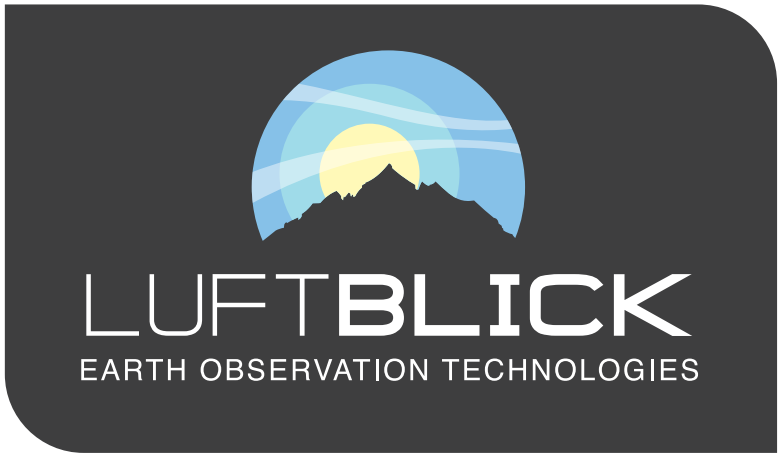


LuftBlick Report 2018013

Pandonia Operations

Calibration results document

Version 7.0, 29th Feb 2020

	Name	Company
prepared by	Moritz Müller	LuftBlick
	Martin Tiefengraber	LuftBlick
	Manuel Gebetsberger	LuftBlick

Contents

Document Change Record

Issue	Date	Section	Observations
0.1	26th Nov 2018	All	First draft version
0.2	29th Nov 2018	Summary	Adding software field calibration
2.0	30th Nov 2018	All	Minor changes, first version 2
3.0	28th Feb 2019	All	Minor changes, First version 3
4.0	27th May 2019	Calibration frequency	Minor changes, First version 4
5.0	27th Aug 2019	Calibration frequency	First version 5, updated figures and explanations, changes in section B.2
6.0	30th Nov 2019	Update of figures section, minor changes in section B	
7.0	29th Feb 2020	All	Update of figures and tables

Acronyms and Abbreviations

NO_2	Nitrogene dioxide
O_3	Ozone
BlickC	Blick Calibration Analysis Software
FCS	Field Calibration Set
FRM4AQ	Fiducial Reference Measurements for Air Quality
ILB	Instrument Log Book
mFCT	Mobile Field Calibration Tool
MLE	Modified Langley Extrapolation
MobRef	Mobile Reference Pandora
PGN	Pandonia Global Network
rms	Root Mean Square
WP	Work Package

1 Introduction

This report is deliverable 6 (D6) of the ESA project "Pandonia Operations" (POp) [4, 5] and covers the last quarter from 1st December to 29th February 2020. Further, it provides an overview about calibration activities of Pandora instruments from the beginning of 2018 and an outlook of calibration activities for the next quarter.

1.1 Applicable Documents

[1] CCN1 to ESA Ground-based Air-Quality Spectrometer Validation Network Uncertainties Study [Proposal, Proposal 201705A, Issue 2, 2017.

[2] CCN1 to ESA Ground-Based Air-Quality Spectrometer Validation Network and Uncertainties Study [Statement of Work], ESA-EOPG- MOM-SOW-1, Issue 1, Revision 1, 2017.

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

[4] Pandonia Operations [Proposal], LuftBlick Proposal 201804OPE, Issue 1, 2018.

[5] Pandonia Operations [Contract and Statement of Work], ESA Contract No. 4000124223/18/I-SBo, 2018.

[7] J. Herman, A. Cede, E. Spinei, G. Mount, M. Tzortziou, and N. Abuhassan. NO_2 column amounts from ground-based Pandora and MFDOAS spectrometers using the direct-sun DOAS technique: Intercomparisons and application to OMI validation. *Journal of Geophysical Research (Atmospheres)*, 114:D13307, July 2009. doi: 10.1029/2009JD011848.

1.2 Reference Documents

[7] J. Herman, A. Cede, E. Spinei, G. Mount, M. Tzortziou, and N. Abuhassan. NO_2 column amounts from ground-based Pandora and MFDOAS spectrometers using the direct-sun DOAS technique: Intercomparisons and application to OMI validation. *Journal of Geophysical Research (Atmospheres)*, 114:D13307, July 2009. doi: 10.1029/2009JD011848.

2 Calibration overview

2.1 Explanation

Explanation of the figures which are shown on the next two pages:

- **Lab** stands for laboratory, **Fld** for field, **Ana** for analysis, **Haw** for hardware and **Ref** for reference.
- **HawLab** means measurements in the laboratory in order to determine instrument specific characteristics, more information is given in section A.
- **AnaLab** is the analysis of the measurements taken in the laboratory (details are provided in section B).
- **AnaFld** is a field calibration where solar based L0 data and L1 data are used, for more information refer to section B.1.
- **HawFld** is a field calibration where measurements are done with the mobile field calibration tool mFCT, further information is given in section C.

- **RefFld** denotes the visit of the field calibration set FCS, for details go to section D.

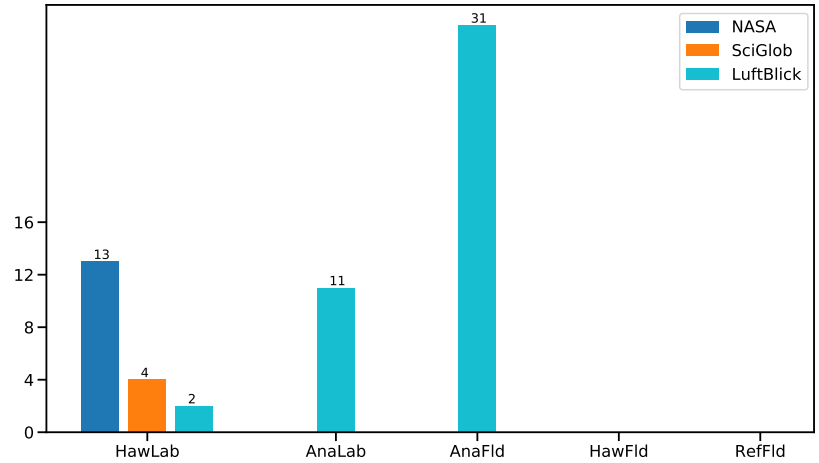
All Pandoras, official PGN and non-official PGN Pandora instruments are taken into account.
All finished laboratory measurements are listed in the figures, this means no sessions which had to be redone (explained further in A). For analysis sessions, only calibration sessions are listed which have been finished and data has been processed with these calibrations (B). Measurements with the mFCT and calibrations towards a planned mobile reference instrument are also shown for completeness.

2.2 Calibration frequency

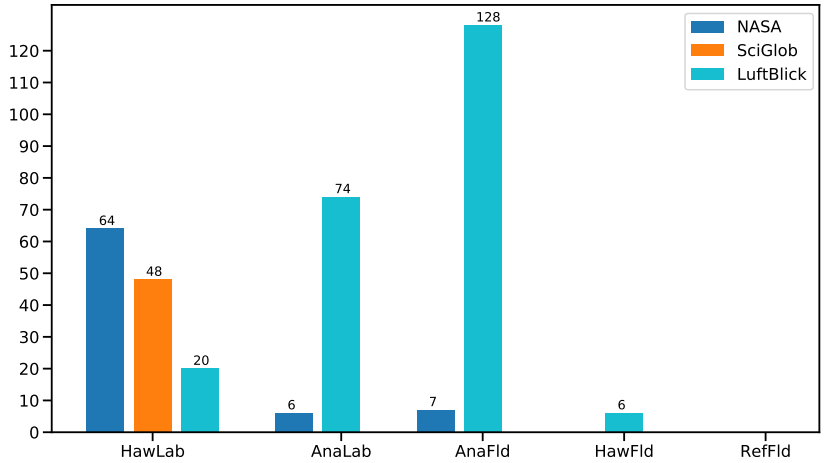
In the last quarter many laboratory calibrations have been done by NASA and a lot of lab analysis work and field calibrations by LuftBlick. The reason therefore is the data submission for several instruments with long timeseries. The NASA calibration team consists now of two people. LuftBlick is still giving support with regular telecons and private discussions. For some calibration steps, technical support is given and the final checks for calibrations, laboratory measurements and also the QA/QC is still done by LuftBlick. The reasons why there are no calibrations listed for NASA is mainly because the finished calibrations have not been checked by LuftBlick so far and the NASA group is currently working on some calibrations which are expected to be finished soon.

Figure 1: Calibration activities

(a) 1st November 2019 to 29th February 2020



(b) 1st January 2018 to 29th February 2020.



A detailed list of the calibration analysis work for the last quarter:

Instrument ID	Location	Nr. of AnaFld	Purpose
59, s1	MaunaLoaHI	2	Re-calibration of whole timeseries with newest software, QA the dataset to prepare for EVDC
101, s1	Izana	2	Re-calibration of whole timeseries with newest software, QA the dataset to prepare for EVDC
105, s1	Innsbruck	1	Calibration of testing period in Innsbruck, available on the live data folders
106, s1	Innsbruck	6	Re-calibration of whole timeseries with newest software, QA the dataset to prepare for EVDC
110, s1	Innsbruck	7	Re-calibration of whole timeseries with newest software, QA the dataset to prepare for EVDC
121, s1	Izana	4	Re-calibration of whole timeseries with newest software, QA the dataset to prepare for EVDC
123, s1	StonyPlain	1	Calibration to have the operational data product and QA to be able to submit data
124, s1	ComodoroRivadavia	4	Calibration to have the operational data product and QA to be able to submit data
125, s1	Cordoba	1	Calibration to have the operational data product and QA to be able to submit data
133, s1	Gobabeb	2	Calibration of whole dataset to QA a first dataset and have it on the operational processing
160, s1	Beijing	1	Initial calibration for live processing

2.3 Calibrations foreseen between 29th February and 31st May

There are two main calibration tasks in the next quarter:

1. Laboratory calibrations due to new instruments and hardware upgrades
2. Re-calibrations and QA of whole datasets due to several quality issues. This will be the main focus instead of starting calibrations of new instruments

Calibration activity	Expected number	Details
HawLab	> 6	initial calibrations by NASA & SciGlob, in Innsbruck it is planned to calibrate P111, P117 and P130 in the next quarter
AnaLab	> 10	re-calibrations of P65, P108, P111, P115, P140; analysis of P111, P117, P130 and NASA calibrations
AnaFld	> 10	field calibrations for the instruments mentioned in AnaLab
HawFld	-	-
RefFld	-	-

A Calibration measurements in the laboratory

The first step after the assembling of an instrument is the initial calibration in a laboratory. Currently, three institutions are doing laboratory measurements of the Pandora spectrometer system:

- SciGlob
- NASA
- LuftBlick.

Before shipping an instrument after the initial calibration, the measurements are checked by LuftBlick. Some of the measurements have to be redone since they are not of best possible quality. An example would be bad alignment of the calibration lamp or an unstable laboratory setup. Another case, in which laboratory measurements have to be redone, is the situation that an instrument does not work properly during the field testing period and repair work has to be done. Then, a new laboratory session is performed. The numbers in the overview figures in section 2 do not include laboratory sessions which had to be re-done because of the mentioned reasons. So, the number of laboratory measurements in the figures 1b and 1a can be lower than the actual number of laboratory sessions. One full calibration, without unpacking, installing and testing the instrument lasts about 2.5 days. This includes dark signal and wavelength calibration at three different temperatures in order to determine the temperature dependence of these two properties.

B Analysis of the laboratory measurements

Since the workshop in May 2019 in Innsbruck, when three NASA colleagues and one EPA colleague have been taught in the analysis of laboratory measurements, LuftBlick gets support with the calibration work. In the NASA team just two people are working on the analysis of laboratory data anymore. To keep the NASA and EPA colleagues informed about changes in the calibration procedures and to calibrate the instruments in a homogenous way, regular telecons are held and individual support is given by LuftBlick. Although the BlickC is a semi-automated software, still some experience is needed to operate it and to finally produce a proper calibration analysis. As always, in the overview figures in section 2, just analysis sessions are shown which have finally been pushed on the server and are being used for data processing. This means it is either under live processing or on EVDC.

B.1 Field calibration

A crucial part of the calibration procedure for Pandoras is the field calibration. Part of this step is to detect a possible change in the spectral dispersion (wavelength shift). Such changes might appear e.g. during the shipping of the instrument or if the fiber is unplugged. Furthermore, for NO_2, a reference is created from Pandoras own measurements and a MLE (explained in [7]), is done in the field calibration. For

this MLE we need some weeks or even months of field measurements, depending on the location and weather conditions.
So, new field calibrations are necessary for the following scenarios:

- Initial calibration of an instrument.
- If there is a jump in the data quality parameters (e.g. wrms or wavelength shift) which can e.g. come from repairing works or location changes.
- When the data quality exceeds certain thresholds which will be determined by the rMLE (explained in detail in B.2).

The amount of field calibrations is relatively high at the moment since we are re-calibrating and re-processing the datasets.

B.2 Data quality checks

In order to have continuous data quality checks, the final NO_2 and O_3 total column data is checked manually. Different data quality parameters and the total column amounts of NO_2 and O_3 are taken into account. Right now, these checks are mainly done offline. Whole timeseries are checked, i.e. the data of the whole time period when an instrument was operational (timeseries go up to now if it is still operational), is processed and checked manually. Therefore, data quality parameters are taken into account which give information about changes in the instrument. An example would be that the fiber gets unplugged, because it is impossible to plug it in again exactly the same way and the instrument is slightly different than it has been before. This can be seen in the wavelength shift and the rms. An information about the quality of the alignment is given in the uncertainty. Mainly these three parameters, together with the final data, are screened for magnitude and jumps. Sometimes it can be the case that these parameters are not enough and we take all information given in the data files and from the ILB to evaluate the data quality. If an instrument gets an initial calibration, we have an idea about the order of magnitude of these quality parameters at a certain location. If there is a significant jump in one of these parameters, we have already a good reason for a new calibration since something changed in the instrument. In combination with the information about the instrument performance from the ILB, this is used for detecting when a new calibration has to be done to have highest data quality possible. Most of it is currently done offline, but the live vizualisation is already used to detect these data jumps as well. The long term plan is to base the decision, of when a new calibration has to be done, on what is seen in the live vizualisation. With this tool, Pandoras, which need a new calibration can immediately be detected.
In the FRM4AQ project, WP4 (refer to [3]) this and other QA/QC procedures will be further studied and refined.

C Measurements with the mFCT

In WP 2 of the Pandonia CCN project [1] [2], a mFCT has been developed. The idea is to track changes of the instrument without the need to dismount and ship it to a laboratory. For the following scenarios, measurements with the mFCT will be done:

- After hardware changes and other repair work on the instrument.
- After actions on the instrument like unplugging the fiber or dismounting the instrument, in order to keep track of changes of the spectral response and to update the absolute calibration.
- After a long period of time in order to track changes and degradation of the hardware, e.g. of the filters.

D Calibration towards a reference instrument

The network strategy foresees a FCS which consists of the mFCT and a MobRef. For details refer to [4]. The acquisition of a MobRef through FRM4AQ is planned for 2019. Actions with the FCS will be done and listed in this report as soon as it is operationally utilized.