinction process $j$ at wavelength $\lambda$ (no dimension)
$qs_j(\lambda)$	Relative slant column amount for extinction process $j$ at wavelength $\lambda$ (no dimension)
$m_j(\lambda)$	AMF (or optical mass) for extinction process $j$ at wavelength (no dimension) $\lambda$
$q_j$	Relative vertical column amount extinction process $j$ (no dimension)

For the standard vertical optical depth  $\tau_{STDj}(\lambda, T_j)$ , BlickSFA uses the settings as listed in table 20. Note that introducing  $\tau_{STDj}$  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  $\tau_{STDj}$  would not change the results, as long as they are in a similar order of magnitude.

### 6.4.2 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  $F(\lambda)$  with the slit function  $S_i(\lambda)$  at the center wavelength  $\lambda_i$  of the pixel.

$$L1_i = F_i = \int_{\Delta\lambda_i} F(\lambda) \cdot S_i(\lambda_i - \lambda) \cdot d\lambda \quad (80)$$

$\Delta\lambda_i$  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 78 yields:

$$F_i = \int_{\Delta\lambda_i} F_0(\lambda) \cdot \exp\left(-\sum_{j=1}^{n_{EX}} \tau_{Sj}(\lambda)\right) \cdot S_i(\lambda_i - \lambda) \cdot d\lambda \quad (81)$$

Equation 81 is the fundamental equation for another type of trace gas retrieval algorithm, often called "Direct fitting algorithm". In such algorithm all unknowns in equation 81 (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 practical for near real time data processing. Therefore the Blick Software Suite uses the following approximation of equation 81:

$$F_i = F_{0i} \cdot \exp\left(-\sum_{j=1}^{n_{EX}} \tau_{Sji}\right) \quad (82)$$

$F_0(\lambda)$  is the convoluted top-of-atmosphere spectrum given by equation 83 and  $\tau_{Sji}$  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.

$$F_{0i} = \int_{\Delta\lambda_i} F_0(\lambda) \cdot S_i(\lambda_i - \lambda) \cdot d\lambda \quad (83)$$

### 6.4.3 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  $\lambda_i$ ,  $\tau_{Sji}$ , at different relative slant columns  $qs_j$ , .

$$\tau_{Sji}(\lambda_i, qs_j) = -\ln \left[ \frac{\int_{\Delta\lambda} F_0(\lambda) \cdot \exp\left(-qs_j \cdot \tau_{STDj}(\lambda, T_j)\right) \cdot S_i(\lambda_i - \lambda) \cdot d\lambda}{\int_{\Delta\lambda} F_0(\lambda) \cdot S_i(\lambda_i - \lambda) \cdot d\lambda} \right] \quad (84)$$

All variables are as in equations 79 and 81. Equation 84 is calculated for  $qs_j$  values ranging from 1 to 9.

The second step consists in expressing the  $\tau_{Sji}$  as a function of  $qs_j$  using so-called OD-fitting parameters  $A_{ji}$ ,  $B_{ji}$  and  $C_{ji}$ .

$$\begin{aligned} \tau_{Sji} &= A_j(\lambda_i, T_j) \cdot qs_j^{1+B_j(\lambda_i, T_j)+C_j(\lambda_i, T_j) \cdot \ln(qs_j)} \\ &= A_{ji} \cdot qs_j^{1+B_{ji}+C_{ji} \cdot \ln(qs_j)} \end{aligned} \quad (85)$$

Equation 85 is a more general approach than what is usually used in classical Differential Optical Absorption Spectroscopy (DOAS) [26], 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 $\tau_{sji}(\lambda_i, q_{sj}=1)$ from equation 84 is used as an approximation of $\tau_{sji}$ . 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 $\tau_{sj}(\lambda_i, q_{sj})$ calculated at $q_{sj}$ 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 $\ln[\tau_{sj}(\lambda_i, q_{sj})]$ calculated at $q_{sj}$ ranging from 1 to 9 as a function of $\ln[q_{sj}]$ . For this method OD-fitting parameter B differs from zero and C is zero.
OD Fitting Method 3	A quadratic fit is done for $\ln[\tau_{sj}(\lambda_i, q_{sj})]$ calculated at $q_{sj}$ ranging from 1 to 9 as a function of $\ln[q_{sj}]$ . 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 [36]. Method 3 is an extension of method 2 as a novel approach of BlickSFA.

The different OD-fitting methods are illustrated in figure 24. 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.

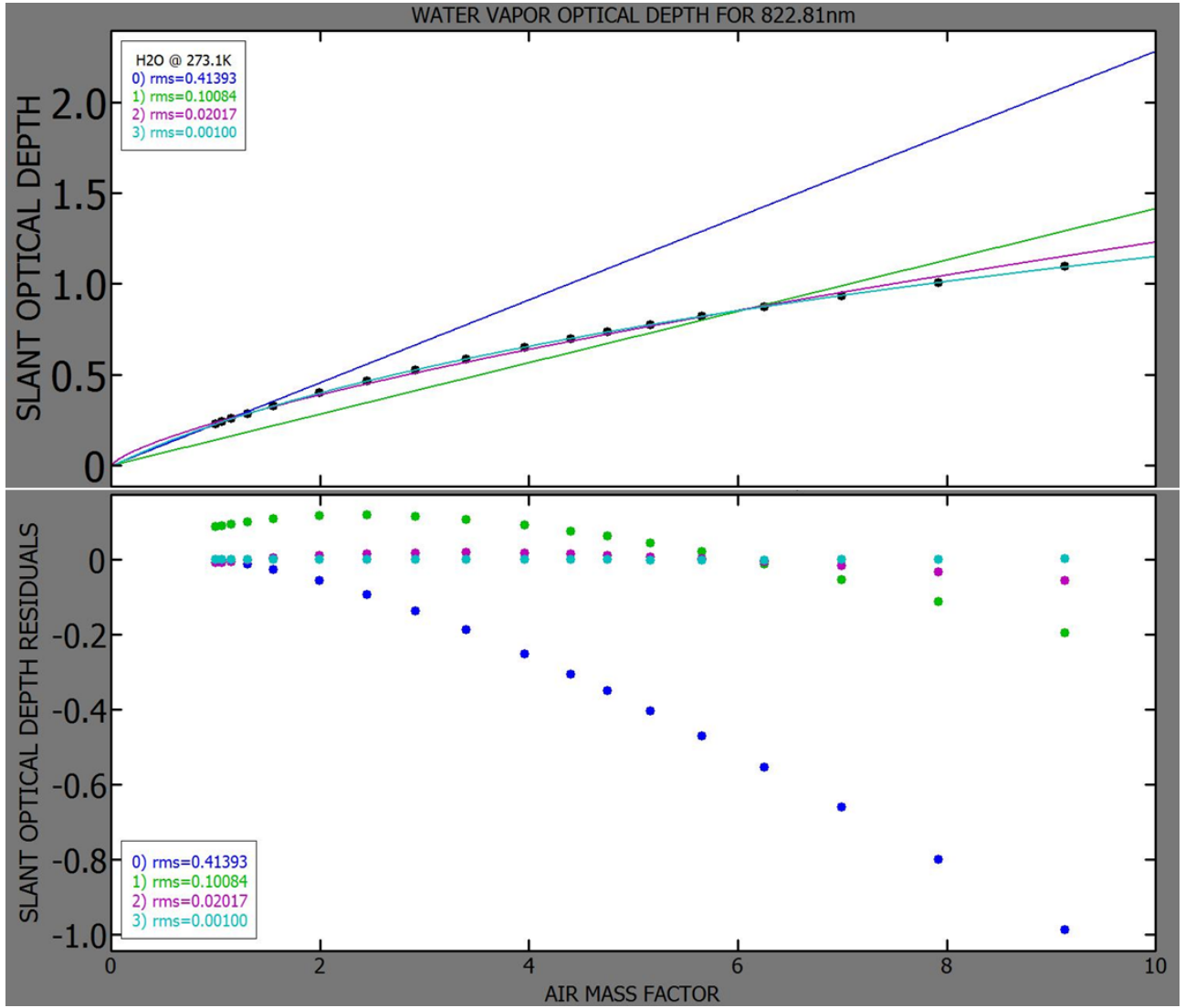


Figure 24: Top: Slant optical depth as a function of the AMF for a vertical column amount of 1 cm precipitable water calculated for AMFs from 1 to 9.3 (black dots) at a strong water vapor line (822.81 nm). Colored lines are different fits in the black dots using 1 (dark blue and green), 2 (magenta) or 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 85 are in general a function of the effective gas temperature  $T_j$ . The BlickSFA allows a temperature dependence up to order 2.

$$A_{ji} = A_{jCi} + A_{jLi} \cdot \frac{T_j - T_{jREF}}{T_{SCALE}} + A_{jQi} \cdot \left( \frac{T_j - T_{jREF}}{T_{SCALE}} \right)^2 \quad (86)$$

$A_{jCi}$ ,  $A_{jLi}$  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 25 and  $T_{SCALE}$  is a temperature scale factor given in the ICF (usually 50 K). The same equation 86 is used for OD-fitting parameters B and C.

## 6.4.4 Basic Fitting Equation

Taking the logarithm of equation 82 and rearranging we obtain:

$$\ln F_{0i} - \ln F_i = \sum_{j=1}^{n_{EX}} \tau_{Sji} \quad (87)$$

The following extinction processes are included in the right side of the equation:

- Molecular absorption by gases (see table 20)
- Rayleigh and Raman scattering by air molecules
- Mie scattering and absorption by aerosols

In addition there are instrumental effects, which can alter equation 87:

- 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 23) 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 87 accordingly. Details to each term are given in the next section 6.4.5.

$$\ln F_{0i} - \ln (F_i + P_{OFFSi}) - \tau_{SFiXi} = \sum_{j=1}^{n_{GAS}} \tau_{Sji}(q_{Sj}, T_j) + \tau_{RINGi} \cdot q_{SRING} + P_{SMOi} + P_{RESCi} \quad (88)$$

i	Index for pixel inside the limits of the fitting window, i=1 to n; the center-wavelength of pixel i is $\lambda_i$
$F_{0i}$	Reference spectrum at pixel i used in the fitting (see table 24)
$F_i$	L1 data for pixel i
$P_{OFFSi}$	Offset polynomial evaluated at pixel i
$\tau_{SFiXi}$	"Known" slant optical depth at pixel i
j	Index for atmospheric absorber, j=1 to $n_{GAS}$
$\tau_{Sji}$	Slant optical depth of absorber j for slant column $q_{Sj}$ and effective temperature $T_j$ at pixel i (see section 6.4.3)
$q_{SRING}$	"Equivalent" slant column amount of the Ring effect
$\tau_{RINGi}$	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

## 6.4.5 Terms of Basic Fitting Equation

### $\tau_{\text{FIX}i}$

The "known" slant optical depth  $\tau_{\text{FIX}i}$  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  $\tau_{\text{SCAI}}$  for the given conditions is added to  $\tau_{\text{FIX}i}$ .  $\tau_{\text{SCAI}}$  is calculated by:

$$\tau_{\text{SCAI}} = \frac{p}{p_{\text{STAN}}} \cdot \tau_{\text{SCAI}} \quad (89)$$

$p$  is the estimated air pressure at the measurement site (calculated using the station altitude),  $p_{\text{STAN}}$  is the standard pressure (=1013.25hPa) and  $\tau_{\text{SCAI}}$  is the standard molecular optical depth for pixel  $i$ . BlickSFA uses molecular scattering cross sections based on the work of *Bodhaine et al.* [7] and *Owens* [23] for 1 standard atmosphere of dry air molecules ( $2.1533 \times 10^{25}$  molc/cm<sup>2</sup>) containing 400 ppm of CO<sub>2</sub>. The effective height (see equation 2) is estimated to  $h_{\text{SCAEFF}}=6.2$  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  $\tau_{\text{FIX}i}$ . Those values are taken from L2Fit data from other fitting setups, of which the numbers are listed in FSE "Fixed Numbers".

### $P_{\text{OFFS}i}$

The offset polynomial  $P_{\text{OFFS}i}$  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.

$$P_{\text{OFFS}i} = \bar{F} \cdot \sum_{k=0}^{\text{noffs}} P_{\text{OFFS}k} \cdot \lambda_i^k \quad (90)$$

$\bar{F}$  is the mean over the  $F_i$ , the  $p_{\text{OFFS}k}$  are the coefficients of the offset polynomial and the  $\lambda_i$  are the scaled wavelength-centers for each pixel  $i$  (scaling with equation 4 and  $x_{\text{MIN}}$  and  $x_{\text{MAX}}$  being the minimum and maximum nominal wavelength of the instrument's total wavelength range).

### $\tau_{\text{RING}i}$

If FSE "Ring" is set to "YES", the Ring spectrum [13] is also fitted by the BlickSFA. The standard vertical optical depth of the Ring effect  $\tau_{\text{RING}i}$  is given in the ICF.

### $P_{\text{SMO}i}$

The purpose of the smooth-part polynomial  $P_{\text{SMO}i}$  is to "absorb" all smooth structures in equation 88, e.g. Rayleigh scattering if it has not been included in  $\tau_{\text{FIX}i}$ , or the instrument spectral sensitivity for the case the unit is not absolutely calibrated.

$$P_{\text{SMO}i} = \sum_{k=0}^{\text{nsmo}} P_{\text{SMO}k} \cdot \lambda_i^k \quad (91)$$

The  $p_{\text{SMO}k}$  are the coefficients of the smooth-part polynomial and the  $\lambda_i$  are as in equation 90.

### $P_{\text{RESC}i}$

The resolution change polynomial  $P_{\text{RESC}i}$  is given by

$$P_{\text{RESC}i} = \Delta_{\text{RESC}i} \cdot \sum_{k=0}^{\text{nresc}} P_{\text{RESC}k} \cdot \lambda_i^k \quad (92)$$

The  $p_{\text{RESC}k}$  are the coefficients of the resolution change polynomial and the  $\lambda_i$  are as in equation 90.  $\Delta_{\text{RESC}i}$  is the estimated change of equation 88 for a 1 % change in the instrument's resolution. It is calculated by

$$\Delta_{\text{RESC}i} = m_i \cdot \Delta\tau_{\text{TOT}i} - \Delta \ln F_{0i} \quad (93)$$

$\Delta \ln F_{0i}$  is the relative change (or absolute change of the logarithm) of  $F_{0i}$  for a 1 % increase in the instrument's resolution.

$$\Delta \ln F_0(\lambda_i) = \ln F_{0\text{RESC}}(\lambda_i) - \ln F_0(\lambda_i) \quad (94)$$

$\ln F_{0\text{RESC}}$  is the logarithm of the reference spectrum for a 1 % increased resolution and is given in the ICF.  $\Delta\tau_{\text{TOT}i}$  is the absolute change of the standard total optical depth for a 1 % increase in the instrument's resolution.

$$\Delta\tau_{\text{TOT}}(\lambda_i) = \tau_{\text{TOTRESC}}(\lambda_i) - \tau_{\text{TOT}}(\lambda_i) \quad (95)$$

$\tau_{\text{TOT}i}$  and  $\tau_{\text{TOTRESC}i}$  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.

## 6.4.6 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  $n_{\text{PAR}}$  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 23). BlickSFA requires  $n_{\text{PAR}} \leq n$ . The total number of output-parameters is given by:

$$n_{\text{PAR}} = n_{\text{GAS}} + n_{\text{TEMP}} + n_{\text{RING}} + (n_{\text{PAR}} + 1) + (n_{\text{OFFS}} + 1) + (n_{\text{WLC}} + 1) + (n_{\text{RESC}} + 1) \quad (96)$$

$n_{\text{GAS}}$	Number of absorbers, for which slant columns are fitted; this is the length of FSE "Fitted Gases"; $n_{\text{GAS}} \geq 0$
$n_{\text{TEMP}}$	Number of absorbers, for which effective gas-temperatures are fitted; this is the length of FSE "Fitted Temps"; $0 \leq n_{\text{TEMP}} \leq n_{\text{GAS}}$
$n_{\text{RING}}$	=1 if the Ring effect is fitted (FSE "Ring" equals YES); =0 if the Ring effect is NOT fitted (FSE "Ring" equals YES)
$n_{\text{SMO}}$	Order of the smooth-part polynomial; from FSE "npol"
$n_{\text{OFFS}}$	Order of the offset polynomial; from FSE "noffs"
$n_{\text{WLC}}$	Order of the wavelength change polynomial; from FSE "nwlc"
$n_{\text{RESC}}$	Order of the resolution change polynomial; from FSE "nresc"

A value of -1 for  $n_{\text{SMO}}$ ,  $n_{\text{OFFS}}$ ,  $n_{\text{WLC}}$  or  $n_{\text{RESC}}$  means the respective polynomial is not used in the fitting process. The residuals  $\xi_i$  are the differences between the left side and the right side of the basic fitting equation.

$$\xi_i = \ln F_{0i} - \ln (F_i + P_{\text{OFFS}i}) - \tau_{\text{SFIX}i} - \sum_{j=1}^{n_{\text{GAS}}} \tau_{\text{S}ji} - \tau_{\text{RING}i} \cdot q_{\text{S}RING} - P_{\text{SMO}i} - P_{\text{RESC}i} \quad (97)$$

The BlickSFA minimizes the residuals in a least squares sense.

$$\sum_{i=1}^n \left( \frac{\xi_i}{\sigma_i} \right)^2 \rightarrow \text{Minimum} \quad (98)$$

$\sigma_i$  is the noise in the measurements. If FSE "Uncertainty" is set to "NO", then all elements of  $\sigma_i$  are set to one, i.e. the noise is not included. Otherwise  $\sigma_i$  is a combination of the noise in the L1 measurements  $\sigma_{\text{MEAS}i}$  and in the reference  $\sigma_{0i}$ .

$$\sigma_i = \sqrt{\sigma_{\text{MEAS}i}^2 + \sigma_{0i}^2} \quad (99)$$

$\sigma_{\text{MEAS}i}$  is given in the L1 data and  $\sigma_{0i}$  may or may not be given depending on the chosen reference. E.g. if FSE "Reference" equals "ExtRef", then  $\sigma_{0i}$  is not given, while if FSE "Reference" equals "Meas" it is usually given. If FSE "Uncertainty" is set to "MEAS", then the measured (instrumental plus atmospheric) uncertainty from the L1 data is used, and if FSE "Uncertainty" is set to "INSTR" the instrumental uncertainty from the L1 data is used. Equation 99 assumes that the noise in the measurements and in the reference are uncorrelated, which is not always the case, e.g. in the trivial case where the measurements and the reference are the same spectra.

### 6.4.7 Linear Fitting

BlickSFA consists of a linear and a non-linear part. First, equation 88 is linearized and solved. Second, if requested and necessary, the results of the linear fitting are used as first guesses for a non-linear fitting process. The least squares fitting in the BlickSFA follows the description of *Press et al.* [28], chapter 15. In order to linearize equation 88, the "measurement term" is linearized for offset and wavelength change in a way as described by *Beirle et al.* [5] and shown in equation 100:

$$\ln [F_i (\lambda_i + P_{\text{WLC}i}) + P_{\text{OFFSi}}] = \ln F_i + P_{\text{WLC}i} \cdot F'_i / F_i + P_{\text{OFFSi}} / F_i \quad (100)$$

$P_{\text{WLC}i}$  is the wavelength change polynomial as defined in equation 15.  $F'_i$  is the derivative of  $F_i$  with wavelength, which is calculated using the reference spectrum. The fully linearized form of equation 88 is finally given by 101:

$$\begin{aligned} \ln F_{0i} - \ln F_i - \tau_{\text{FIX}i} = & \sum_{j=1}^{n_{\text{GAS}}} A_{jCi} \cdot q_{sj} + \sum_{j=1}^{n_{\text{TEMP}}} A_{jLi} \cdot \Delta T_j \cdot q_{sj} + \tau_{\text{RING}i} \cdot q_{\text{SRING}} \\ & + P_{\text{SMO}i} + P_{\text{RESC}i} + P_{\text{OFFSi}} / F_i + P_{\text{WLC}i} \cdot F'_i / F_i \end{aligned} \quad (101)$$

$A_{jCi}$  and  $A_{jLi}$  are the constant and linear terms in temperature of OD-fitting parameter A (see equation 86) and  $\Delta T_j$  is the scaled temperature difference to the reference temperature.

$$\Delta T_j = \frac{T_j - T_{j\text{REF}}}{T_{\text{SCALE}}} \quad (102)$$

All variables in 102 are as in equation 86. 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 101 can be written in matrix form

$$\vec{Y} = \mathbf{M} \cdot \vec{X} \quad (103)$$

$\vec{Y}$  is a  $(n,1)$ -vector. Its elements  $Y_i$  are given by

$$Y_i = \ln F_{0i} - \ln F_i - \tau_{\text{FIX}i} \quad (104)$$

$\vec{X}$  is a  $(n_{\text{PAR}},1)$ -vector

$$\vec{X} = [q_{S_1}, \dots, q_{S_{n_{GAS}}}, \Delta T_1 \cdot q_{S_1}, \dots, \Delta T_{n_{TEMP}} \cdot q_{S_{n_{TEMP}}}, q_{S_{RING}}, p_{SMO_1}, \dots, p_{SMO_{n_{SMO}}}, p_{RESC_1}, \dots, p_{RESC_{n_{RESC}}}, p_{OFFS_1}, \dots, p_{OFFS_{n_{OFFS}}}, p_{WLC_1}, \dots, p_{WLC_{n_{WLC}}}]^T \quad (105)$$

$\mathbf{M}$  is a  $(n, n_{PAR})$ -matrix. One row of  $\mathbf{M}$  is given by

$$\begin{aligned} \vec{M}_{i:} = & [A_{1Ci}, \dots, A_{n_{GAS}Ci}, \\ & A_{1Li}, \dots, A_{n_{TEMP}Li}, \\ & \tau_{RINGi}, 1, \lambda_i, \lambda_i^2, \dots, \lambda_i^{n_{SMO}}, \\ & \Delta_{RESCi}, \Delta_{RESCi} \cdot \lambda_i, \dots, \Delta_{RESCi} \cdot \lambda_i^{n_{RESC}}, \\ & \bar{F}/F_i, \bar{F}/F_i \cdot \lambda_i, \dots, \bar{F}/F_i \cdot \lambda_{n_{OFFS}}, \\ & F'_i/F_i, F'_i/F_i \cdot \lambda_i, \dots, F'_i/F_i \cdot \lambda_{n_{WLC}}] \end{aligned} \quad (106)$$

Each element of vector  $\vec{Y}$  and each column of matrix  $\mathbf{M}$  are divided by  $\sigma_i$  to include the uncertainty in the fitting.  $\mathbf{M}^*$  is called the design matrix of the fitting problem [28].

$$Y^*_{:i} = \frac{Y_i}{\sigma_i} \quad \vec{M}^*_{:i} = \frac{\vec{M}_{i:}}{\sigma_i} \quad (107)$$

BlickSFA solves for  $\vec{Y}$  in equation 108 using the `linalg.lstsq`-routine of Python's `numpy` module (see section 2.4).

$$\vec{Y}^* = \mathbf{M}^* \cdot \vec{X} \quad (108)$$

BlickSFA returns two versions of the root mean square of the spectral fitting residuals. `rms` (equation 109) is called "rms of unweighted spectral fitting residuals". `wrms` (equation 110) is called "Normalized rms of fitting residuals weighted with measured uncertainty" if the measured uncertainty is used for  $\sigma_i$  and "Normalized rms of fitting residuals weighted with instrumental uncertainty" if the instrumental uncertainty is used for  $\sigma_i$ .

$$rms = \sqrt{\frac{\sum_{i=1}^n \xi_i^2}{n - n_{FIT}}} \quad (109)$$

$$wrms = \sqrt{\frac{\sum_{i=1}^n \left(\frac{\xi_i}{\sigma_i}\right)^2}{\sum_{i=1}^n \left(\frac{1}{\sigma_i}\right)^2} \cdot \frac{n}{n - n_{FIT}}} \quad (110)$$

In both equations the residuals  $\xi_i$  are calculated inserting the output parameters retrieved in the spectral fitting process in equation 97 setting  $n_{FIT}=n_{PAR}$ .

In addition to `rms` and `wrms`, BlickSFA also calculates the expected rms based on the input uncertainties only, i.e. not using the residuals  $\xi_i$ . `rmsu` (equation 111) is called "Expected rms based on measured uncertainty" if the measured uncertainty is used for  $\sigma_i$  and "Expected rms based on instrumental uncertainty" if the instrumental uncertainty is used for  $\sigma_i$ . In the same way, `wrmsu` (equation 112) is called "Expected normalized

weighted rms based on measured uncertainty" if the measured uncertainty is used for  $\sigma_i$  and "Expected normalized weighted rms based on instrumental uncertainty" if the instrumental uncertainty is used for  $\sigma_i$ . They can be used to estimate of how much of the rms can be explained by instrumental and atmospheric noise in the data.

$$\text{rmsu} = \sqrt{\frac{\sum_{i=1}^n \sigma_i^2}{n - n_{\text{FIT}}}} \quad (111)$$

$$\text{wrmsu} = \sqrt{\frac{n}{\sum_{i=1}^n \left(\frac{1}{\sigma_i}\right)^2} \cdot \frac{n}{n - n_{\text{FIT}}}} \quad (112)$$

To obtain the effective gas temperature-difference  $\Delta T_j$ , BlickSFA divides the output parameter  $\Delta T_j \cdot q_{sj}$  by the corresponding output parameter  $q_{sj}$ .

BlickSFA also calculates the uncertainty  $\sigma_{Xj}$  for each element of  $X$ . The covariance matrix  $C$  is given as the inverse of the matrix product of  $\mathbf{M}^*$  transposed times  $\mathbf{M}^*$ .

$$\mathbf{C} = \text{inv}(\mathbf{M}^{*T} \cdot \mathbf{M}^*) \quad (113)$$

The main diagonal elements of  $C$  are the variances of the  $X_j$  and hence the uncertainty of  $X$  is given by:

$$\sigma_{Xj} = \sqrt{C_{jj}} \quad (114)$$

Equation 114 is only used for the case, where the measured uncertainty or the instrumental uncertainty are used for  $\sigma_{Xj}$ . In the case, where the fitting was done without using any input uncertainty, i.e.  $\mathbf{M}^*$  equals  $\mathbf{M}$ , we assume a Gaussian distribution of the input uncertainty and estimate the uncertainty of  $X$  by:

$$\sigma_{Xj}(\sigma_i = 1) = \text{rms} \cdot \sqrt{C_{jj}} \quad (115)$$

It must be noted that the  $\sigma_{Xj}$  are not the accuracy of the output parameters. They are the statistical uncertainty or noise of the output parameters based on the uncertainty or noise in the measurements.

If no non-linear fitting is needed ( $n_{\text{OFFS}}=-1$ ,  $n_{\text{WLC}}=-1$ , 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.

## 6.4.8 Non-linear Fitting

The non-linear fitting minimizes the residuals in equation 97 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. Equations 109 to 112 also apply to the non-linear fitting. While the linear fitting is always a very fast process (<0.1 s per fit), the non-linear fitting can take up to a couple of seconds per fit in the worst case.



## 6.5 L2 Algorithms

The Blick Software Suite includes some L2 algorithms, which produce atmospheric data such as total or tropospheric vertical column amounts and surface concentrations of trace gases. All L2 algorithms in the Blick Software Suite have several characteristics in common:

- They are not using any external data, i.e. only measurements from Pandora.
- Only L2Fit data from one single routine (i.e. one measurement sequence) are used. This means they can be applied in real time directly after the measurement sequence is finished.
- They are not performing radiative transfer calculations (RTC) and are consequently very fast.
- They do not require any special software license to run and the source code is provided with the standard installation of the Blick Software Suite.

We envision that, at a later stage, there will also be additional algorithms developed for the PGN. 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.

The existing L2 algorithms are described in the sections below.

### 6.5.1 Direct Algorithm

This algorithm is used for direct sun and direct moon measurements and produces total vertical column amounts. The L2Fit data return the slant column amount  $q_j$  for absorber  $j$ . To convert to the vertical column amount  $q_j$ , the slant columns are divided by the direct sun (or moon) AMF for extinction process  $j$ ,  $m_{DIRj}$ . It is estimated by

$$m_{DIRj}(ZA) = \sec \left( \arcsin \left[ \left( \frac{R}{R + h_{EFFj}} \right) \cdot \sin(ZA^*) \right] \right) \quad (116)$$

$R$  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 the extinction process  $j$  taken from table 20.

### 6.5.2 Five Angles O2O2-Ratio Algorithm

This algorithm has been developed in collaboration with Elena Spinei from NASA/Goddard Space Flight Center. It estimates the surface concentration (vmr) and the tropospheric column (qt) of a trace gas based on sky measurements at 5 pointing zenith angles (PZA) at a fixed azimuth. The 5 PZAs are 0°, 60°, 75°, one angle above 87° (the "largest angle") and one angle 1° smaller than the largest angle. The largest 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, the lowest 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°.

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 (assuming the largest angle is 89°) is 0°, 60°, 75°, 88°, 89°, 88°, 75°, 60°, 0°. The V-shape allows to interpolate all measurements to the central

measurement and therefore avoids systematic errors at larger SZAs. The central measurement is used as a reference in the spectral fitting. Besides the slant column amounts  $q_s$  of the trace gas, for which  $v_{mr}$  and  $q_t$  should be determined, the algorithm also needs the slant columns of the oxygen dimer  $q_{sO_4}$  for all the angles, since it is based on the assumption of similar AMFs for the trace gas and  $O_2O_2$ . Here we will use indices 0 to 4 for the angles, where index 0 corresponds to the largest PZA, 1 to the second largest PZA, 2 to  $PZA=75^\circ$ , 3 to  $60^\circ$  and 4 to  $0^\circ$ . Since the largest PZA is used as a reference,  $q_{s0}$  and  $q_{sO_40}$  equal 0 by definition. Here is a step-by-step description of the algorithm:

### Step 1: Extract Viewing Angles

In the case more than just the required 5 angles were measured, in this step the data are reduced to the 5 angles only.

### Step 2: Interpolate or extrapolate the $O_2O_2$ slant columns to the effective fitting wavelength

The goal of this step is to use  $O_2O_2$  slant columns in the algorithm, which are matching as good as possible the 'true'  $O_2O_2$  slant columns at the effective wavelength of the trace gas. If r-code entry 'f-codes' lists only one f-code for this algorithm, then the fitted  $O_2O_2$  slant columns are not altered. If exactly two f-codes are listed, then the unaltered fitted  $O_2O_2$  slant columns from the second f-code are used in the algorithm (see table 27). If more than two f-codes are listed, then the fitted  $O_2O_2$  slant columns are linearly inter- or extrapolated in wavelength to the effective fitting wavelength of the trace gas (see equation 17) using f-codes, 2, 3, etc. Note that the linear fit is also using the uncertainty of the  $O_2O_2$  slant columns.

### Step 3: Interpolate $q_s$ to central measurement

If V-shape was measured, the fitted slant columns at each PZA are interpolated in time to the central measurement. After this step there are 8 effective data inputs left, which are  $q_{s1}$  to  $q_{s4}$  and  $q_{sO_41}$  to  $q_{sO_44}$ .

### Step 4: Extrapolate to $PZA=90^\circ$

Since we actually would like to have the largest PZA at  $90^\circ$ , but in general cannot measure this, the following extrapolations is done to get the estimated differential slant column between  $PZA=90^\circ$  and  $PZA=0^\circ$   $q_{sh}$  in the case the largest viewing angle  $PZA_0$  was below  $90^\circ$ :

$$q_{sh} = q_{s1} \cdot \frac{PZA_0 - 90}{PZA_0 - PZA_1} - q_{s4} \quad (117)$$

This step is also done in the same way to obtain  $q_{shO_4}$ .

### Step 5: Modifications to account for the heterogeneous case

RTCs have shown that tropospheric AMFs of  $O_2O_2$  within the lowest 100 m are ranging between 0.5 and 3 when considering scenarios with different SZAs, low to high AODs, different aerosol phase functions etc. Therefore we are using an empirical correction on the  $O_2O_2$  slant columns to adjust for the case of not equal mixing conditions:

$$q_{shO_4c} = \frac{q_{shO_4}}{q_{sO_42} - q_{sO_44}} \cdot nO_4 \cdot heffO_4 \quad (118)$$

The estimation in equation 118 is sensitive to clouds, especially low clouds when multiple scattering within the cloud or up-down the cloud changes the photon path differently for the trace gas and  $O_2O_2$  due to difference in profiles.  $heffO_4$  in equation 118 is the estimated effective  $O_2O_2$  height calculated with equation 2.  $nO_4$  is the estimated  $O_2O_2$  surface concentration, calculated by:

$$nO_4 = \left( \frac{P_{surf} \cdot f_{O_2}}{T_{surf} \cdot k_{Boltz}} \right)^2 \quad (119)$$

$P_{\text{surf}}$  is the surface pressure,  $f_{\text{O}_2}$  the  $\text{O}_2$  mixing ratio,  $T_{\text{surf}}$  is the surface temperature and  $k_{\text{Boltz}}$  the Boltzmann constant. Blick Software Suite uses  $f_{\text{O}_2}=0.20946$  and calculates  $P_{\text{surf}}$ ,  $T_{\text{surf}}$  and  $\text{heffO}_4$  from a climatology [1] based on the season, latitude and height a.s.l. of the location. The values for sea level are shown in figure 25.

The same correction as in equation 118 is also applied to  $qs_{\text{O}_4}$ .

$$qs_{4\text{O}_4\text{c}} = \frac{qs_{\text{O}_4}}{qs_{\text{O}_4} - qs_{\text{O}_4}} \cdot n_{\text{O}_4} \cdot \text{heffO}_4 \quad (120)$$

### Step 6: Get the surface concentration

First four different estimations of the surface concentration are calculated, called  $\text{vmr}_1$  to  $\text{vmr}_4$ .

$$\begin{aligned} \text{vmr}_1 &= \frac{qs_4 \cdot P_{\text{surf}} \cdot f_{\text{O}_2}}{qs_{\text{O}_4} \cdot T_{\text{surf}} \cdot k_{\text{Boltz}}} \\ \text{vmr}_2 &= \frac{qsh \cdot P_{\text{surf}} \cdot f_{\text{O}_2}}{qsh_{\text{O}_4} \cdot T_{\text{surf}} \cdot k_{\text{Boltz}}} \\ \text{vmr}_3 &= \frac{-qs_4 \cdot P_{\text{surf}} \cdot f_{\text{O}_2}}{qs_{4\text{O}_4\text{c}} \cdot T_{\text{surf}} \cdot k_{\text{Boltz}}} \\ \text{vmr}_4 &= \frac{qsh \cdot P_{\text{surf}} \cdot f_{\text{O}_2}}{qsh_{\text{O}_4\text{c}} \cdot T_{\text{surf}} \cdot k_{\text{Boltz}}} \end{aligned} \quad (121)$$

For the final best guess of the surface concentration the largest value among  $\text{vmr}_1$  to  $\text{vmr}_4$  is picked. The index of the largest  $\text{vmr}$  (between 1 and 4) is called the "surface concentration index". As a rough estimation of the uncertainty  $u_{\text{vmr}}$  of the final  $\text{vmr}$ , the algorithm uses simply the standard deviation over the 4 values  $\text{vmr}_1$  to  $\text{vmr}_4$ . Note that this is a different approach for the uncertainty than used in all other uncertainties, since it is not the propagated instrumental and atmospheric noise. Finally the so-called "heterogeneity flag" is calculated. This flag equals 0, if the ratio  $\text{vmr}/u_{\text{vmr}}$  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.

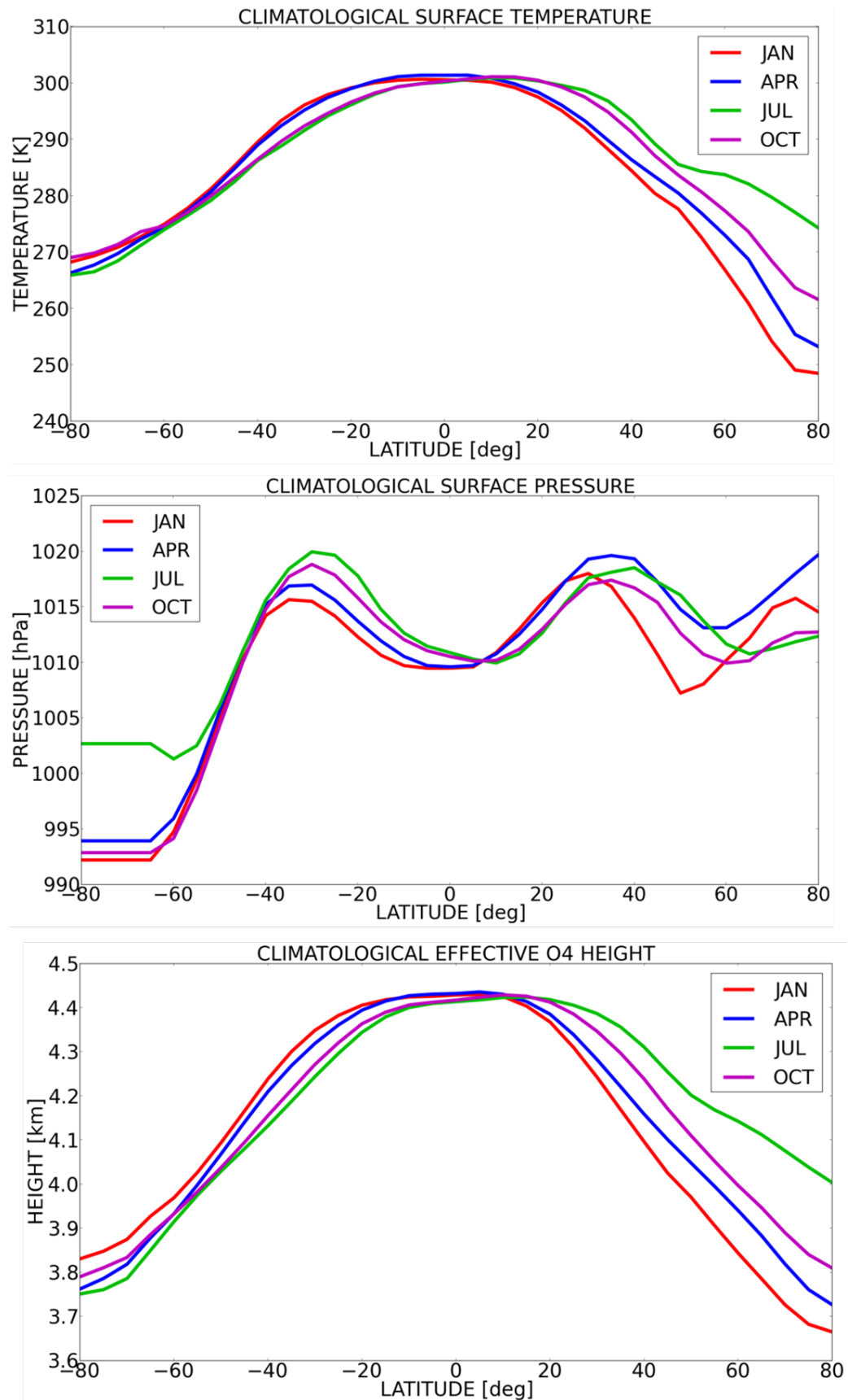


Figure 25: Climatological [1] surface temperature (top), surface pressure (middle) and effective  $O_2O_2$  height (bottom) at sea level\* for the months of January, April, July and October as a function of latitude. \*For latitudes below 60 deg South the values are actually not at sea level, but at the average height of the surface in Antarctica.

### Step 7: Get air mass factors for the tropospheric column

For the tropospheric column amount  $q_t$  the important VZAs are  $60^\circ$  and  $75^\circ$ . The best guess AMF results from a modified geometrical approach. Two more AMFs, AMF1 and AMF2 are also calculated to get an uncertainty estimation of  $q_t$ .

$$\begin{aligned} \text{AMF} &= \frac{q_{sO_4_2} - q_{sO_4_3}}{n_{O_4} \cdot \text{heff}_{O_4}} + 2 \\ \text{AMF1} &= \frac{q_{sO_4_2} - q_{sO_4_3}}{n_{O_4} \cdot \text{heff}_{O_4}} + \frac{q_{s_2} - q_{s_4}}{(q_{s_3} - q_{s_4}) \cdot 2} \\ \text{AMF2} &= 1 \end{aligned} \quad (122)$$

### Step 8: Get the tropospheric column

Three different estimations of the tropospheric column are calculated, called  $q_t$ ,  $q_{t1}$  and  $q_{t2}$ .

$$\begin{aligned} q_t &= \frac{q_{s_2} - q_{s_4}}{\text{AMF}} \\ q_{t1} &= \frac{q_{s_2} - q_{s_4}}{\text{AMF1}} \\ q_{t2} &= \frac{q_{s_3} - q_{s_4}}{\text{AMF2}} \end{aligned} \quad (123)$$

For the final best guess of the tropospheric columns  $q_t$  is taken. As a rough estimation of the uncertainty  $u_{q_t}$  of the final  $q_t$ , the algorithm uses simply the standard deviation over the 3 values  $q_t$ ,  $q_{t1}$  and  $q_{t2}$ . As for the surface concentration this is a different approach for the uncertainty than used in all other uncertainties, since it is not the propagated instrumental and atmospheric noise.

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