



LuftBlick Report 2018013

Pandonia Operations

Calibration results document

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Document Change Record

Issue	Date	Section	Observations
0.1	26 th Nov 2018	All	First draft version
0.2	29 th Nov 2018	Summary	Adding software field calibration
2.0	30 th Nov 2018	All	Minor changes, first version 2
3.0	28 th Feb 2019	All	Minor changes, First version 3
4.0	27 th May 2019	Calibration frequency	Minor changes, First version 4
5.0	27 th Aug 2019	Calibration frequency	First version 5, updated figures and explanations, changes in section B.2
6.0	30 th Nov 2019	Update of figures section, minor changes in section B	
7.0	28 th Feb 2020	All	Update of figures and tables
8.0	31 st May 2020	All	Update of figures and tables
9.0	31 st August 2020	All	Update of figures and tables
10.0	30 th November 2020	All	Update of figures and tables
11.0	28 th February 2021	All	Update of figures and tables
12.0	31 st May	All	Update of figures and tables
13.0	31 st August	All	Update of figures and tables
14.0	30 th November	All	Update of figures and tables

Issue	Date	Section	Observations
15.0	14 th January	All	Update of figures and tables
15.1	28 th February	All	Update of figures and tables
15.2	7 th March	D	Update of section D
16	30 th May 2022	1,2,2.2.3,A,B	Update of figures and tables and explanations how calibrations are counted

Acronyms and Abbreviations

NO ₂	Nitrogene dioxide
O ₃	Ozone
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 March 2022 to 24th May 2022. Further, it provides an overview about calibration activities of Pandora instruments from the beginning of 2018 and an outlook of calibration activities for the weeks until the end of this projects 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. NO₂ 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. NO₂ 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.

Laboratory measurements are counted as unique instruments if there have been any measurements (explained further in A). For analysis sessions, only calibration sessions are listed which have been finished and resulted in a calibration file (B). Measurements with the mFCT and calibrations towards a planned mobile reference instrument are also shown for completeness.

2.2 Calibration frequency

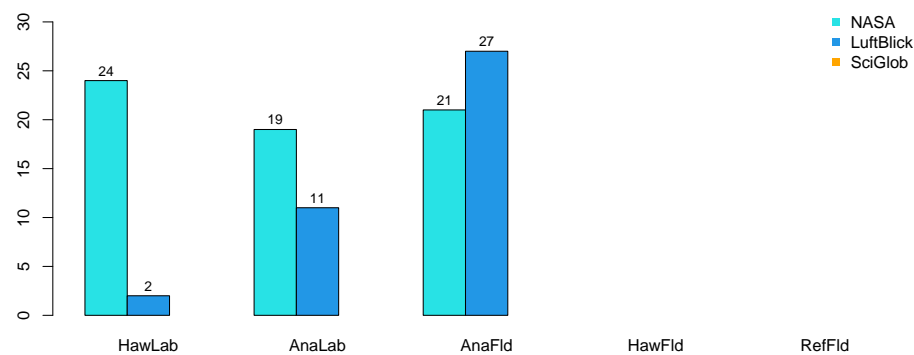
In the last quarter, 24 new or recently upgraded instruments have been calibrated in the laboratory of NASA. In Innsbruck, Pandora 209 (s1,s2) has been calibrated after a filter upgrade of the instrument.

Beside clearing, which is mainly done by NASA personnel, the main operational calibration task is still the re-calibration of longer timeseries with the 1.8 software.

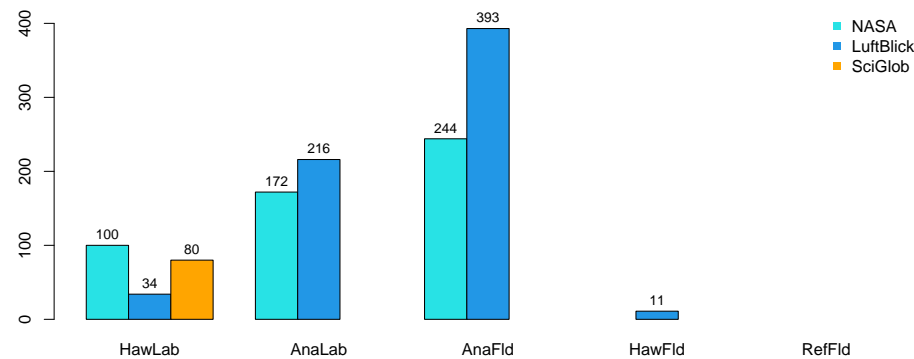
At NASA, 19 calibrationfiles have been created which also included the analysis of lab calibrations, and 11 on the LuftBlick side. On NASA site, this is mostly related to clearing. We see these numbers also in the amount of related field calibrations, where the preparation of longer timeseries can include more field calibrations.

Figure 1: Calibration activities

(a) 1st March 2022 to 30th May 2022



(b) 1st January 2018 to 30th May 2022



A detailed list of the calibration analysis work for the last quarter. The main operational calibration task right now is the clearing, mainly done by NASA, and the re-calibration of datasets with the 1.8 software.

Instrument ID	Location	Nr. of AnaFld	Purpose
2	GreenbeltMD	1	1.8 data preparation
11	LaPorteTX	1	TRACER-AQ data preparation
24	GreenbeltMD	1	Clearance
30	Juelich	1	AnaFld
49	GreenbeltMD	2	Clearance
58	GreenbeltMD	1	Clearance
59	GreenbeltMD	1	Clearance
61	AldineTX	2	TRACER-AQ data preparation
63	LaPorteTX	2	TRACER-AQ data preparation
71	GreenbeltMD	1	1.8 data preparation
75	GreenbeltMD	1	Clearance
76	GreenbeltMD	2	Clearance
77	GreenbeltMD	1	Clearance
78	GreenbeltMD	2	Clearance
79	GreenbeltMD	1	Clearance
105	Helsinki	5	AnaFld

Instrument ID	Location	Nr. of AnaFld	Purpose
117	Rome-SAP	1	AnaFld
128	AliceSprings,GreenbeltMD	2	1.8 data preparation,Clearance
146	Yokosuka	1	AnaFld
148	AldineTX	1	TRACER-AQ data preparation
150	Ulsan	1	AnaFld
154	GreenbeltMD	1	Clearance
157	MexicoCity-Vallejo	1	AnaFld
162	Brussels-Uccle	1	AnaFld
165	GreenbeltMD	1	Clearance
170	Downsview	5	1.8 data preparation
179	GreenbeltMD	1	Clearance
180	BronxNY	1	1.8 data preparation
198	Kobe	1	AnaFld
206	GreenbeltMD	1	Clearance
209	Innsbruck-FKS	2	Clearance
220	GreenbeltMD	1	Clearance
221	GreenbeltMD	1	Clearance

2.3 Calibrations foreseen between 1st June and 30th August

The main calibration tasks in the next weeks:

1. The data quality checks raise our attention to instruments which are having data quality issues. These instruments have high priority and will be calibrated with BlickC 1.8
2. Calibrations of datasets with 1.8
3. Calibrations of datasets with 1.8 where the 1.7 datasets have already been used for satellite validation have higher priority.
4. Field clearing instruments

Calibration activity	Expected number	Details
HawLab	> 6	Initial calibrations by NASA
AnaLab	> 10	Field clearance for instruments which are measured in the laboratory. Recalibration of datasets.
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 and NASA, respectively. 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 is lower than the actual number of laboratory sessions finished. 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

During a workshop in May 2019 in Innsbruck, three NASA colleagues and one EPA colleague have been taught in the analysis of laboratory measurements. Currently, the NASA team consists of only one person. On the LuftBlick side, the core calibration team consists of four people, where two are in an intensive training phase since February 2022.

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 a finished documentation and which lead to an approved calibrationfile usable for processing data.

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 visualization 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 visualization. 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

At the start of the project, the network strategy has foreseen a FCS consisting of the mFCT and a MobRef. The acquisition of a MobRef through FRM4AQ was initially planned for 2021. The additional value of a FCS is currently still evaluated due to substantially improved field calibration techniques. Depending on the results, it is still being decided if a MobRef will be bought within the project.