LuftBlick Report 2023002

New Algorithm and Product Plan

Project “Fiducial Reference Measurements for Air Quality 2.0”

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Prepared by

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1 Contents

2 Document Change Record

Issue	Date	Sections	Updates
0	9 Dec 2022	All	First version
1	28 Feb 2023	5 Product Status Table	Updated numbers of PGN and EVDC datasets.
1.1	6 Mar 2023	5 Product Status Table	Corrected numbers for EVDC datasets.
2	31 May 2023	4.6 Column “Uncertainty readiness”, 5 Product Status Table	New column added to product status table that describes the maturity of the uncertainty reporting. Numbers (PGN and EVDC datasets) have been updated.
3	31 Aug 2023	4.4 “#” Columns 5 Product Status Table	Changed counting of data product numbers. Updated numbers of PGN and EVDC datasets
4	22 Nov 2023	5 Product Status Table	Updated numbers of PGN datasets
5	29 Feb 2024	5 Product Status Table	Updated numbers of PGN datasets
6	28 May 2024	5 Product Status Table	Updated numbers of PGN datasets
7	31 Aug 2024	5 Product Status Table	Updated numbers of PGN datasets
8	29 Nov 2024	5 Product Status Table	Updated numbers of PGN datasets

3 Introduction

This report is deliverable D10 of ESA project “Fiducial Reference Measurements for Air Quality 2.0" (FRM4AQ-2) as described in the technical proposal and shown in the gantt chart. It makes references to the project "Pandonia Operations 2.0" (POp-2)”, since the work in both projects is complementary.

Its precursor is deliverable D11 from the predecessor project “Fiducial Reference Measurements for Air Quality”, which was running from 2019 to 2022. This report was updated semi-annually (e.g. version 7 from 30 Jun 2022) and is called “D11-1” in this document. D10 differs from the predecessor in the way that it is more an overview document, focusing on the key parameters for each data product such as when was it planned to be developed, when has the research started, when was it made operational, how was it validated etc. The core part of this report is the Product Status table in section 5. The meaning of the columns in the table is explained in section 4.

The data processing is done by the BSS, which is at version 1.8.45 at the beginning of this project in Jan 2023. Since Jul 2022 the BSS versioning is part of the POp-2 project and is documented in the project’s “Software Status Report” (e.g. the version from 30 Nov 2022). Therefore this element is NOT part of FRM4AQ-2 anymore and is not covered by D10.

3.1 Acronyms and Abbreviations:

AOD: Aerosol Optical Depth
BIACET: Biacetyl
BrO: Bromine oxide
BSS: Blick Software Suite
CH4: Methane
ClO: Chloride oxide
CO2: Carbon dioxide
D11-1: Deliverable D11 of FRM4AQ-1
ESA: European Space Agency
EVDC: ESA Data Validation Center
FRM4AQ: Fiducial Reference Measurements for Air Quality
GLY: Glyoxal
HCHO: Formaldehyde
HONO: Nitrous acid
H2O: Water vapor
ICE: Ice
IO: Iodine monoxide
I2: Molecular iodine
LuftBlick: LuftBlick OG, Innsbruck, Austria
MAXDOAS: Multi-Axes Differential Optical Absorption Spectrometry
MGLY: Methylglyoxal
NO2: Nitrogen dioxide
NO3: Nitrate
OBrO: Bromine dioxide
OClO: Chloride dioxide
OH: Hydroxyl radical
OIO: Iodine dioxide
O2: Oxygen
O2O2: Oxygen dimer
O3: Ozone
Pandora: Pandora Spectrometer System
PGN: Pandonia Global Network
POp: Pandora Operations
PYRAC: Pyruvic Acid
QA/QC: Quality Assurance and Quality Control
SO2: Sulfur dioxide
SW: Software
WAT: Liquid water

4 Product Status Table Description

The “Product Status Table” is a living document, of which at the end of each quarterly cycle (end of Feb, May, Aug and Nov) a snapshot is taken and inserted into section 5 of this document.

The rows of the table are split into groups for the different trace gasses (NO2, O3, etc.) and followed by the group “Aerosols”. Data products to support QA/QC procedures are listed at the end. Within each group the different data products, which can in principle be retrieved by a Pandora, are listed.

4.1 Column “Product”

This column lists the different PGN product types. For trace gasses, those types are:

- **Direct Sun Total Column, Direct Moon Total Column**: They are derived from direct sun (or moon) viewing geometry (see section 4.1 of the PGN Data Products Readme File) and retrieved with the “Direct Algorithm”, which is described in detail in section 6.6 of the BSS SW Manual.
- **TropCol, SurfConc, Profile:** This stands for Tropospheric Column, Surface Concentration and Vertical Profile respectively. They are derived from MAXDOAS viewing geometry (see section 4.2 of the PGN Data Products Readme File) and are retrieved with the “Air_ratio Sky Algorithm”, which is described in detail in section 6.7 of the BSS SW Manual. Note that these parameters are by default not retrieved for O2 and O2O2, since those species are used as reference in the algorithm.

For aerosols, those products are Direct Sun AOD, Direct Moon AOD, “Aerosol Params from Sky”, which stands for Aerosol Parameters derived from sky observations, which could be Single Scattering Albedo, Particle Size Distribution, etc. Since none of them is operational yet, they are not fully described in any manual yet. Nevertheless an analysis of the possibility of AOD retrievals from Pandora is given in appendix B of this LuftBlick report.

4.2 Column “Version”

This column lists the “product version”, which is the combination of the retrieval details (r-code) and the processor version. The r-code is described in section 5.10.4 of the BSS SW Manual. Retrieval details for the respective r-code can be found in section 2 of the PGN Data Products Readme File). Note that not all product versions that have been used historically in the PGN are listed in the table, just the operational ones starting from processor version 1.7.

4.3 “Start Dates” columns

There are 5 columns with “Start dates”. The background color of the row depends on whether a start date is set. If no date is set, the background color is white.

- **Planned**: this refers to the date, when the decision to develop this product was made, which is usually a FRM4AQ-2 progress meeting. If this date is set and none of the dates in the columns to the right, then the background color of the entire row is light red.
- **Develop**: this refers to the date, when the development of this product was started. If this date is set and none of the dates in the columns to the right, then the background color of the entire row is light yellow.
- **Validation**: this refers to the date, when the validation of this product was started (see also section 4.4). If this date is set and none of the dates in the columns to the right, then the background color of the entire row is light blue.
- **Release**: this refers to the date, when the product was officially released and the data started to be uploaded on the PGN data server. If this date is set and none of the dates in the columns to the right, then the background color of the entire row is light green.
- **EVDC**: this refers to the date, when the first data of this product was uploaded on EVDC. If this date is set and none of the dates in the columns to the right, then the background color of the entire row is green.

Note that it is possible that some of the dates are not given, even if a product already exists. E.g. for NO2 Direct Sun Total Column nvs1, no dates for Planned, Develop or Validation are given. This can have different reasons:

- The exact date, when a respective action was started, is not known anymore. This usually happens for products, which have been established a rather long time ago.
- The version is an update to a previous version for the same data product, where the different development stages were done rather fast.

4.4 "#" Columns

Column "# PGN" gives the number of processed and downloadable PGN data products (i.e. at the date of the report). Column "# EVDC" gives the number of PGN data products available on EVDC.

Note that "# PGN" also contains data products from instruments that are not yet fully quality assured. Hence this number is higher than "# EVDC" where datasets have been quality assured before its initial upload.

Moreover, the number of data products which exist for multiple processor versions (e.g. direct sun total column NO_2 for p1-7 and p1-8), will decrease over time for older versions, since it is replaced by the latest official product version.

4.5 Column "Validation type"

Column "Validation type" describes whether and how the respective product was validated. The options are:

- **Unval**: this means that a product is in the pipeline, but no validation has been started yet.
- **Intern**: this means (only) internal validation is being done or has been done. Internal validation basically means that the results of collocated Pandoras are compared to each other, checked for homogeneity and possibly also compared to models or climatologies. Internal validation is done for each data product. If this entry is set, then it means that no external validation could be done. The reason is usually that the respective data product is not measured by any other remote sensing instrument or that no other remote sensing instrument measuring the same quantity is collocated with a PGN instrument.
- **ExtLB**: this means that in addition to internal validation, external validation is being done or has been done by LuftBlick staff. External validation means that the PGN data are compared to data from other instruments.
- **ExtOut**: this means that in addition to internal validation and external validation performed by LuftBlick staff, external validation performed by people from an institution other than Luftblick is being done or has been done.
- **ExtPub**: this means that internal validation and external validation performed by LuftBlick staff and possibly also by people from an institution other than Luftblick has been done and the results are already published in a peer reviewed paper.

4.6 Column "Uncertainty maturity"

The uncertainty maturity level is reported for three uncertainty components that represent different correlation lengths in time (from zero to infinity). Details are outlined in the Blick Software manual or the PGN data products readme file. For simplicity, we encode the maturity level as L (=low), M (=medium) and H (=heigh). E.g. "HMH" would tell us that the maturity level of the independent uncertainty (correlation length = zero) is H(eigh) the structured uncertainty (correlation lengths between zero and infinity) is M(edium) and the common uncertainty (infinite correlation length) is also H(eigh).

4.7 Columns “Key aspects / remarks” and “Literature”

Column “Remarks” gives additional comments on the respective product, such as “Retrieves effective O3 temperature”.

Column “Literature” gives links with literature in relation to the data product other than the BSS SW Manual and the PGN Data Products Readme File. The link points to a report, paper or presentation. Note that these links are focused on literature that describes the data product itself or the research performed to develop it or how it was validated. General papers using the data for air quality, atmospheric modeling or satellite validation purposes are not listed, but most of them can be found on the publication section of the PGN webpage.

5 Product Status Table

The PGN Product Status Table described in section 4 is displayed on the next pages.

Product	Version	Planned	Develop	Validation	Release	EVDC	# PGN	# EVDC	Validation type	Uncertainty maturity	Key aspects / remarks	Literature
		Dates of first accomplishment										
NO2												
Direct Sun Total Column	**rnvs1p1-7**				Dec-2019	Feb-2020	12	17	ExtPub	HLL	short fitting window, fixed effective parameters (temperature, height)	Wang et al, 2010, Diemoz et al., 2021
	rnvs3p1-8	Jul-2019			Sep-2021	May-2022	135	58	Intern	HMH	long fitting window, climatological effective parameters (temperature, height)	Section 3.3 of D11-1
Direct Moon Total Column	**rnvm0p1-8**	Jan-2021	Jul-2017						Unval	HLL	short fitting window, fixed effective parameters (temperature, height), reference spectrum from solar measurements	Section 3.4 of D11-1
	rnms0p1-8	Nov-2020	Sep-2021	Dec-2021					Intern	HMM	long fitting window, climatological effective parameters (temperature, height), reference spectrum from solar measurements	Section 3.4 QA4EO deliverable, Section 3.4 of D11-1
TropCol, SurfConc, Profile	**rnvh3p1-8**	Jul-2019	May-2020	May-2020	Sep-2021		176	0	ExtPub	HLM	V-shaped measurement geometry, parameterized algorithm using look-up tables, sequential reference spectrum used; EVDC-GEOMS template still missing	Roscoe et al. 2010, Kreher et al. 2020, Tirpitz et al. 2021, Section 3.15 of D11-1
O3												

Direct Sun Total Column	rout0p1-7			Aug-2012	Dec-2019		12	0	ExtPub	HLL	no spectral straylight correction, fixed effective parameters (temperature, height)	Tzortziou et al. 2012, Herman et al. 2015, Zhao et al. 2016, Robinson et al. 2020, Zhao et al. 2021
	rout2p1-8	Jul-2019	Jan-2020	Jan-2021	Sep-2021	May-2022	178	37	ExtLB	HML	no spectral straylight correction, climatological effective parameters (temperature, height)	Section 3.5 of D11-1
	rous1p1-8	Jul-2019	Jun-2020	Jan-2021	Sep-2021				ExtLB	HMH	with spectral straylight correction, effective O3 temperature retrieved, climatological effective height	Section 3.5 of D11-1
Direct Moon Total Column	roms0p1-8	Nov-2020	Sep-2021	Dec-2021					Intern	HMH	Chappuis band from VIS Pandora channel	Section 3.4 QA4EO deliverable
TropCol, SurfConc, Profile											Ongoing O3 profile algorithm project	Kreher et al. 2020
SO2												
Direct Sun Total Column	rsus1p1-8	Jul-2019	Jun-2020	Jan-2021	Sep-2021	May-2022	135	50	Intern	HMH	O3 effective temperature is fitted, reference spectrum is O3 absorption free	Section 3.6 of D11-1
Direct Moon Total Column												
TropCol, SurfConc, Profile												
HCHO												

Direct Sun Total Column	**rfus5p1-8**	Jul-2019	Jul-2019	Jan-2021	Sep-2021	May-2022	135	46	ExtPub	HMH	extended-MLE used for calbration	Spinei et al. 2018, Spinei et al. 2021, Section 3.7 of D11-1
Direct Moon Total Column												
TropCol, SurfConc, Profile	**rfuh5p1-8**	Jul-2019	May-2020	May-2020	May-2021		176	0	Unval	HML	V-shaped measurement geometry, parameterized algorithm using look-up tables, sequential reference spectrum used	Pinardi et al. 2013, Kreher et al. 2020, Section 3.17 of D11-1
H2O												
Direct Sun Total Column	**rwvt1p1-8**	Jul-2019	Jan-2022	Jan-2022	Mar-2023		178	0	ExtLB	HML	fitting window around 505 nm band using literature reference spectrum	Section 3.11 of D11-1
Direct Moon Total Column	**rwms0p1-8**	Nov-2020	Sep-2021	Dec-2021					Intern	HMM	fitting window around 505 nm band using measured solar reference, calibrated towards rwvt0p1-8	Section 3.4 QA4EO deliverable
TropCol, SurfConc, Profile	**rnvh3p1-8**	Jul-2019	Jan-2017		Sep-2021		176	0		HML	same fitting setup as rnvh3p1-8	Section 3.17 of D11-1
HONO												
Direct Sun Total Column	**raus0p1-8**	Jun-2020	Dec-2021							HMH	current limitation: spectral feature from the band pass filter setup disturbs the retrieval	Section 3.8 of D11-1
Direct Moon Total Column												
TropCol, SurfConc, Profile		Jun-2020										

GLY												
Direct Sun Total Column	**rgvs0p1-8**	Jan-2020	Jun-2022							HMH	current limitation: unidentified spectral feature around 450 nm disturbs the retrieval	Section 3.9 of D11-1
Direct Moon Total Column												
TropCol, SurfConc, Profile		Jan-2020										
NO3												
Direct Moon Total Column	**rrvs0p1-8**	Jan-2020	Sep-2021	Dec-2021						HMH	VIS Pandora channel	Section 3.4 QA4EO deliverable
BrO												
Direct Sun Total Column		Jun-2020										
Direct Moon Total Column												
TropCol, SurfConc, Profile		Jun-2020										
Aerosols												
Direct Sun AOD		Jul-2019	Jul-2017							HLL	current limitation: radiometric stability and calibration transfer	Section 3.21 & appendix B of D11-1, D4 of Pandonia CCN, D6 of Pandonia CCN

Direct Moon AOD												
Aerosol Params from Sky		May-2020	May-2020							LLL		DIVA-2 D4, DIVA-2 D5
QAQC support products												
O2O2												
Direct Sun Total Column	**rovs0p1-8**	Jul-2019	Jun-2021						Intern	HMH		Section 3.10 of D11-1, Section 6.3 of D5
Direct Moon Total Column												
O2												
Direct Sun Total Column	**rdvs0p1-8**	Jul-2019	Dec-2021						Intern	HMH		Section 3.10 of D11-1, Section 6.3 of D5
Direct Moon Total Column												