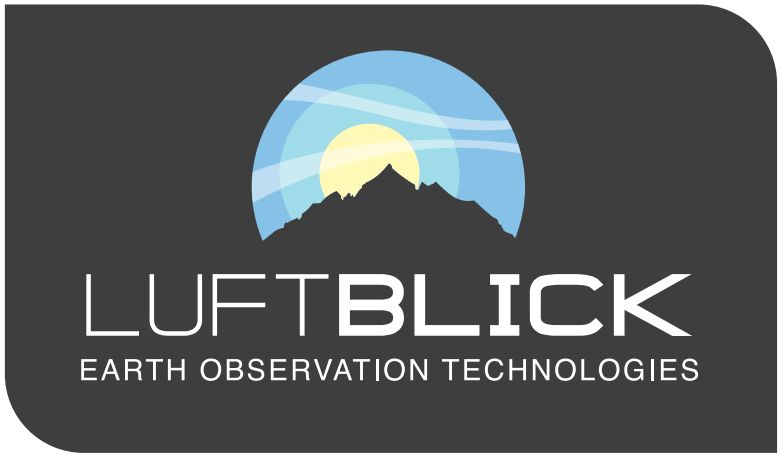

LuftBlick Report 2019003

Fiducial Reference Measurements for Air Quality

Calibration Procedures Document

Version 3, 28th Jun 2020

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Document Change Record

Issue	Date	Section	Observations
1	30th Jun 2019	All	First version
2	31st Dec 2019	Minor changes, added summary section	First version 2
3	28th Jun 2020	Changes in section 5	First version 3

Acronyms and Abbreviations

NO_2	Nitrogene Dioxide
AMF	Air Mass Factor
BlickM	Blick Monitoring Software
CPD	Calibration Procedures Document
ESA	European Space Agency
EVDC	ESA Atmospheric Validation Data Centre
FRM4AQ	Fiducial Reference Measurements for Air Quality
GSFC	Goddard Space Flight Center
ICF	Instrument calibration file
IOF	Instrument Operation File
NASA	National Aeronautics and Space Administration
O3	Ozone
Pandora	Pandora spectrometer system
PGN	Pandonia Global Network
QA	Quality Assurance
QC	Quality Control
SciGlob	SciGlob LLC, Elkridge, Maryland, USA
SOP	Standard Operating Procedure

1 Introduction

This Calibration Procedures Document (CPD) is deliverable 2 (D2) of the ESA project "Fiducial Reference Measurements for Air Quality" (FRM4AQ) [1, 2]. It describes the currently applied procedures performed to calibrate a Pandora spectrometer system (Pandora) within the Pandonia Global Network (PGN).

This document describes what calibration procedures are done and in what order, but does not describe the physical understanding of each step. For the "Why?" we refer to *Cede* [4]. The calibration procedure is split into two parts:

- Laboratory calibration, section 2: these are the calibration steps taken before the instrument is deployed at its final location. Note that any "hardware" calibration steps such as ensuring proper alignment of all optical elements or putting the lens in focus, are not described here. Hence we assume the instrument is already in its final configuration.
- Field calibration, section 3: these are the calibration steps using data from the instrument at its final location. It includes quality assurance/quality control (QA/QC).

Section 5 provides an outlook about changes in the procedure and the organization of all calibration activities.

1.1 Applicable Documents

[1] Fiducial Reference Measurements for Air Quality [Proposal], LuftBlick Proposal 201805DEV, Issue 1, 2018.

[2] Fiducial Reference Measurements for Air Quality [Statemet of Work], ESA ESA-EOPG-MOM-SOW-0046, Issue 1, Revision 5, 2018.

1.2 Reference Documents

[3] A. Cede. *Manual for Blick Software Suite 1.3, Version 7*, 2017. URL `http://pandonia.net/media/documents/BlickSoftwareSuite_Manual_v7.pdf`.

[4] A. Cede. ESA Ground-Based Air-Quality Spectrometer Validation Network and Uncertainties Study, LuftBlick Report 2018005: Final Pandonia report, 2018.

2 Laboratory Calibration

Before a Pandora is installed at its final measurement location, it undergoes the following actions:

- Installation and initial testing of its performance in the laboratory.
- Measurements in the laboratory, section 2.1.
- Analysis of the laboratory measurements, section 2.2
- Updating the instrument operation file (IOF) and clearing the instrument for shipping to its final destination.

2.1 Laboratory measurements

Laboratory measurements can currently be done at three different locations:

- LuftBlick lab at Innsbruck, Austria
- NASA/GSFC lab at Geenbelt, Maryland, USA
- SciGlob lab at Elkridge, Maryland, USA

The laboratory protocols from LuftBlick are used in all labs to have homogeneous and high quality lab measurements. This section summarizes these steps. More details can be found in the laboratory documentation, which is listed in section 2.4.

The measurements in the laboratory always follow the same "routine sequences" (for meaning of routines see *Cede* [3]). This guarantees the same measurement procedure for all laboratories. E.g. for the dark characterization there is a routine called "L2". So the laboratory personnel has to execute this routine and always the same measurement sequence is performed for different instruments. These routines are existing for every single calibration step and are summarized here:

- L2: Dark measurements at different integration times. Measured at three different temperatures for the determination of the so-called dark map.
- L3: "Bright" measurements at different integration times for the determination of parameters such as non-linearity and pixel response non-uniformity.
- L4: Wavelength calibration for the determination of the dispersion and resolution; done at three different temperatures to account for the temperature dependence of the dispersion and the resolution. The measurements are done with different spectral lamps. The different laboratories are having different spectral lamps, but the most important, i.e. the strongest lamps with the most pronounced spectral lines for the wavelength range we are working with, e.g. a mercury lamp, are existing in every laboratory.
- L5: Straylight characterization, done with a different number of lasers. GSFC lab currently has the best equipped laboratory with six lasers below 540 nm, while LuftBlick currently has three. SciGlob has no laser so far, so instruments calibrated in this laboratory cannot have a straylight characterization.
- L6: Determination of the transmission of the neutral density attenuation filters.
- L7: Absolute radiometric calibration for the case a certificate for the lamp is given. If no certificate is given, the transmissions of the functional filters are determined with this measurement.
- LT: Bright measurements at different temperatures to characterize the radiometric temperature dependence.

2.2 Analysis of laboratory measurements

For the analysis of the measurements a semi-automated software, called BlickC is used. BlickC is built in a way, that the user can analyze each measurement from section 2.1. For some analysis steps no user input is required, but in several steps the software user has to select and adjust different parameters in order to describe the Pandora in the best way. All these parameters are already pre-selected in a reasonable way, but it is still the task of the user to refine the selection. To ensure that similar parameters are used for every instrument and also to detect outliers (i.e. an instrument with an unusual behaviour regarding a calibration step) we set up a standard operating procedure (SOP), where thresholds for the parameters are defined.

2.3 Update IOF and clear unit

Every IOF is called PandoraX_OF_vVdYYYYMMDD.txt, where X is the instrument number, V the version number and YYYYMMDD the operational validity starting date. A new version number is given, when entries in the IOF are changed, but the validity starting date stays the same. The validity date changes when the hardware of an instrument changes in a way, that the raw data is different. An operational validity date simply ends with the starting date of the next IOF.
If the analysis reveals no major problems, the IOF is updated with some parameters. These parameters ensure a proper ratio of dark and bright measurements, and that the instrument does not saturate. Because of that, we update the IOF as soon as possible after the calibration measurements, to ensure that an instrument in the field is operating with a perfect setup in order to have best possible measurements. So within this procedure, the IOF version is increased.
Further, the operational data products are compared to the reference instruments at this location. In Innsbruck this is e.g. Pandora 110. So if the data of an instrument does not agree with the reference instrument(s), the reason therefore is examined and if necessary re-calibrated and tested again until the data agrees with the reference.
Finally the instrument is cleared for being shipped to its final destination.

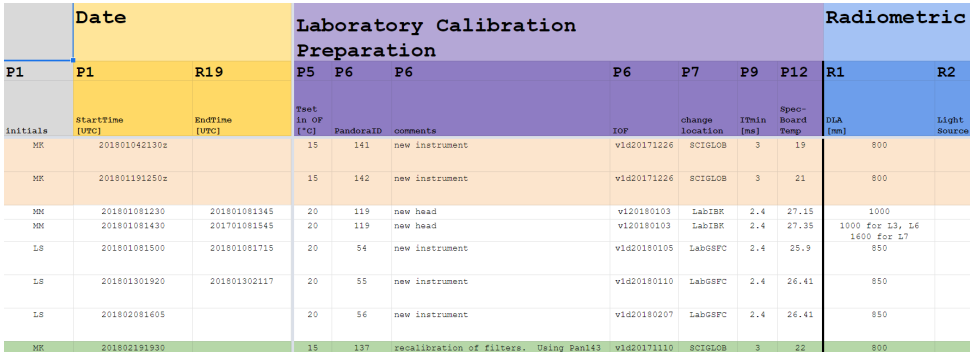
2.4 Laboratory Documentation

Measurement manual The guideline for the work in the laboratory is the Lab-Manual. Every calibration step, starting from setting up the instrument until uploading the data on the server, is described.

Laboratory Log To further have a proper documentation of the measurements, to detect possible instrumental errors and to have a reproduceable and traceable laboratory setup, we are using a Google sheet in which we document all the laboratory calibrations we are doing - the BlickLabLog, shown in figure 1. It goes hand in hand with the Lab-Manual, where every calibration step is explained in great detail. In the BlickLabLog, information such as the distance between the instrument and the lamp, the signal strength, the stability, the temperature and the lamp power is given.

The following information is written down in the lab log:

- Lab personnel.
- Date and time of the measurements.
- Pandora ID and IOF used.
- Temperature.
- Distance between the lamp and the instrument.
- Light source, its power and burning hours.
- Executed measurements.



	Date		Laboratory Calibration Preparation							Radiometric	
P1	P1	R19	P5	P6	P6	P6	P7	P9	P12	R1	R2
initials	StartTime [UTC]	EndTime [UTC]	Tset in OF [°C]	PandoraID	comments	IOF	change location	ITmin [ms]	Spec-Board Temp	DLA [nm]	Light Source
MK	201801042130z		15	141	new instrument	v1d20171226	SCIGLOB	3	19	800	
MK	201801191250z		15	142	new instrument	v1d20171226	SCIGLOB	3	21	800	
MM	201801081230	201801081345	20	119	new head	v120180103	LabIBK	2.4	27.15	1000	
MM	201801081430	201701081545	20	119	new head	v120180103	LabIBK	2.4	27.35	1000 for L3, L6 1600 for L7	
LS	201801081500	201801081715	20	54	new instrument	v1d20180105	LabGSFC	2.4	25.9	850	
LS	201801301920	201801302117	20	55	new instrument	v1d20180110	LabGSFC	2.4	26.41	850	
LS	201802081605		20	56	new instrument	v1d20180207	LabGSFC	2.4	26.41	850	
MK	201802191930		15	137	recalibration of filters. Using Pan143	v1d20171110	SCIGLOB	3	22	800	

Figure 1: Example of the BlickLabLog sheet, where all laboratory sessions are documented. In the upper line, one can see acronyms like P9. This always refers to a certain step in the Lab-Manual.

BlickM For every measurement done in the laboratory, a corresponding checkbox exists in the Blick Monitoring Software (BlickM). The lab personnel can tick off the measured routines. So as soon as measurements are finished, the data files are uploaded on the Google drive and entries are made in BlickM, indicating which measurements have been done. Note that BlickM - the new monitoring tool - is existing since May 2019. Before that date, all the communication regarding lab measurements has been done by E-mail. The people involved in the lab analysis (section 2.2) check BlickM on a regular basis. If the lab analysis reveals that the measurements are good, they are accepted. Otherwise they are rejected and have to

be re-done (unless a heardware problem is detected, in which case this needs to be fixed first).

In figure 2, a screenshot of BlickM regarding calibration entries is given. In this example, a L6 and L7 measurement has been made, but not been verified yet. If this is done, one can tick off the verified checkbox for these measurements. All actions are always given with a date and the lab personnel.

Standard Operating Procedure and analysis manual A very extended, technical manual describes all calibration steps and the parameters in very detail. In addition to the technical manual, there exists a user´s guideline. This was set up during the May 2019 workshop with LuftBlick and NASA and provides thresholds where possible to detect either bad instrumental behaviour or defective laboratory measurements.

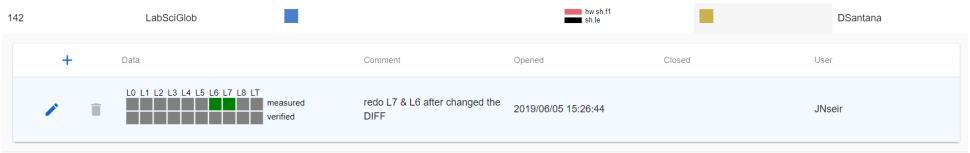


Figure 2: BlickM screenshot

ID	calibration starting date	calibration end date	Op file used for calibration analysis?	lab measurements used	data for MLE	name of final CF	name of new OF	session uploaded + sessions.txt + cslog	CoC for calibration analysis
#	[date]	[date]	[date, version]	[date(s)]	[date(s), amount of data points]	[date, version]	[date, version]		
124	20190415		20160530, v1	20160601-0602	20181004-1022	20181004, v1		☐	☐
144	20190423	20190425	20180302,v2	20180313;20180314;20180316	20190314-0416	20190314, v1	-	☑	☐
119	20190424	20190426	20180103, v1	20180103-0108	20180401-0430	20190801, v4	-	☑	☐
40	20180509		20170420, v1	20170420	20180129-20180331, ~4800 data	20170420, v1	-	☐	☑

Figure 3: Pending sheet

3 Field calibration

To apply a field calibration, the instrument has to be installed and aligned at the measurement location. Then, a few days of data during good atmospheric conditions (clear sky) need to be taken to be analyzed.
Field calibration analysis is also part of BlickC. The first step is to correct for a possible change in the dispersion (wavelength to pixel assignment), which usually happens when moving the instrument from the laboratory to the field, when translocating an instrument or when maintenance work is done, e.g. cleaning the fiber surface.
To obtain column amount of certain gases, e.g. NO_2, it is also necessary to take a reference spectrum which is done by Pandora own measurements [4]. The same sheets and manual as for the analysis of the laboratory measurements are used (section 2.4).

Instrument Calibration File and processing data with the instrument calibration file (ICF).
The ICF 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 on 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. This is e.g. if parameters in the calibration file change because of new measurements or different calibration strategies. The validity simply ends with the starting date of the next ICF. A new validity date is given if the hardware changes, so if there is a new IOF there will also be a new ICF. Another reason for a new validity date would be if we have good reasons that something has changed in the spectral response of the instrument. An example would be if the fiber is unplugged, cleaned and plugged in again. Actions like this are seen in the data and it can be accounted for them in a new field calibration.

4 Blick Operational Processing Progress

Within the Blick Operational Processing Progress, the dataset of an instrument undergoes the current QA/QC procedure, which involves a certain number of of calibrations and re-processing. If the whole procedure has been done for an instrument, then we believe that the best data possible are obtained and this should be the main condition for an instrument to be accepted as part of the PGN. Since on the one hand there are many new instruments coming into the network, on the other hand we have to prepare a lot of historical datasets, which is currently one of the main calibration tasks.

We do not give out data we did not check. That data users and other interested people can still have a look at the data, we have different levels of processing on our servers which are listed in the following sections. This should help to distinguish between quality assured and preliminary data.

4.1 Live processing

For a NO2 field calibration, described in section 3, we typically need a certain amount of data. When installing an instrument for testing, we normally do not have a sufficient amount of field data. Hence, we can just do a preliminary calibration. So when an instrument is in the field-testing period and we made a preliminary calibration file, we can process the data in the live folders and just the last week of data is in the live files. This is very helpful for a first look on the data and to detect errors in the hardware as well in the calibration, also if the field calibration has not been done in a way that the NO2 total column looks perfect. This is e.g. the case if the daily pattern has a strong AMF dependence and the data has an (inverse) U-shape. For O3 we do not need a field calibration and we can get it directly after the laboratory calibration and the analysis of this data. Since sometimes there is no time between the measurements in the lab and the installation in the field to evaluate the data, we might use old calibration files, coming from a previous laboratory calibration. Of course the final data does not give proper results then, but we still get a good idea of how the instrument is working. If the Pandora gets translocated to its final destination, the data still can be processed with this calibration for a first preliminary data product.
At the moment there are two live processing folders. One unofficial which is only for internal access, so that we have a grab on the instrument and data quality but we do not give out the data to avoid that data, which has not undergone the QA/QC procedures, is used for publications. This data should not be supervalued. On the other hand, on the official live processing webpage, the data is having good quality. But per definition they are also not quality assured. So it might be that instruments run out of calibration, e.g. if hardware repairings are done. In these cases we have to do a new field calibration to have good data on the official live processing again. On a long term basis it is of course the goal to have all instruments on the live visualisation with a up-to-date calibration, giving us the best possible data.

4.2 Initial processing

As explained in the previous section 4.1, the first calibration for an instrument is preliminary. If an instrument has collected a good amount of data, i.e. a few weeks or months, we can do a field calibration and continue with the calibration process of this Pandora. Therefore we are doing a NO2 field calibration and process the collected data in the initial processing folder. Then we can evaluate the data quality, e.g. compare to other instruments or detect jumps in the data. If e.g. there was hardware maintenance done on this instrument we have to do a second field calibration. This is a "working" folder in which we process the data with a certain calibration, check the data quality and start the whole process again if necessary. This is done until the data is quality assured and then we can make the data officially available by moving into other folders.

4.3 Backlog processing

If we checked the whole dataset for an instrument at one location, we can put it on the backlog processing, meaning that final L2 data are processed and officially available at the webpage. Per definition, the data is just quality assured until the last calibration file validity date (for detailed information regarding the validity date go to section 3).

4.4 Documentation

Pending sheet Apart from the SOP and the calibration analysis manual, a sheet, in which all the calibrations are listed, is existing. This ensures homogeneous calibrations and an open documentation for all people involved in the calibration activities. We upload all the final calibration results which include the calibration file and figures and a more detailed information about the calibration on the GDrive. The idea behind this is, that the workload can be split between all the people involved in the calibration activities.
The name pending is historical, in the meanwhile it is our working sheet for calibrations. There we write down the calibrations we are working on and highlight the finished ones. In the meanwhile, most of the important information is in the calibration file itself. But for internal work the pending sheet is very helpful. The following information is given in the pending sheet:

- Pandora ID.
- Calibration session.
- Laboratory or field calibration.
- Calibration starting and end date.
- IOF used.
- Lab measurements used.
- Data for field calibration used.
- Name of final IOF and ICF created.

In figure 3, a screenshot of the pending sheet is added where one can see, that Pandora 124 is still being worked on and Pandoras 144, 119 and 40 are finished.

Blick Operational Processing Progress Overview sheet The calibration, processing and data quality status is provided in the Blick Operational Processing Progress Overview (BOPPO) sheet. It gives us an overview about which calibrations have been done for an instrument and how the QA/QC status is. The most important information in it is:

- Pandora ID and location.
- Start and end date of operation.
- Information if all raw data files are on our servers. Especially important for old instruments which were measuring with the old software.
- Is the final data quality approved?
- Is the final data available on the server?
- Where is the processing done: is there live data? Data availability on the backlog? Is there data on EVDC?

To have fixed guidelines within this procedure, a step-by-step list how to complete the BOPPO sheet is existing.

Calibration file overview All the calibration file validity dates are listed in an extra sheet which contains information about when the reference spectra have been taken (information in section 3). Further it is given if the processing has already been done with this ICF.

5 Organization and Outlook

Currently, two LuftBlick people and two NASA people are working on the calibrations. Since four weeks, a calibration intensive period has started, meaning these four people are working around 80% of their time calibrating Pandoras. Because of that, for most instruments which are running operationally without hardware problems, high-quality data is available, meaning the data has been checked by LuftBlick in order to assure highest data quality. The remaining instruments are not yet calibrated since unforeseen problems happened, e.g. errors in the laboratory calibrations. The instruments which are having overlap with TROPOMI data are having second highest priority and within the next quarter these instruments will likely all be calibrated. This means, by the end of next quarter we expect on one side to have all operational instruments being calibrated and on the other side, all campaign/historic datasets having overlap with TROPOMI, will be calibrated as well.
This allows us to monitor the instruments on a weekly basis and to detect errors in the data very fast. This is a very good addition to the network operation since we know that an instrument might be running fine from an operational point of view but in the data we see unexpected issues.
Regarding the calibration procedures, no big changes are expected in the near future except changes in the calibration guidelines, which are more related to the New Algorithm & Product Development Plan, being outlined in D11. The Standard Operating Procedure will further be refined so that all calibration steps have clear thresholds if possible.
Further, we are planning to implement some changes regarding the internal documentation and to make it better accessible for external people. One example would be to have a vizualized calibration file overview, which shows for all instruments the available calibration files and also some metadata. This makes the documentation more easy for us and better visible for users.