

LuftBlick Report 2023009

Fiducial Reference Measurements for Air Quality

Calibration Procedures Document
Version 4, 29 Nov 2024

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Document Change Record

Issue	Date	Section	Observations
1	31 May 2023	All	First version
2	24 Nov 2023	All	2nd version: Additions since June 2023
3	29 May 2024	All	3rd version: Adaptations since December 2023
4	29 Nov 2024	All	4rd version: Adaptations since June 2024

Acronyms and Abbreviations

CPD: Calibration Procedures Document

ESA: European Space Agency

FRM4AQ-2: Fiducial Reference Measurements for Air Quality 2

NDs: Neutral Density filters

OoB: Out of Box data

PGN: Pandonia Global Network

SOPs: Standard Operating Procedures

L6,L7, ...: Laboratory Routines with identifying numbers

S2: spectrometer 2

PRNU: Photo(Pixel) Response Non Uniformity

AXC: Auto Cross Correlation



Introduction

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

Together with the upgrade to the Blick software version 1.8, the documentation of the calibration procedures have been centralized into three living documents. Changes in these documents will be listed in future versions of this report and in the documents themselves. The three main documents are part of this deliverable.

The documents describe what calibration procedures are done and in what order, but do not describe the physical background of each step. The calibration procedures are split into two parts:

Laboratory calibration

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. The corresponding calibration procedures are collected in the document *ManualforLabCal*.

Analysis of laboratory measurements and field calibration

For the analysis of the measurements a semi-automated software, called BlickC, is used to analyze the laboratory measurements and field data, to build a calibration file needed as input for the Blick processing software (BlickP). 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 characterize 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 behavior regarding a calibration step) we set up a step-by-step BlickLabAnalysis manual, where also SOPs are defined in order to ensure calibrations are analyzed in the same way. This document has grown over time as part of this deliverable of the predecessor project, and has been used as a living document until July 2022. At that time, an online CalibrationAnalysisHandbook was released to the calibration team, to ease the introduction of new calibration personnel to BlickC. The major advantage over the prior manual is the user-interactivity, which allows to collapse detailed information by default. This sets the focus more on important analysis actions without flooding the reader with technical details. However, the user is able to open a new layer of information, and is also supported by guidelines and examples on how to overcome certain analysis steps.

Document change logs

The three main documents which are part of this deliverable D2 are the *ManualforLabCal*, the *BlickLabAnalysis Manual* and the *CalibrationAnalysisHandbook*. The last two are very similar from the content and differ mainly in the handling for the user as mentioned above.



Changes for the ManualforLabCal

Date	Change
2023-04-18	Changed order of radiometric calibration so that L7 is run first to determine which internal NDs need to be characterized by L6
2023-07-11	Reorganized and clarified radiometric calibration procedure slightly to be more optimized for S2 instruments
2024-05-28	In the case where the final location of the instrument is unknown the set temperature should be set at 15°C but both, the Radiometric calibration and Stray Light calibration should be run for 15°C and 20°C The minimum temperature for wavelength calibration was changed from 8°C to 10°C

Changes for the CalibrationAnalysisHandbook

Date	Change
2023-04-12	Identify emission lines to be used for wavelength calibration based on theoretical intensity & "neighborhood" and practical appearance for available lamps & according data
2023-07-13	Prepare BlickC_config.txt for easy application of the selected emssionlines
2023-07-13	Update Calibration-Analysis-Handbook for the new procedures

2023-08-10	Add "good lines" for spectrometer 2
2023-08-07	Added instruction for judging retrieved temperature from AXC
2023-08-14	Updated spectral lines library for He-Lamp
2023-9&10	Improve readability and comprehensibility of the document
2023-10-13	Added uncertainty for the smoothed mean within bright analysis for better evaluation of significant PRNU-features
2023-11-13	Updated instructions for selecting reference days for improving SO2-field calibration: Best with lowest air mass factors, meaning noon on summer days.
2023-11-20	Added instructions how to circumvent the BlickC-Bug when using an uncalibrated lamp
2023-11-24	Added an additional page listing changelogs
2024-02-27	Edited informations concerning calibrations of spectrometer 2: Etaloning & LongPassFilter
2023-11-28 - 2024-05-28	Continuous corrections of typos and spellings and minor adaptations (formats,)
2024-08-08	Field Calibration: Added Information about special features in AXC
2024-08-12	Create Reference: Added SOP about correction of sensitivity (if L7 was measured with external ND filter in lab)
2024-09-02	Processing and Quality Iterations: Added recipe for processing on the OVH Adapted the docker run command



2024-09-12	CreateReference: include AOD in stage 1 as it should be done operationally from now on
2024-09-30	Check Filters: Added an image in order to identify a wrongly connected VIS-fiber to Spectrometer 1 right there. Bright Analysis: Added an image in order to identify a wrongly connected VIS-fiber to Spectrometer 1 right there. Sensitivity: Added an image in order to identify a wrongly connected VIS-fiber to Spectrometer 1 right there.
2024-10-16	CreateReference: New feature for estimating aod: Added hint to delete L1 file used for AOD estimation (aodtool.pandonia.net) in stage 1 after usage
2024-10-30	Processing and Quality Iterations: Adaped the processing guideline (paths and links) after the server update
2024-11-11	Processing and Quality Iterations: Additions for QA-Datachecker-launch via fastAPI: /workflows/launch_I2_datacheck
2024-11-18	Create Reference: Additions for ND-filter-falsified sensitivities on how to discriminate different functional filte
2024-11-19	Wavelength Calibration: Improve the clarity of SOPs for selecting the temperature prior to the last step.

Changes for the BlickLabAnalysis1.8

Date	Change
2019-11-26	First version of the BlickC 1.8 specific manual
2021-04-10	start including the SOPs and section preparation steps before the calibration
2021-06-29	minor changes and adding some more figures for SOPs
2021-08-10	added some more key figures in SOP sections; added section Introducing new validity periods
2021-10-08	added new SOP for operational processing
2022-01-14	add new subsection under section 5.2 Processing
2022-01-24	update SOPs regarding field calibration for NO2 (MLE)
2022-03-08	adding QC codes to processing, description how to use centralized visualization and analysis tools
2022-04-27	adding H2O into fieldCalibration
2022-06-03	adding ExtRef H2O to processing procedure
2024-08-12	added SOP in CreateReference stage 3
2024-10-02	added SOP for L0 to L1 correction in CreateReference stage.