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Quality Assurance for Earth Observation - QA4EO

Final Report WP2125 “Qualitative accuracy assessment of operational PGN data products”

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1 Summary and Conclusions

The WP2125 “Pandonia products uncertainty” of the ESA project “Quality Assurance for Earth Observation” (QA4EO) [AD1] had basically three goals. Here the summary and conclusions for each of them.

Goal 1) Analyze the maturity level of the Pandonia Global Network (PGN) at the beginning and the end of phase 1 of this project.

This was done and is described in section 5. During this project the maturity category “Uncertainty quantification” was improved in the following way:

- Status at beginning of phase 1 (Nov 2019): Score 2 “... data may not be well curated or metrologically understood and calibrated.”
- Status at end of phase 1 (Nov 2020): Score 3 “... measurements are better characterised and understood, and intended to be run for the long-term. However, they lack strict traceability and comparability.”

After the next phase of the project (Nov 2021) we intend to reach score 5 “... measurements are very well characterised, with strict traceability and comparability, and robustly quantified uncertainties.”.

Goal 2) Interact with the UK National Physics Laboratory (NPL) about the “correct” nomenclature and usage of the uncertainty output in the PGN data products.

This was done and is described in section 3. The current version V1.7 of the Blick Software Suite, which is the software to process all PGN data, will be soon replaced by V1.8. V1.8 is extensively restructured and updated taking into account the correct nomenclature and usage of data uncertainties as recommended by NPL. We do not expect that this new nomenclature has to be replaced again in the future as it is fully compliant with the newest core principles of the metrological community [RD1].

Goal 3) Determine the impact of uncertainties in the laboratory calibration on the official PGN data products total ozone (O_3) and total nitrogen dioxide (NO_2) column amounts.

This was the task, which consumed the majority of the time and manpower effort in this project as it involved a lot of testing, variation, calculations, etc. It is described in section 4.

All PGN instruments undergo a rigorous laboratory calibration protocol before being deployed. The results of this calibration are used to apply corrections on the raw data (level 0, L0) to produce spectra (level 1, L1) and higher level output products (level 2, L2) such as trace gas column amounts. The calibration parameters determined in this procedure can have errors for the following reasons:

E1) Outdated laboratory equipment: e.g. a calibration lamp is used, which is past its lifetime.
E2) Insufficient laboratory equipment: e.g. the used single line lasers do not cover the hole wavelength range of the spectrometer.

E3) Operator errors during the laboratory measurements: e.g. positioning of the calibration lamp in the wrong distance.
E4) Operator errors in the analysis of the laboratory measurements: e.g. an unreasonable order for the polynomial was used to obtain the dispersion, i.e. the relation between pixel and wavelength.

To minimize these errors the PGN regularly updates and improves the laboratory equipment (E1, E2), and uses experienced operators, who stick to a rigorous procedure for the laboratory measurements (E3) and their analysis (E4). Nevertheless there is still some room for differences in the way the calibration is exactly performed, especially with respect to the data analysis (E4). In this study we have evaluated the uncertainty introduced by a different interpretation of the laboratory measurements from different operators. The results are summarized in table 1.1. Hence the numbers shown are in most cases NOT the error introduced by not applying a certain correction to the L0 data. Such impact would be much larger. Instead the numbers give the effect on the total column amounts caused by a E2 or E4. The only exception is the quantification of the latency effect (here we compare applying or not applying the correction).

Table 1.1: Summary of the impact of the L1 correction steps on the retrieved total O_3 and total NO_2 column amounts, sorted by decreasing impact

L1 correction	**Qualitative impact**	**Impact on total O_3**	**Impact on total NO_2**
Stray light	Moderate	Up to 3%	Up to 2%
Latency effect Radiometric sensitivity Wavelength calibration Non-linearity Flat field	Small	Up to 0.5%	Up to 0.3%
Dark count Temperature sensitivity	Very small	Up to 0.02%	Up to 0.03%

Based on the outcome of this study we have made the following conclusions for the further reduction and description of the uncertainty in PGN data products. The list below also indicates with “**(→ CCN)**”, which of the related tasks will be studied during the next phase of this project going until Nov 2021.

- The impact of E2 and E4 is in general small, except for the stray light correction, where it is moderate. We could determine that this is mostly associated with E2, and not with E4 (see table 1.1 and section 4). Hence in order to reduce the overall PGN data uncertainty, the spectral coverage of the lasers with respect to the stray light calibration needs to be improved. Currently the PGN labs at LuftBlick, Innsbruck, Austria, and SciGlob, Elkridge, MD, USA, are insufficiently equipped with lasers. Only the lab at NASA/Goddard Space Flight Center, in Greenbelt, MD, USA, has a sufficient number of lasers, although still improvable. Therefore we conclude:
    - The training and the standard operation procedure (SOP) for the lab operators are not a significant error source for the PGN data product. Hence as long as their quality does not drop, we do not have to take action on this part.

- A major step to reduce the PGN data uncertainty is to improve the stray light calibration equipment in the PGN laboratories.
- The impact of operator error on the PGN data is small (once the labs have improved their stray light calibration equipment). Therefore we believe that it is not useful to build a mathematical system, which propagates these uncertainties into the L1 and L2 data, since the relation between the needed effort, which would consume the vast majority of the time allocated for the CCN, and the potential improvement in the data uncertainty (<0.5%, see table 1.1), cannot be justified. Instead one shall rather use the time and manpower resources for other tasks listed in the next points.
- The impact of laboratory uncertainties on the L1 data should be included in the Blick processing software (BlickP) as an additional (common) uncertainty, which totals the sum of all effects analyzed in this project. It shall be a function of the air mass factor and needs to be developed in the next year. **(→ CCN)**
- BlickP needs to be modified to propagate this newly developed common uncertainty in the L1 data into the PGN L2Fit data (i.e. the fitted slant columns) and L2 data (i.e. the total columns). **(→ CCN)**

2 Introduction

This is the final report of WP2125 “Pandonia products uncertainty” of the ESA project “Quality Assurance for Earth Observation” (QA4EO) [AD1] for the time period 1 November 2019 to 1 November 2020. The report is structured into the following sections:

- Section 1 - Summary and Conclusions
- Section 2 - Introduction
- Section 3 - Description of the status of the Pandonia Global Network (PGN) ozone and NO_2 data product uncertainty structure introduced within the updated Blick Software Suite V1.8. This was developed in collaboration with NPL (in particular Emma Woolliams).
- Section 4 - Case study of the impacts of the uncertainties in the calibration actions on the corrected spectra (L1 data) and the ozone and NO_2 data products.
- Section 5 - Maturity matrix assessment procedure.

2.1 Acronyms and Abbreviations

AD	Applicable Document
AMF	Air Mass Factor
BlickC	Blick Calibration Software
BlickP	Pandora Processing Software
BMC	Baseline Measurement Capability
CCD	Charge-Coupled Device
CDR	Climate Data Record
CMC	Comprehensive Measurement Capability
DQ	Data quality
DQF	Data quality flag
DSC	Differential Slant Column
DU	Dobson Units
EO	Earth Observation
L0 data	Level 0 data
L1 data	Level 1 data
L2 data	Level 2 data
MM	Maturity Matrix
NO2	Nitrogen Dioxide
O3	Ozone
PGN	Pandonia Global Network
PRNU	Pixel Response Non Uniformity
QA4EO	Quality Assurance Framework for Earth Observation
RD	Reference Document
RMC	Reference Measurement Capability
SZA	Solar Zenith Angle

2.2 Applicable Documents

[AD1] Quality Assurance for Earth Observation project [Annex B, Statement of Work for LuftBlick], SERCO Contract QA4EO/SER/SUB/04, 2020.

2.3 Reference Documents

[RD1] Jonathan Mittaz, Christopher J Merchant, and Emma R Woolliams. Applying principles of metrology to historical earth observations from satellites. Metrologia, 56(3):032002, 2019.
[RD2] Cede A., Manual for Blick Software Suite 1.8, Blick Software Suite Manual Version 1.8.
[RD3] Cede A., Manual for Blick Software Suite 1.7, Blick Software Suite Manual Version 1.7.
[RD4] Thorne, P. W., Madonna, F., Schulz, J., Oakley, T., Ingleby, B., Rosoldi, M., Tramutola, E., Arola, A., Buschmann, M., Mikalsen, A. C., Davy, R., Voces, C., Kreher, K., De Maziere, M., and Pappalardo, G.: Making better sense of the mosaic of environmental measurement networks: a system-of-systems approach and quantitative assessment, Geosci. Instrum. Method. Data Syst., 6, 453–472, https://doi.org/10.5194/gi-6-453-2017, 2017.
[RD5] Su, Z., Timmermans, W., Zeng, Y., Schulz, J., John, V.O., Roebeling, R.A., Poli, P., Tan, D., Kaspar, F., Kaiser-Weiss, A.K., Swinnen, E., Toté, C., Gregow, H., Manninen, T., Riihelä, A., Calvet, J.-C., Ma, Y., Wen, J.: An overview of european efforts in generating climate data records. Bull. Am. Meteorol. Soc. 99 (2), 349–359. https://doi.org/10.1175/BAMS-D-16-0074.1, 2018.

3 Status of the current V1.8 PGN data uncertainties

The data uncertainty in the Blick Software Suite V 1.8 has been extensively restructured and updated from previous versions taking into account the correct nomenclature and usage of data uncertainties based on core principles of metrological traceability. This was done under the guidance of Emma Woolliams from the UK National Physics Laboratory (NPL).

The main output products of BlickP are spectra (L1), slant columns (L2Fit) and total and tropospheric column amounts or profiles or surface concentrations (L2). Most of these data come with associated uncertainties. For the naming and meaning of the uncertainties, the Blick Software Suite follows the guidelines laid out by Mittaz et al. [RD1]. Three types of errors are distinguished, which differ from each other by the correlation length along a certain "dimension". In the Blick Software Suite, this dimension is wavelength for L1 data and time for L2Fit and L2 data.

- **Independent error:** The correlation length along the dimension for the independent error is zero. An example for L1 data is the read noise in a certain pixel (i.e. at a certain wavelength), which is totally uncorrelated to the read noise in any other pixel (wavelength). An example for L2Fit data is the photon noise propagated into the slant column amount measured at a certain moment, which is totally uncorrelated to the propagated photon noise for measurements taken at any other time. The uncertainty associated with an independent error is called "Independent uncertainty" and is symbolized with U_I.
- **Common error:** The correlation length along the dimension for the common error is infinite. An example for L1 data is a bias in the radiometric calibration due to a faulty positioning of the calibration lamp in the laboratory. This bias affects each wavelength for the same amount, e.g. +3%, hence the error in one pixel is fully correlated to the error in any other pixel. An example for L2Fit data is an error in the assumed slant column in the reference spectrum. This error affects all retrieved slant columns using the same reference spectrum in the same way, hence the error at a certain measurement is fully correlated to the error for measurements taken at any other time. The uncertainty associated with a common error is called "Common uncertainty" and is symbolized with U_C.

- **Structured error:** The correlation length along the dimension for the structured error is larger than zero, but not infinite. An example for L1 data is an error in the flat field correction around a certain wavelength region. Such an error affects all the pixels inside this wavelength region in the same way but is uncorrelated to pixels at a different part of the spectrum. An example for L2Fit data is a difference between the effective temperature of a trace gas used in the spectral fitting (assuming that the temperature is NOT fitted itself) and the true effective temperature of this gas in the atmosphere. This introduces an error in the retrieved slant column, which is highly correlated to measurements taken around the same time, but in general not correlated to measurements taken at times farther away. E.g. if an effective ozone temperature of 225 K is used in the spectral fitting, but the true effective ozone temperature is 228 K at 10:00 in the morning of 27 October, this causes approximately a -1% error in the retrieved ozone slant column. The next measurement on this day at 10:02 will still suffer nearly exactly the same error, since the true temperature has hardly changed in the 2 minutes. However a few days later, on 3 November, the true temperature has in general changed and might be 225 K, which means the error due a mismatch of the effective temperature is then 0 and not correlated to the error from 27 October at 10:00. The uncertainty associated with a structured error is called "Structured uncertainty" and is symbolized with U_S.

For the total uncertainty U of a single (L1, L2Fit or L2) data point, we combine U_I, U_C and U_S as shown in equation:

$$\mathrm{U} = \sqrt{\mathrm{U}_\mathrm{I}^2 + \mathrm{U}_\mathrm{C}^2 + \mathrm{U}_\mathrm{S}^2}$$

When the data are averaged, e.g. by building the mean spectrum over a certain wavelength range, or the mean column amount over a certain time interval, the total uncertainty of the mean is a combination of the individual $U_I(i)$, $U_C(i)$ and $U_S(i)$. i=1 to n is the index for a single data point out of the n data points averaged. Here we look at the two "extreme" cases.

In the first situation the structured errors are fully correlated along the dimension. In this "short" case the total uncertainty of the mean value, called U(n,short), is given by:

$$\mathrm{U(n,short)} = \frac{1}{\mathrm{n}} \cdot \sqrt{\sum_{i=1}^{\mathrm{n}} \left[\mathrm{U_I\,(i)}^2\right] + \left[\sum_{i=1}^{\mathrm{n}} \mathrm{U_C\,(i)}\right]^2 + \left[\sum_{i=1}^{\mathrm{n}} \mathrm{U_S\,(i)}\right]^2}$$

Hence the independent uncertainty of the mean is "reduced" compared to the individual values, but the common and structured uncertainties are not. An example for this would be the mean column amount over a rather short time period, e.g. 10 min, in which we assume the data with respect to mismatch of the true and assumed effective trace gas temperature to be fully correlated.

The other extreme case assumes the structured uncertainties to be uncorrelated along the dimension. In this"long" case the total uncertainty U(n,long), is given by:

$$\mathrm{U(n,long)} = \frac{1}{\mathrm{n}} \cdot \sqrt{\sum_{i=1}^{\mathrm{n}} \left[\mathrm{U_I\,(i)}^2\right] + \left[\sum_{i=1}^{\mathrm{n}} \mathrm{U_C\,(i)}\right]^2 + \sum_{i=1}^{\mathrm{n}} \left[\mathrm{U_S\,(i)}^2\right]}$$

Here the structured uncertainty "behaves" like the independent uncertainty. An example for this would be the mean column amount over a long time period, e.g. one year, when we assume that the temperature used in the spectral fitting is from a climatology that represents very well the average true effective temperature over this year. Then we could say that the temperature errors are a mixture of over- and underestimations and can therefore be approximated as uncorrelated overall.

It is important to note that not all possible uncertainty sources are included in the Blick Software Suite at this moment and therefore even the total uncertainty is still incomplete. Therefore the output products also include data quality flags (DQF) in addition to the uncertainty information. These DQF are required since the current PGN data product uncertainties do not cover all sources that may contribute to a decrease in the data quality. In other words, there are effects, from which we know they are affecting the data quality, but the current Blick Software Suite retrieval version is either not taking them into account at all, or does not include an estimation of how much they affect the uncertainty in a quantitative way. The plan is to add the uncertainty sources not taken into account at later versions of the software. This is briefly discussed in Section 5.2.

4 Impacts of calibration uncertainties on PGN data products

To investigate possible impacts of laboratory calibration uncertainties on the PGN L1 data and the final ozone and NO_2 data products, direct sun measurements made with the Pandora #67 located at Greenbelt/USA on 12 March 2019 are used for a case study. The study was done by performing the processing steps using the Blick Calibration Software (BlickC) while introducing just one modification at a time to a standard session and then comparing the final 'modified' PGN products with the results from that standard session.

The analysis and calibration processing steps - or calibration actions - are listed here in the order in which they are applied to the L0 raw data:

1. Dark correction
2. Non-linearity correction
3. Latency correction
4. Flat field correction
5. Temperature correction
6. Stray light correction
7. Sensitivity correction
8. Wavelength correction

It is important to note that the order in which the correction steps are applied cannot be changed since they are not commutative and when a modification is, for example, introduced during the dark correction, all following steps have to be repeated to ensure that the impact of the modification in the dark correction is carried through the processing chain correctly. The impact of the introduced changes are discussed and shown graphically for total column ozone and NO_2 (figures 4.1-4.10) for the whole day and as well as presented in tables for selected SZAs (tables 4.1-4.2).

The following sections discuss the particular modification to a key parameter of a specific laboratory calibration action. The impact of each of these modifications is then carried through the processing chain to the final PGN data product which is then compared to the value of the standard session. Note that this section does NOT describe the details of the correction itself. For this we refer to the Blick Software Suite Manual Version 1.8 (BM1.8) [RD2]. BM1.8 is still under development and will be published at the release of the PGN v1.8 data in early 2021. It is cited here as several new developments in the data processing, which are also related to the QA4EO project, did not exist and are consequently not described in the current official Blick Software Suite Manual Version 1.7 [RD3].

4.1 Uncertainty investigation in the stray light correction

To investigate the uncertainty in the stray light correction, several parameters important for the stray light calibration action were varied and compared to the standard data analysis session. Figures 4.1 and 4.2 show examples for the PGN ozone vertical columns and the NO_2 vertical columns, respectively. Both ozone and NO_2, are plotted against the airmass factor (AMF) for the standard session (black symbols) and several modified sessions (colour symbols).

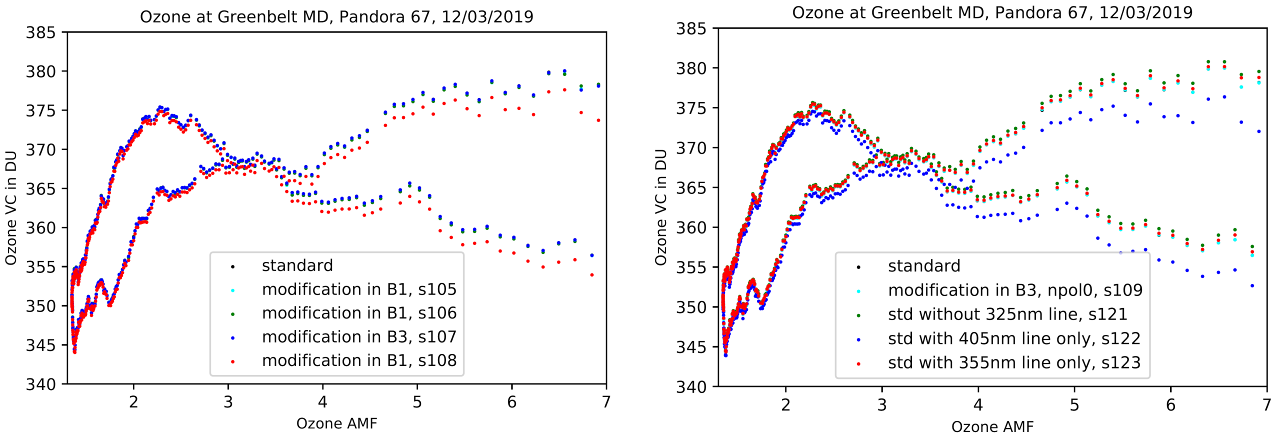


Figure 4.1 Ozone vertical columns measured with Pandora 67 at Greenbelt, USA on 12 March 2019. The diurnal variation of the standard session is displayed in black in each of the two panels while four different sessions with one modification each in the stray light correction calibration action are shown in colour.

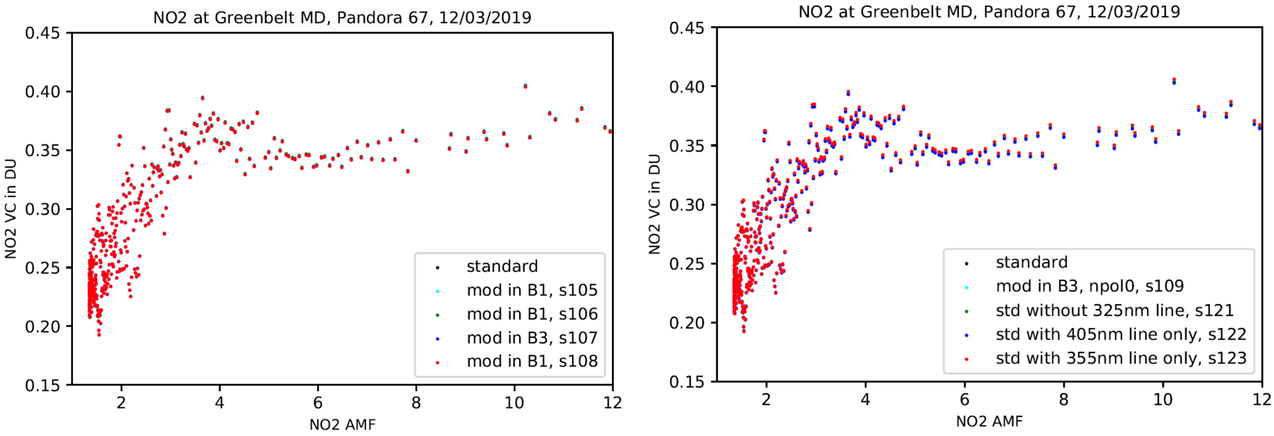


Figure 4.2 NO_2 vertical columns measured with Pandora 67 at Greenbelt, USA on 12 March 2019. The diurnal variation of the standard session is displayed in black in each of the two panels while four different sessions with one modification each in the stray light correction calibration action are shown in colour.

Figures 4.3 and 4.4 display the differences in ozone (left panel) and NO_2 (right panel) vertical columns between the modified sessions and the standard session which are shown in figures 4.1 and 4.2. The same format will also be used for the figures in the following subsections investigating the uncertainty in all the other processing correction steps listed in the introduction above. Three solar zenith angles (SZAs) are indicated with dashed lines with the AMF of 1.55 corresponding to an SZA of 50°, an AMF of 2.85 to 70° and an AMF of 5.20 to 80° for ozone. Similarly for NO_2, an AMF of 1.55 is corresponding to an SZA of 50°, an AMF of 2.90 to 70°, an AMF of 5.50 to 80°, and in addition an AMF of 9.86 for 85°.

Sessions 105 to 108 differ from the standard session by a change in the polynomial used for the wavelength inter- and extrapolation of the stray light parameters needed to define the stray light correction matrix. B1 (related to the stray light near field) and B3 (related to the stray light far field) are the slit function parameters and one specific change is made to either the B1 or B3 polynomial used in the stray light correction. A rather extreme change from order 1 to 0 for the B1 polynomial leads to a change of approximately 0.7 DU (approx. 0.2%) for 70° and 1.9 DU (approx. 0.5%) for 80° SZA (session 108) while the other three modifications lead to smaller changes of 0.2 DU (approx. 0.05%) and less for the whole SZA range (sessions 105 - 107).

The same changes in the order of polynomial for the slit function parameters B1 and B3 lead to a different impact on NO_2 with a change of 0.001 DU (approx. 0.3%) or less for all 4 modifications with sessions 105 and 106 having a slightly greater impact than sessions 107 and 108 (figure 4.3, right panel).

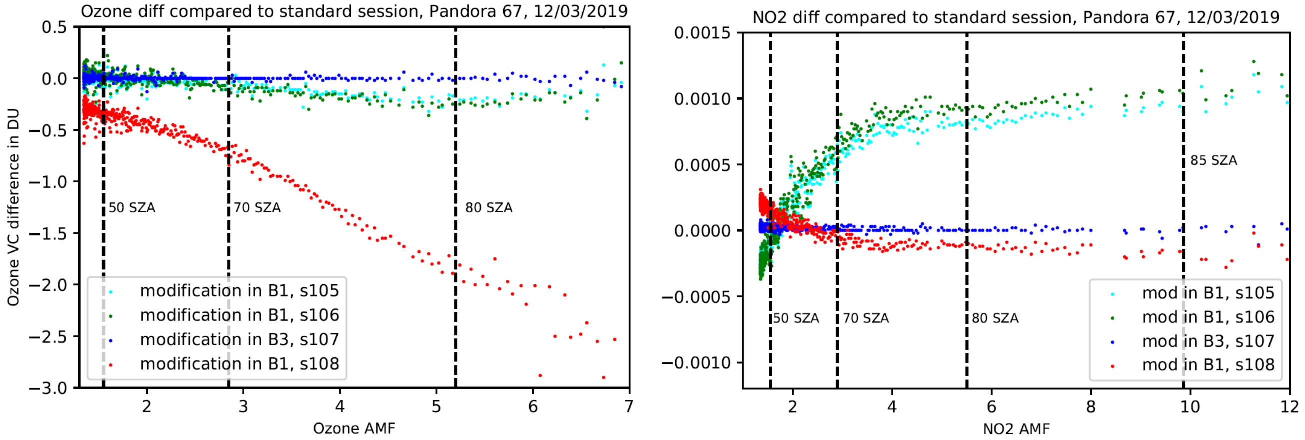


Figure 4.3 shows the difference between four modified sessions to the standard session for ozone vertical columns in DU (left panel) and NO_2 vertical columns in DU (right panel).

Figure 4.4 shows another set of modifications introduced in the stray light correction processing step. Session 109 features a further modification in the slit function parameter B3 (left panel, cyan symbols) while the other 3 sessions (121 - 123) include a modification in the usage of the laser lines used for the stray light correction. The standard session includes 5 laser lines (at 514, 532, 355, 488 & 325nm) to determine the instrument's full slit function while session 121 excludes the 325 nm line. For session 122, only one laser line at 405 nm is used for the stray light correction instead of the five lines used for the standard case and this session, like session 108, illustrates again a more extreme case with a difference of about 3 DU (approx. 0.8%) for ozone at 80° SZA. An impact of this modification can also be seen in L1 data. For session 123, also only one laser line at 355 nm is used but the impact on ozone is clearly much lower while this session shows a slightly higher impact on NO_2 with a change of 0.002 DU (approx. 0.6%) than the other sessions investigated as part of the stray light correction.

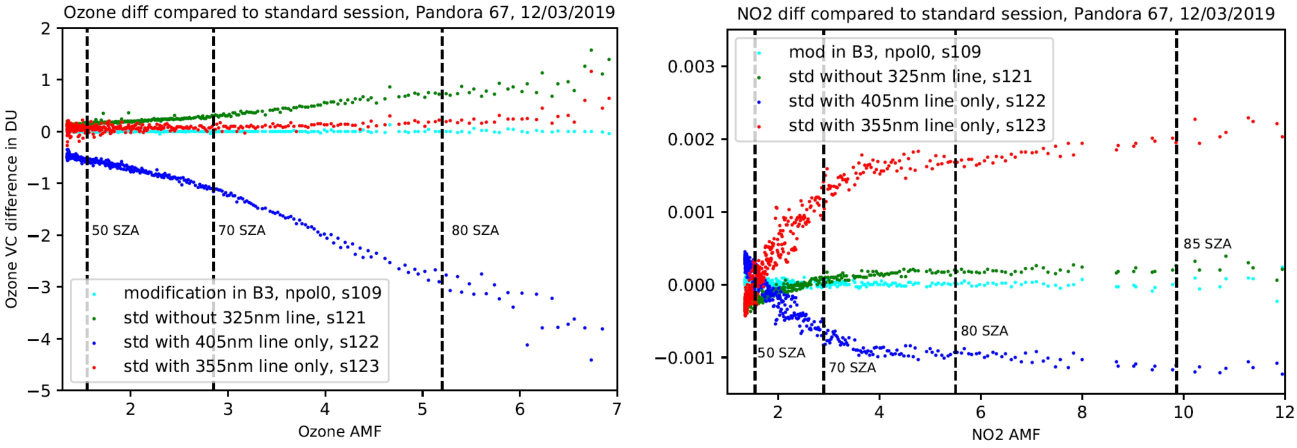


Figure 4.4 shows the difference between four modified sessions to the standard session for ozone vertical columns in DU (left panel) and NO_2 vertical columns in DU (right panel).

As expected, the greatest impact on ozone and NO_2 based on any stray light correction modifications can be seen in session 110 where only a very simplified approach is used to correct for stray light (the signal below 290 nm is assumed to be zero). This is shown in figure 4.5 (cyan symbols) below, with a change in ozone around 9 DU for 80^o SZA and 0.006 DU (or 1.7%) for NO_2. A change of 9 DU in ozone was by far the greatest change observed in this study. As anticipated, session 110 also shows a clear impact on the L1 data.

4.2 Uncertainty investigation in latency and sensitivity correction

In addition to the stray light correction, figure 4.5 also shows an example each of the effect of a modification in the latency (red symbols) and sensitivity correction (blue symbols). The latency effect in CCD detectors can cause the readings in a pixel to be influenced by the readings in the previously read pixel. For example, if there are many subsequent high readings followed by very low readings, then the first low readings can be biased high, since the residual charge from the previous readings is still in the readout electronics capacitor. The standard session does not include a latency correction but in session 136, latency parameters are introduced to determine the effect on the ozone and NO_2 data. The ozone determined for session 136 shows a change of 1.2 DU (approx. 0.3%) for 80^o SZA in comparison to the standard session while the change in NO_2 is truly negligible.

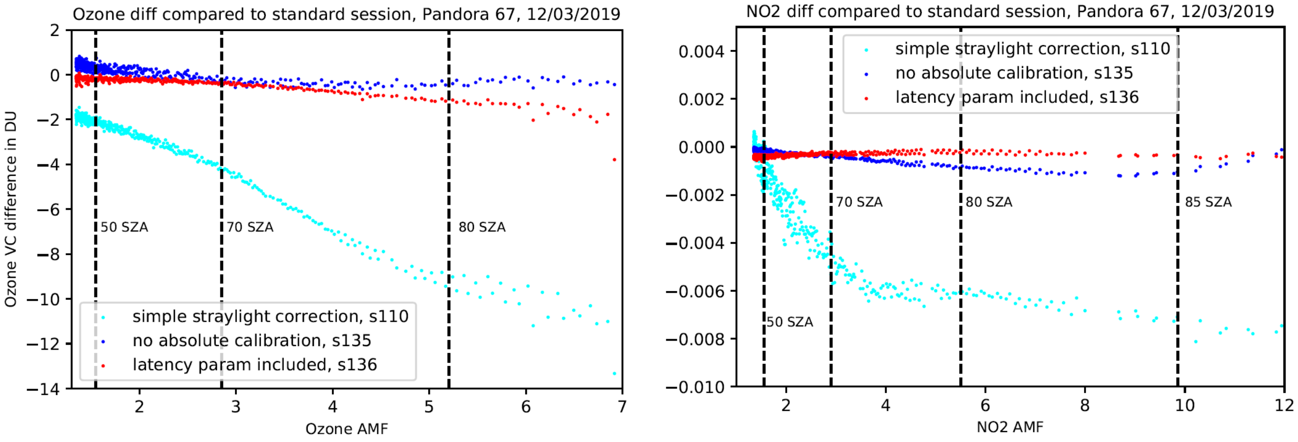


Figure 4.5 shows the difference between four modified sessions to the standard session for ozone vertical columns in DU (left panel) and NO_2 vertical columns in DU (right panel).

As part of the sensitivity correction, a radiometric calibration of the Pandora instrument is done using an ANSI standard 10000 watt quartz halogen lamp. If a certificate exists for this lamp, which gives the absolute output of the lamp for a given input current and at a given distance from it, then the sensitivity correction applies an absolute calibration to the data and the unit of the L1 data changes from [counts/s] to [W/m^2/nm] for direct sun observations. If there is no certificate, then the calibration is used to determine the filter transmission and the unit after the correction stays [counts/s]. Session 135 (blue symbols in figure 4.5) shows that the omission of the absolute calibration has only a very small impact on both final data products. This is, however, different for the L1 data which are definitely impacted if no absolute calibration is used.

4.3 Uncertainty investigation in wavelength correction

All modified sessions shown in figures 4.6 and 4.7 differ from the standard case in the variation of parameters relevant for the wavelength correction. In this processing step, the measured spectra are shifted to the nominal wavelength grid using a corresponding "standard spectrum" and this action analyzes the laboratory measurements to determine the instrument's dispersion and slit function.

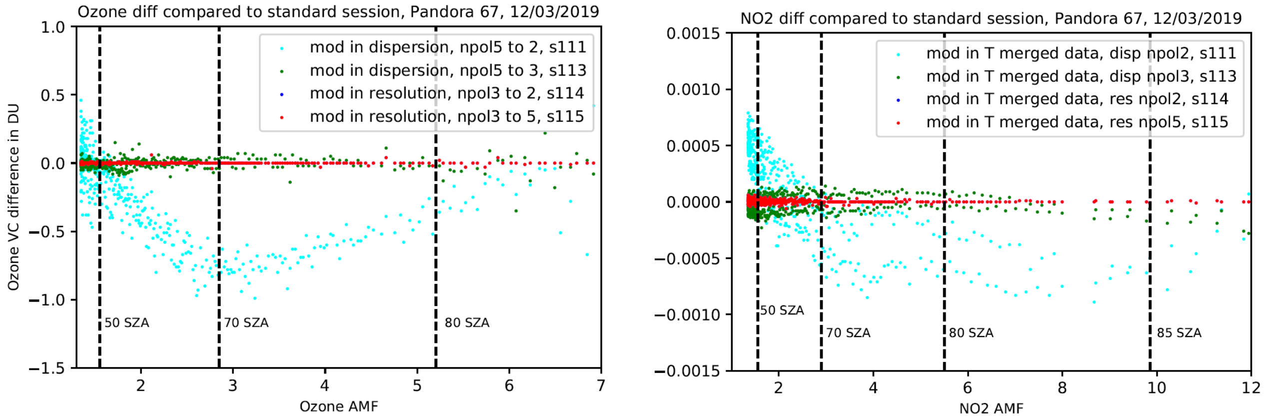


Figure 4.6 shows the difference between four modified sessions to the standard session for ozone vertical columns in DU (left panel) and NO_2 vertical columns in DU (right panel).

The strongest effect is visible in session 111 for ozone of up to 1 DU (approx. 0.3%) around 70° SZA (Figure 4.6, left panel, cyan symbols), with a change from a 5th order to a 2nd order polynomial in the dispersion of the temperature merged data. NO_2 also shows a corresponding change of up to 0.0009 DU (approx. 0.25%). The other changes in the polynomials for the dispersion (from 5th order to 3rd order polynomial in session 113) and for the resolution of the temperature merged data set (from the 3rd order to 2nd or 5th order) show an - in comparison - negligible effect on ozone and NO_2.

Figure 4.7 shows further modified sessions regarding the wavelengths correction. In these four sessions, changes to the fitting parameters of the slit function A2 and A3 from the temperature merged data are applied. A change to the polynomial for A2 from 3rd order to 2nd and 5th order are applied in sessions 116 and 117, respectively, and to the polynomial for A3 also from 3rd order to 2nd and 5th order in sessions 118 and 119, respectively. Here the greatest impact is on ozone measured at higher SZAs for the change in the polynomial for A3 from 3rd to 2nd order with up to 0.7 DU (approx. 0.2%) at 80° SZA followed by the change also in A3 from a 3rd to 5rth order polynomial with up to 0.5 DU (approx. 0.14%) at 80° SZA. For NO_2, the greater effect is seen in the variation of the fitting parameter for A3 than A2 with up to 0.0005 DU (approx. 0.14%) at 85° SZA.

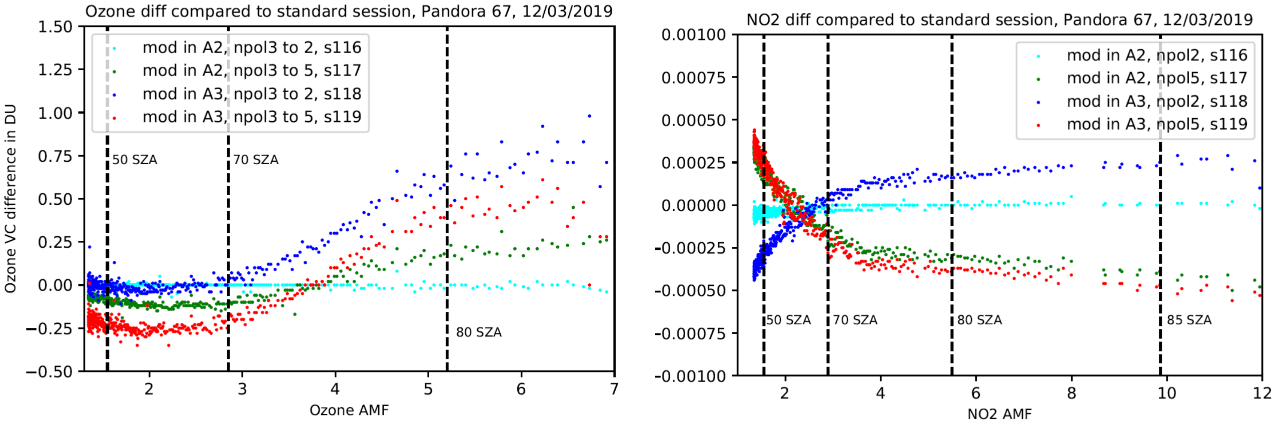


Figure 4.7 shows the difference between four modified sessions to the standard session for ozone vertical columns in DU (left panel) and NO_2 vertical columns in DU (right panel).

4.4 Uncertainty investigation in the correction of non-linearity, flat field and temperature dependence

Image sensors are in general not linear, i.e. they do not return a doubled signal when they are illuminated by the double amount of light. The non-linearity of Pandora instruments is typically a few percent for not too low counts. For very low counts, the non-linearity leaves the range of a few percent correction, i.e. the instrument returns significantly more signal than it should if it was linear. For the linearity correction a reference count value, ccref, needs to be chosen by the calibration scientist. The linearity is characterized in the laboratory and is not dependent on the temperature.

The impact of changes in the parameters affecting the non-linearity correction is investigated in sessions 124 and 125 (figure 4.8) and session 133 (figure 4.9). For session 124, where the ccref value is changed to a rather extreme value (1000 instead of the 6000 which is used for the standard case), ozone shows some effect with close to 0.6 DU (approx. 0.16%) higher than the standard case for around 80° SZA. The modification introduced in session 124 also shows some impact on the L1 data.

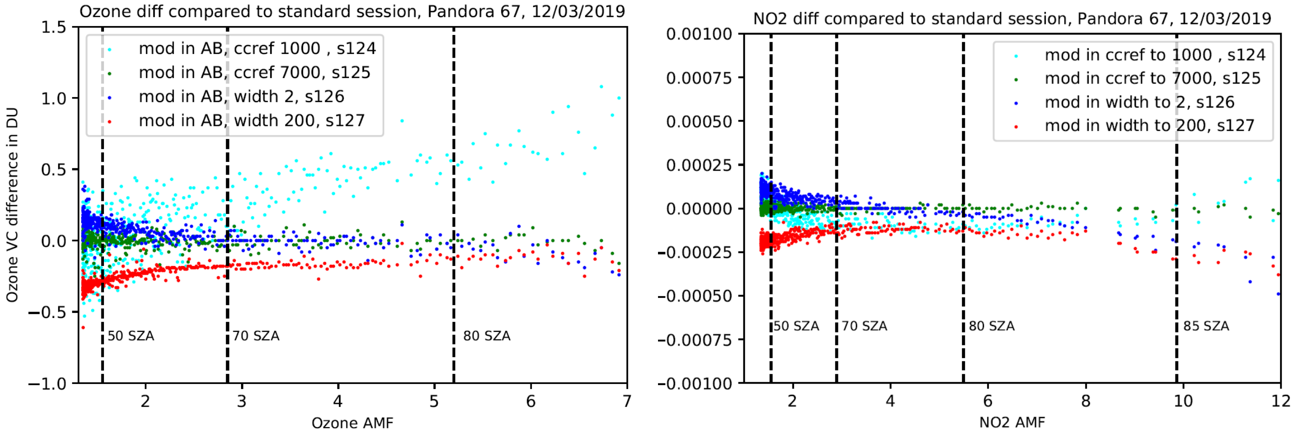


Figure 4.8 shows the difference between four modified sessions to the standard session for ozone vertical columns in DU (left panel) and NO_2 vertical columns in DU (right panel).

Sessions 126, 127 and 134 investigate the flat field characteristics or "Pixel Response Non Uniformity" (PRNU) response. Even when each pixel is illuminated by the same amount of light, they all return slightly different signals. This is called PRNU and is caused by physical differences in the pixels. The PRNU is determined during the radiometric calibration. Note that if the lamp signal is not smooth as a function of wavelength, lamp features might falsely be interpreted as PRNU. Therefore only selected lamps can be used for the radiometric calibration. The PRNU impact of the modifications can mainly be seen at higher SZAs (figure 4.7, blue and red symbols and figure 4.8, red symbols) with the diurnal variation in the difference to the standard session being very similar for both ozone and NO_2. For NO_2, session 127 with a variation in width for the smoothing of the lamp spectrum shows the highest impact for 50° - 85° SZA with up to 0.0003 DU (approx. 0.12%).

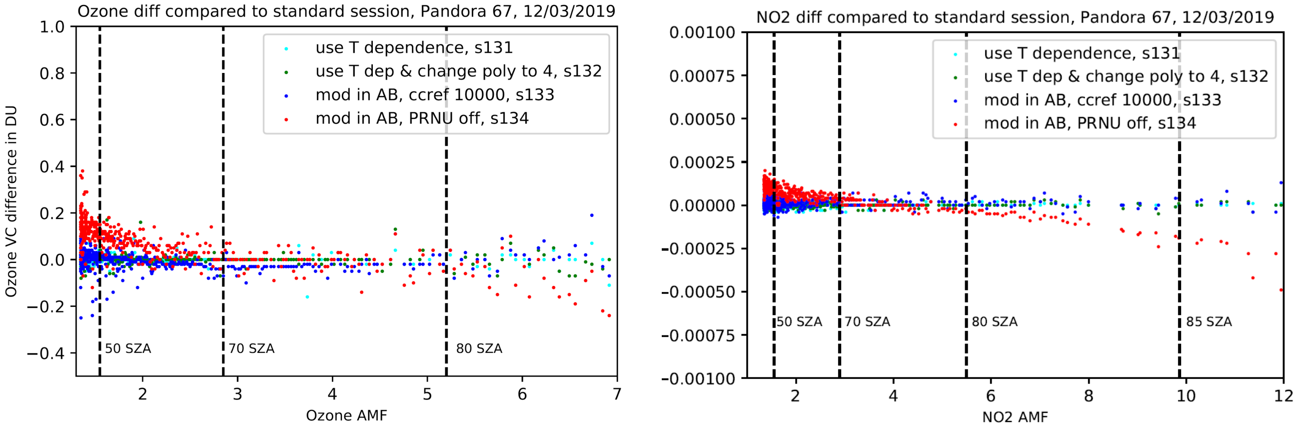


Figure 4.9 shows the difference between four modified sessions to the standard session for ozone vertical columns in DU (left panel) and NO_2 *vertical columns in DU (right panel).*

In order to determine the temperature sensitivity of a Pandora, the radiometric calibration is performed in the laboratory at three different spectrometer temperatures. If a Pandora is in good condition, it has only very small radiometric temperature sensitivity, which means no temperature correction needs to be applied to the data. In the case a signal change as a function of temperature is noted, the instrument will give false calibration results for the other tests as well, thus leading to an investigation of a hardware problem, e.g. moisture inside the optical bench. In the standard case, no temperature correction is applied. Hence, to test a possible effect of the temperature correction, session 131 has the temperature correction applied. For session 132, the temperature correction is applied as well but additionally the order of the fitted polynomial to describe the temperature sensitivity is changed from 0 to 4. Both sessions show a negligible effect for both ozone and NO_2.

4.5 Uncertainty investigation in dark correction

The first correction from L0 (raw data) to L1 data is the dark correction, where an estimation for the dark counts are subtracted from the measured bright counts. Pandora can measure dark counts by setting the filter-wheel in a position to block the light input.

The dark count is the sum of the dark offset (given by an electronic bias of the read-out electronics) and the dark slope (charge produced by thermal electrons). The Pandora dark count depends on the detector it is using. The dark offset is usually about 1-2 % (of the saturation value) and the dark slope is about 1-2 % per second at the current operational temperature. For our standard 16-bit AD converter, this corresponds to about 1000 counts dark offset and 1000 counts/s dark slope at a detector temperature of about 25°C.

There are two methods to estimate the dark count. For the "Immediate dark method", only the dark count measured immediately after the regular measurements (with light input) is used to estimate the dark count included in the regular data. For the "Dark map method", the immediate dark measurements are used in combination with the "dark fine structure map", which has been determined during calibration.

The advantage of the immediate dark measurements is that the conditions (temperature, state of the instrument, etc.) are basically the same as for the actual measurements. The disadvantage is that in order to optimize the signal to noise of the L1 data, the system needs to spend quite some time doing dark count measurements, which could be better used to make actual measurements. For the dark mapping it is the opposite. Using this method, much less time is spent in doing dark count measurements, but there is the risk that the dark map is not entirely representative for the measured spectra, since the conditions (temperature, state of the instrument, etc.) might have changed between the time the dark map was created and the time of the measurements were made.

To investigate the potential impact of changes in the dark correction on the observations, three modified sessions were run. For the first 2 sessions, the fitting parameter for the dark count background was changed from 6 to 2 (session 128) and to 8 (session 129). For session 130, the dark map was switched off while the standard session has the dark mapped switched on. As can be seen clearly in figure 4.10, these changes have only a minimal impact on ozone and NO_2. However, in particular session 128 does show an impact on the L1 data. Also do note, that the application of a dark correction is essential for good data quality and while the variations to the dark correction, investigated in this study, have only a negligible impact on the final data products, it is vital that any raw data is always corrected for the dark count.

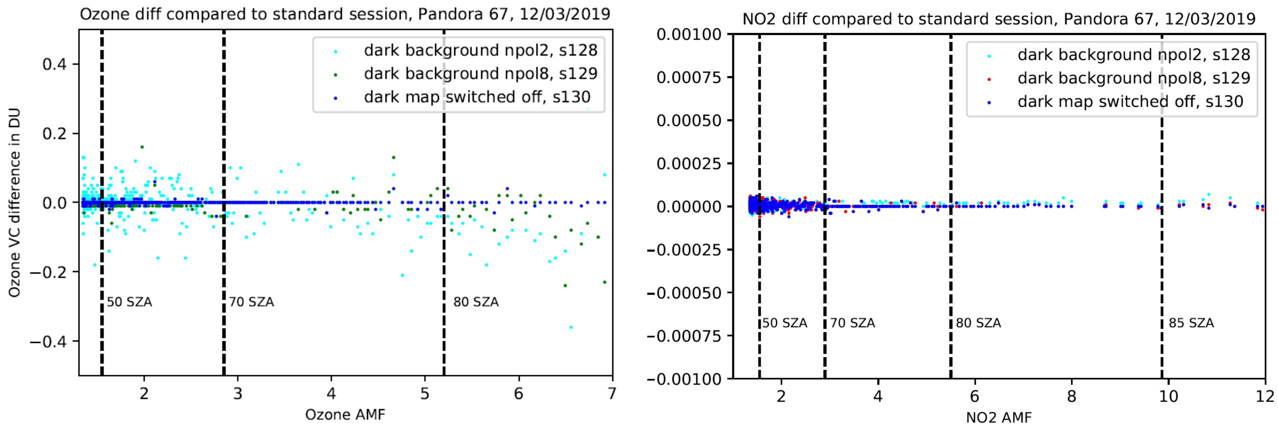


Figure 4.10 shows the difference between three modified sessions to the standard session for ozone vertical columns in DU (left panel) and NO_2 vertical columns in DU (right panel).

4.6 Summary of impact study

All modifications shown and discussed in the previous subsections are also summarized in the following two tables for ozone and NO_2. When comparing the values in the tables one needs to keep in mind that the tables contain a snapshot at a particular SZA while the figures show the diurnal variation for the whole day. For ozone, the figures only show data where the L2 data quality flag indicates high or medium quality and hence the measurements with higher SZA are omitted from the ozone figures while the table still contains the ozone values for 85 SZA.

Table 4.1 List of the differences between the modified and standard sessions for the PGN ozone data product measured with the Pandora #67 at Greenbelt/Maryland on 12 March 2019. The first 2 columns provide the session number and investigated correction, and the following 8 columns show the ozone differences as absolute values in DU and as percentage change (in brackets) relative to the ozone measured in the standard session.

	Difference in ozone in DU (and in %) between modified and standard session at the approx. SZA								
Session#	Corrected effect	. 85 SZA am	80 SZA am	70 SZA am	50 SZA am	50 SZA pm	70 SZA pm	80 SZA pm	85 SZA pm
105	stray light	0.48 (0.15)	-0.17 (-0.05)	-0.11 (-0.03)	0.02 (0.01)	0.01 (0.0)	-0.04 (-0.01)	-0.21 (-0.06)	1.14 (0.38)
106	stray light	1.29 (0.4)	-0.25 (-0.07)	-0.11 (-0.03)	0.05 (0.01)	0.05 (0.01)	-0.04 (-0.01)	-0.25 (-0.07)	1.69 (0.57)
107	stray light	0.1 (0.03)	-0.02 (-0.01)	0.0 (0.0)	-0.01 (-0.0)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	0.91 (0.31)
108	stray light	-4.04 (-1.27)	-1.89 (-0.5)	-0.84 (-0.23)	-0.31 (-0.09)	-0.34 (-0.1)	-0.67 (-0.18)	-1.81 (-0.5)	-2.38 (-0.8)
109	stray light	-0.03 (-0.01)	0.0 (0.0)	0.0 (0.0)	-0.01 (-0.0)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	0.11 (0.04)
110	stray light	-12.39 (-3.88)	-9.44 (-2.51)	-4.35 (-1.17)	-2.12 (-0.59)	-2.05 (-0.59)	-4.17 (-1.13)	-9.02 (-2.5)	-10.51 (-3.54)
111	wavelength	2.9 (0.91)	-0.52 (-0.14)	-0.81 (-0.22)	0.0 (0.0)	-0.06 (-0.02)	-0.82 (-0.22)	-0.36 (-0.1)	1.17 (0.39)
113	wavelength	0.02 (0.01)	-0.02 (-0.01)	-0.04 (-0.01)	-0.03 (-0.01)	-0.03 (-0.01)	0.03 (0.01)	-0.02 (-0.01)	0.15 (0.05)
114	wavelength	-0.02 (-0.01)	-0.02 (-0.01)	0.0 (0.0)	-0.01 (-0.0)	0.0 (0.0)	0.0 (0.0)	0.02 (0.01)	-0.01 (-0.0)
115	wavelength	-0.02 (-0.01)	-0.02 (-0.01)	0.0 (0.0)	-0.01 (-0.0)	0.0 (0.0)	0.0 (0.0)	0.02 (0.01)	-0.01 (-0.0)
116	wavelength	0.08 (0.03)	-0.02 (-0.01)	0.0 (0.0)	-0.01 (-0.0)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	0.3 (0.1)
117	wavelength	0.31 (0.1)	0.18 (0.05)	-0.11 (-0.03)	-0.09 (-0.03)	-0.08 (-0.02)	-0.11 (-0.03)	0.23 (0.06)	1.22 (0.41)

118	wavelength	1.05 (0.33)	0.58 (0.15)	0.03 (0.01)	0.05 (0.01)	-0.02 (-0.01)	0.0 (0.0)	0.69 (0.19)	1.25 (0.42)
119	wavelength	0.29 (0.09)	0.39 (0.1)	-0.18 (-0.05)	-0.17 (-0.05)	-0.26 (-0.07)	-0.25 (-0.07)	0.46 (0.13)	0.35 (0.12)
121	stray light	2.41 (0.76)	0.72 (0.19)	0.28 (0.08)	0.15 (0.04)	0.14 (0.04)	0.31 (0.08)	0.73 (0.2)	1.81 (0.61)
122	stray light	-4.62 (-1.45)	-2.9 (-0.77)	-1.16 (-0.31)	-0.58 (-0.16)	-0.55 (-0.16)	-1.1 (-0.3)	-2.77 (-0.77)	-3.79 (-1.28)
123	stray light	1.84 (0.58)	0.22 (0.06)	0.03 (0.01)	0.08 (0.02)	0.07 (0.02)	0.1 (0.03)	0.19 (0.05)	1.35 (0.45)
124	non-linearity	2.6 (0.81)	0.56 (0.15)	0.1 (0.03)	-0.05 (-0.01)	-0.07 (-0.02)	0.1 (0.03)	0.53 (0.15)	1.02 (0.34)
125	non-linearity	0.22 (0.07)	0.0 (0.0)	-0.04 (-0.01)	0.04 (0.01)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	0.27 (0.09)
126	PRNU	0.66 (0.21)	-0.05 (-0.01)	0.0 (0.0)	0.15 (0.04)	0.1 (0.03)	0.03 (0.01)	0.04 (0.01)	0.47 (0.16)
127	PRNU	0.23 (0.07)	-0.13 (-0.03)	-0.18 (-0.05)	-0.29 (-0.08)	-0.3 (-0.09)	-0.18 (-0.05)	-0.11 (-0.03)	1.78 (0.6)
128	dark count	0.96 (0.3)	-0.04 (-0.01)	-0.04 (-0.01)	0.0 (0.0)	0.01 (0.0)	0.03 (0.01)	-0.04 (-0.01)	-2.06 (-0.69)
129	dark count	-0.72 (-0.23)	-0.02 (-0.01)	0.0 (0.0)	-0.01 (-0.0)	0.0 (0.0)	0.0 (0.0)	0.04 (0.01)	-1.19 (-0.4)
130	dark count	-0.03 (-0.01)	-0.02 (-0.01)	0.0 (0.0)	-0.01 (-0.0)	0.0 (0.0)	0.0 (0.0)	0.02 (0.01)	0.0 (0.0)
131	temperature	0.05 (0.02)	-0.02 (-0.01)	0.0 (0.0)	0.04 (0.01)	-0.03 (-0.01)	0.0 (0.0)	0.02 (0.01)	0.41 (0.14)
132	temperature	0.48 (0.15)	-0.02 (-0.01)	0.0 (0.0)	0.04 (0.01)	-0.03 (-0.01)	0.0 (0.0)	0.04 (0.01)	0.85 (0.29)
133	non-linearity	0.16 (0.05)	-0.02 (-0.01)	-0.07 (-0.02)	-0.01 (-0.0)	0.01 (0.0)	-0.04 (-0.01)	0.04 (0.01)	0.51 (0.17)
134	PRNU	0.66 (0.21)	-0.05 (-0.01)	0.0 (0.0)	0.15 (0.04)	0.1 (0.03)	0.03 (0.01)	0.04 (0.01)	0.47 (0.16)
135	sensitivity	0.01 (0.0)	-0.46 (-0.12)	-0.25 (-0.07)	0.14 (0.04)	0.16 (0.05)	-0.25 (-0.07)	-0.4 (-0.11)	-0.83 (-0.28)
136	latency	-2.87 (-0.9)	-1.18 (-0.31)	-0.46 (-0.12)	-0.18 (-0.05)	-0.15 (-0.04)	-0.36 (-0.1)	-1.13 (-0.31)	-2.06 (-0.69)

Table 4.2 List of the differences between the modified and standard sessions for the PGN NO$_2$ data product measured with the Pandora #67 at Greenbelt/Maryland on 12 March 2019. The first 2 columns provide the session number and investigated correction, and the following 8 columns show the NO$_2$ differences as absolute values in DU and as percentage change (in brackets) relative to the NO$_2$ measured in the standard session.

		Difference in NO$_2$ in DU (and in %) between modified and standard session at the approx. SZA							
Session#	Corrected effect	85 SZA am	80 SZA am	70 SZA am	50 SZA am	50 SZA pm	70 SZA pm	80 SZA pm	85 SZA pm
105	stray light	0.0009 (0.25)	0.00081 (0.24)	0.00045 (0.15)	-0.00026 (-0.12)	-2e-05 (-0.01)	0.00065 (0.18)	0.00082 (0.24)	0.00094 (0.26)
106	stray light	0.00104 (0.29)	0.00092 (0.27)	0.00055 (0.18)	-0.00023 (-0.11)	-1e-05 (-0.0)	0.00072 (0.2)	0.00093 (0.27)	0.00106 (0.29)
107	stray light	2e-05 (0.01)	0.0 (0.0)	-1e-05 (-0.0)	0.0 (0.0)	3e-05 (0.01)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)
108	stray light	-0.00016 (-0.05)	-0.0001 (-0.03)	-1e-05 (-0.0)	0.00015 (0.07)	0.00011 (0.04)	-7e-05 (-0.02)	-9e-05 (-0.03)	-0.00016 (-0.04)
109	stray light	3e-05 (0.01)	1e-05 (0.0)	-1e-05 (-0.0)	-1e-05 (-0.0)	4e-05 (0.01)	0.0 (0.0)	2e-05 (0.01)	0.0 (0.0)
110	stray light	-0.00709 (-2.0)	-0.00604 (-1.77)	-0.00405 (-1.35)	-0.0002 (-0.1)	-0.00145 (-0.52)	-0.00532 (-1.45)	-0.00606 (-1.77)	-0.00727 (-2.0)
111	wavelength	-0.0005 (-0.14)	-0.00028 (-0.08)	-0.0001 (-0.03)	0.00052 (0.25)	5e-05 (0.02)	-0.00055 (-0.15)	-0.0006 (-0.17)	-0.00063 (-0.17)
113	wavelength	-6e-05 (-0.02)	7e-05 (0.02)	6e-05 (0.02)	0.0 (0.0)	-0.00013 (-0.05)	-7e-05 (-0.02)	-6e-05 (-0.02)	-0.00017 (-0.05)
114	wavelength	-1e-05 (-0.0)	0.0 (0.0)	-1e-05 (-0.0)	-4e-05 (-0.02)	-2e-05 (-0.01)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)
115	wavelength	-1e-05 (-0.0)	0.0 (0.0)	-1e-05 (-0.0)	-4e-05 (-0.02)	-2e-05 (-0.01)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)
116	wavelength	0.0 (0.0)	0.0 (0.0)	-3e-05 (-0.01)	-0.0001 (-0.05)	-6e-05 (-0.02)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)
117	wavelength	-0.00039 (-0.11)	-0.00029 (-0.08)	-0.00012 (-0.04)	0.00021 (0.1)	0.00018 (0.06)	-0.00021 (-0.06)	-0.00031 (-0.09)	-0.0004 (-0.11)
118	wavelength	0.00025 (0.07)	0.00016 (0.05)	-2e-05 (-0.01)	-0.00036 (-0.17)	-0.00028 (-0.1)	7e-05 (0.02)	0.00016 (0.05)	0.00023 (0.06)
119	wavelength	-0.00047 (-0.13)	-0.00037 (-0.11)	-0.00015 (-0.05)	0.00027 (0.13)	0.00021 (0.08)	-0.00028 (-0.08)	-0.00039 (-0.11)	-0.00048 (-0.13)
121	stray light	0.00026 (0.07)	0.00018 (0.05)	0.0 (0.0)	-0.00032 (-0.15)	-0.00014 (-0.05)	3e-05 (0.01)	0.0002 (0.06)	0.0002 (0.05)
122	stray light	-0.00111 (-0.31)	-0.00093 (-0.27)	-0.00057 (-0.19)	0.00021 (0.1)	3e-05 (0.01)	-0.00083 (-0.23)	-0.00093 (-0.27)	-0.00117 (-0.32)

123	stray light	0.00195 (0.55)	0.00168 (0.49)	0.00104 (0.35)	-0.00024 (-0.11)	0.00019 (0.07)	0.00141 (0.38)	0.00168 (0.49)	0.00201 (0.55)
124	non-linearity	2e-05 (0.01)	-0.0001 (-0.03)	-0.00011 (-0.04)	3e-05 (0.01)	3e-05 (0.01)	-0.00014 (-0.04)	-9e-05 (-0.03)	-7e-05 (-0.02)
125	non-linearity	-1e-05 (-0.0)	0.0 (0.0)	1e-05 (0.0)	-2e-05 (-0.01)	0.0 (0.0)	3e-05 (0.01)	2e-05 (0.01)	-1e-05 (-0.0)
126	PRNU	-0.00019 (-0.05)	-4e-05 (-0.01)	4e-05 (0.01)	7e-05 (0.03)	7e-05 (0.03)	3e-05 (0.01)	-2e-05 (-0.01)	-0.00018 (-0.05)
127	PRNU	-0.00029 (-0.08)	-0.00011 (-0.03)	-0.00014 (-0.05)	-0.00025 (-0.12)	-0.00022 (-0.08)	-0.00011 (-0.03)	-0.00013 (-0.04)	-0.00029 (-0.08)
128	dark count	3e-05 (0.01)	1e-05 (0.0)	0.0 (0.0)	-4e-05 (-0.02)	-2e-05 (-0.01)	3e-05 (0.01)	0.0 (0.0)	1e-05 (0.0)
129	dark count	-1e-05 (-0.0)	0.0 (0.0)	0.0 (0.0)	-6e-05 (-0.03)	-2e-05 (-0.01)	0.0 (0.0)	0.0 (0.0)	-1e-05 (-0.0)
130	dark count	-1e-05 (-0.0)	0.0 (0.0)	-2e-05 (-0.01)	-4e-05 (-0.02)	-1e-05 (-0.0)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)
131	temperature	0.0 (0.0)	1e-05 (0.0)	-1e-05 (-0.0)	-4e-05 (-0.02)	-2e-05 (-0.01)	0.0 (0.0)	0.0 (0.0)	-1e-05 (-0.0)
132	temperature	1e-05 (0.0)	0.0 (0.0)	0.0 (0.0)	-4e-05 (-0.02)	0.0 (0.0)	3e-05 (0.01)	0.0 (0.0)	-1e-05 (-0.0)
133	non-linearity	4e-05 (0.01)	1e-05 (0.0)	2e-05 (0.01)	-6e-05 (-0.03)	0.0 (0.0)	3e-05 (0.01)	3e-05 (0.01)	4e-05 (0.01)
134	PRNU	-0.00019 (-0.05)	-4e-05 (-0.01)	4e-05 (0.01)	7e-05 (0.03)	7e-05 (0.03)	3e-05 (0.01)	-2e-05 (-0.01)	-0.00018 (-0.05)
135	sensitivity	-0.00105 (-0.3)	-0.0008 (-0.23)	-0.0004 (-0.13)	-0.00032 (-0.15)	-0.00019 (-0.07)	-0.00042 (-0.11)	-0.00088 (-0.26)	-0.00111 (-0.31)
136	latency	-0.00033 (-0.09)	-0.00013 (-0.04)	-0.00024 (-0.08)	-0.00047 (-0.22)	-0.00049 (-0.18)	-0.00035 (-0.1)	-0.00024 (-0.07)	-0.00036 (-0.1)

Based on the discussion above and the two overview tables, the impact of the modifications in the laboratory calibration steps on the PGN L1 data, and the final ozone and NO_2 data products, can be rated in importance and summarized as described in the following.

The modifications to the stray light correction have by far the greatest impact and hence efforts in improving the stray light correction as well as a better understanding of the uncertainty quantification of stray light will potentially be the most effective. This is followed by a more moderate impact of modifications in the correction of latency, sensitivity, wavelength, non-linearity and flat field (PRNU). The last group contains the processing steps dealing with the dark correction and the temperature dependence. For an indication in terms of numbers, table 4.3 makes an attempt at providing an overview of the impact of the eight correction steps on the data processing of the PGN ozone data product.

Table 4.3 List of the L1 data processing steps in order of impact of the investigated modifications and the impact on the PGN ozone data product (usually at 80^o SZA or smaller unless otherwise explicitly mentioned) for the case study.

L1 data processing steps	Impact of modification on ozone in DU
Stray Light correction	up to 9 DU
Latency	up to 1.2 DU (up to 3 DU at 85^o SZA)
Wavelengths	up to 0.8 DU
Non-linearity	up to 0.6 DU
Sensitivity	up to 0.5 DU
Flat field correction (PRNU)	up to 0.3 DU
Dark correction	up to 0.04 DU (up to 2.1 DU at 85^o SZA)
Temperature correction	up to 0.04 DU (up to 0.9 DU at 85^o SZA)

5 Maturity assessment procedure and results

As part of this project, a maturity assessment of the PGN ozone and NO_2 data products has been made in collaboration with Emma Woolliams from the UK National Physics Laboratory (NPL). The result of this assessment was that the section “Uncertainty quantification” is the one, where the PGN is still farthest away from maturity and therefore being able to improve this section within QA4EO is of high importance to the PGN. The final aim of the further planned improvements is to have full uncertainty in the PGN L2 total trace gas column data.

The 3 tables further below show the PGN maturity matrix (MM) assessment. The tables show three versions of the PGN MM assessment:

- Table 5.1: MM for October 2019 - status at the start of QA4AO
- Table 5.2: MM for October 2020 - status at the end of phase 1 of this project
- Table 5.3: MM predicted for October 2021: status expected if the improvements outlined in Section 5.2 will be achieved.

The measurement system MM approach used here, as defined in [RD4], is a tool to assess various facets of a measurement series or measurement network. It assesses to what extent measurement best practices have been met, and the assessment can be performed either on individual instruments/sites or for entire networks.

There are six mandatory and one optional categories where assessments are made, which overlap with but are not identical to those used to assess CDRs under CORECLIMAX (e.g. [RD5]). The assessment categories are:

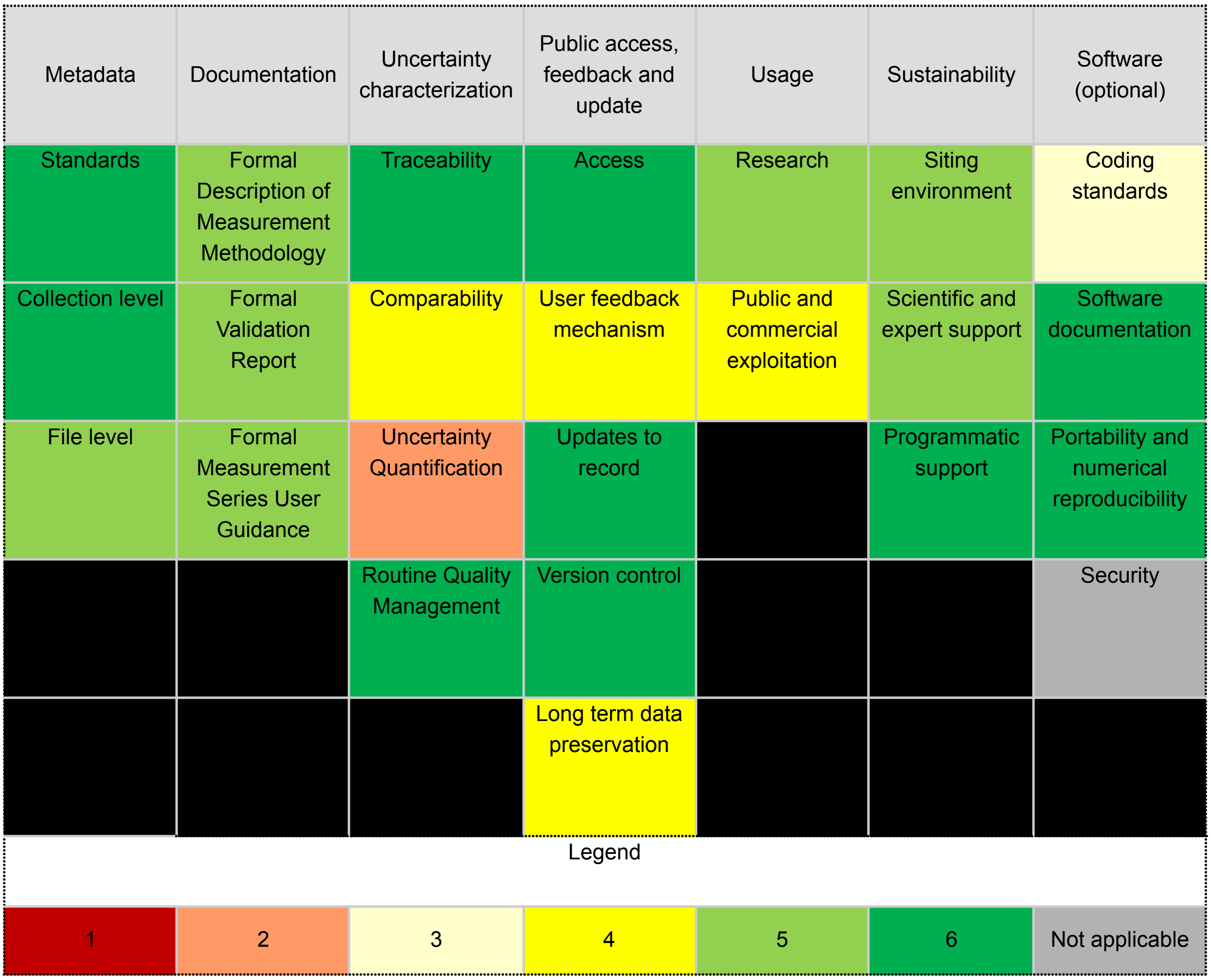
- metadata,
- documentation,
- uncertainty characterisation,
- public access, feedback and update,
- usage,
- sustainability,
- software (optional).

Within each category, there are a number of subcategories. For each of these subcategories, the assessment will assign a score from 1 to 6 (sometimes 6 is not used and/or 1 and 2 are identical criteria), reflecting the maturity of that aspect of the measurement system. The maturity can be considered in three broad categories that give information on the scientific grade and sustainability of the measurements being assessed:

- Maturity scores 1 and 2 establish comprehensive measurement capability (CMC, comprehensive network type measurements): The instruments are placed in the field and recording data but may not be well curated or metrologically understood and calibrated.
- Maturity scores 3 and 4 establish a baseline measurement capability (BMC, baseline network type measurements): These measurements are better characterised and understood, and intended to be run for the long-term. However, they lack strict traceability and comparability.

- Maturity scores 5 and 6 establish a reference measurement capability (RMC, reference network type measurements): These measurements are very well characterised, with strict traceability and comparability, and robustly quantified uncertainties. The measurements are actively managed and curated, and envisaged as a sustained contribution.

Table 5.1: MM assessment for PGN for October 2019.

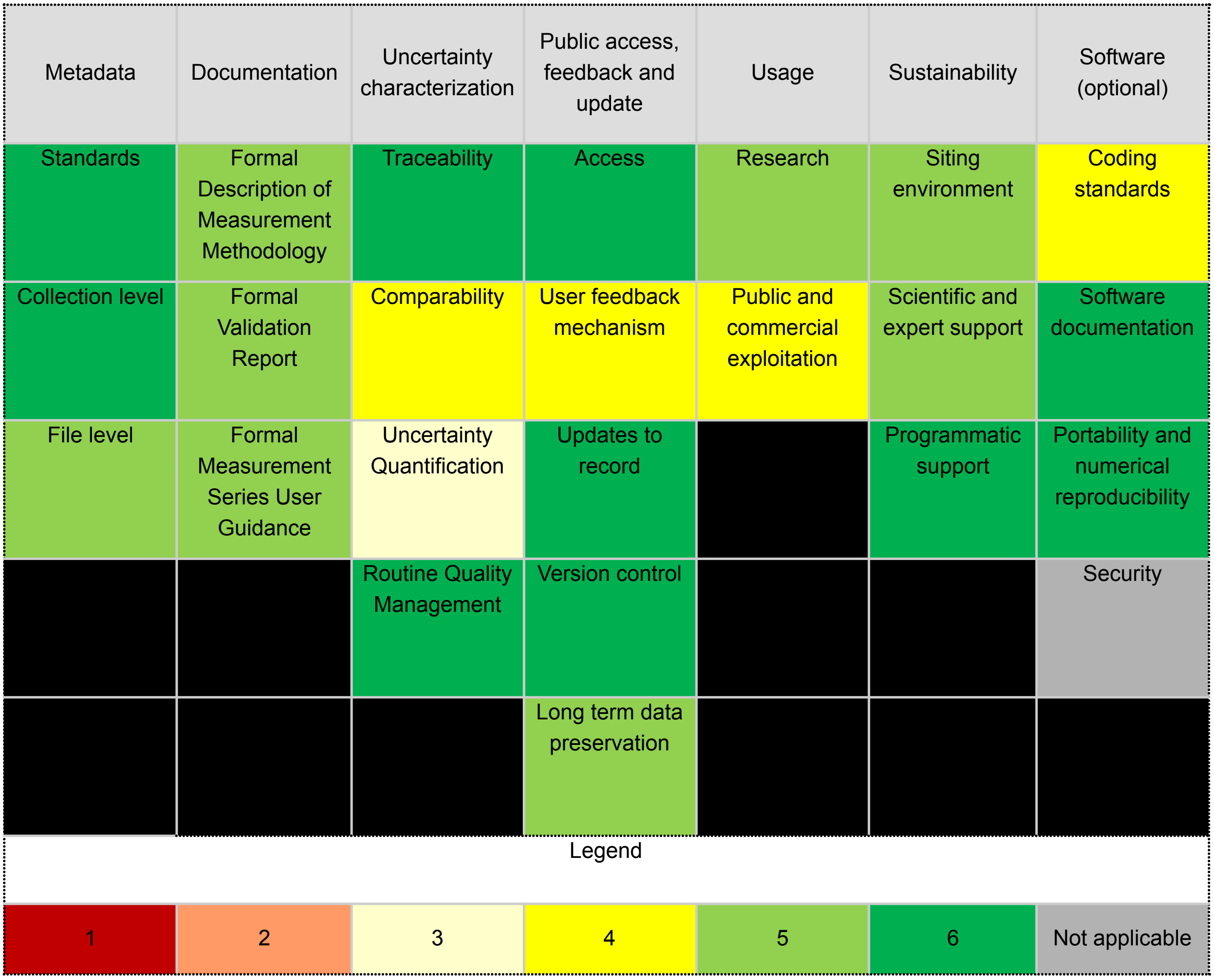


Metadata	Documentation	Uncertainty characterization	Public access, feedback and update	Usage	Sustainability	Software (optional)
Standards	Formal Description of Measurement Methodology	Traceability	Access	Research	Siting environment	Coding standards
Collection level	Formal Validation Report	Comparability	User feedback mechanism	Public and commercial exploitation	Scientific and expert support	Software documentation
File level	Formal Measurement Series User Guidance	Uncertainty Quantification	Updates to record		Programmatic support	Portability and numerical reproducibility
		Routine Quality Management	Version control			Security
			Long term data preservation			

Legend

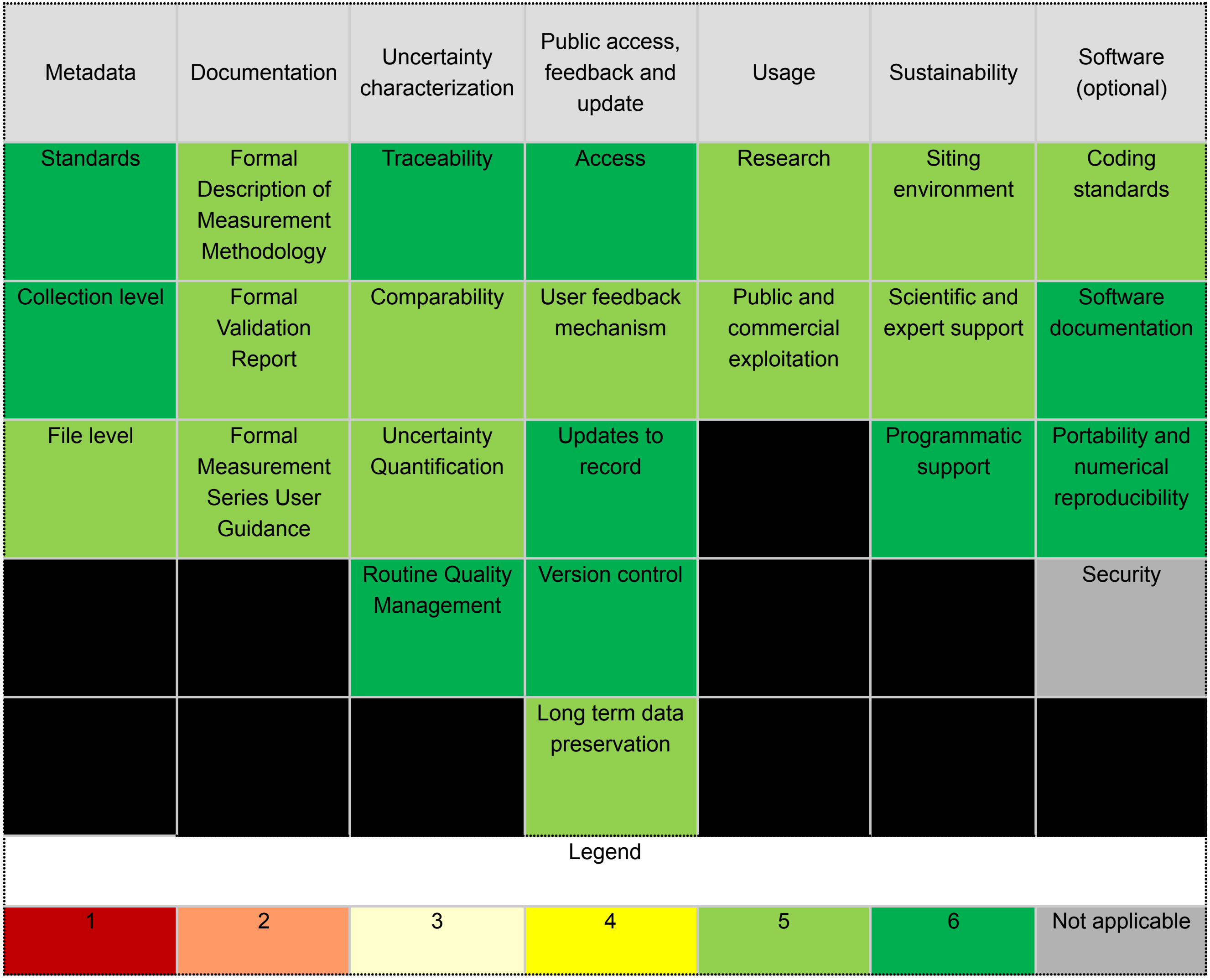
1	2	3	4	5	6	Not applicable

Table 5.2: MM assessment for PGN for October 2020. Note in particular the change in the 'Uncertainty Quantification' panel compared to the assessment made for the previous year.



Metadata	Documentation	Uncertainty characterization	Public access, feedback and update	Usage	Sustainability	Software (optional)
Standards	Formal Description of Measurement Methodology	Traceability	Access	Research	Siting environment	Coding standards
Collection level	Formal Validation Report	Comparability	User feedback mechanism	Public and commercial exploitation	Scientific and expert support	Software documentation
File level	Formal Measurement Series User Guidance	Uncertainty Quantification	Updates to record		Programmatic support	Portability and numerical reproducibility
		Routine Quality Management	Version control			Security
			Long term data preservation			
			Legend			
1	2	3	4	5	6	Not applicable

Table 5.3: Expected maturity matrix assessment for PGN for October 2021 after implementation of suggested improvements. Note in particular the change in the ‘Uncertainty Quantification’ panel compared to the assessments made for the previous 2 years.



Metadata	Documentation	Uncertainty characterization	Public access, feedback and update	Usage	Sustainability	Software (optional)
Standards	Formal Description of Measurement Methodology	Traceability	Access	Research	Siting environment	Coding standards
Collection level	Formal Validation Report	Comparability	User feedback mechanism	Public and commercial exploitation	Scientific and expert support	Software documentation
File level	Formal Measurement Series User Guidance	Uncertainty Quantification	Updates to record		Programmatic support	Portability and numerical reproducibility
		Routine Quality Management	Version control			Security
			Long term data preservation			
Legend						
1	2	3	4	5	6	Not applicable

Table 5.4: Reasons for PGN maturity level limitations for each category.

CATEGORY	**SUBCATEGORY**	**SCORE / LIMITATION**		
		Oct 2019	**Oct 2020**	**Oct 2021**
Uncertainty characterization	Uncertainty quantification	2 / Missing comprehensive information on uncertainty arising from systematic and random effects in the measurement.	3 / No quantitative estimates of uncertainty provided within the measurement products characterising more or less uncertain data points.	*Matured to reference measurement capability*
	Comparability	4 / Not compared regularly to at least one measurement that has a traceability score >=5.		*Matured to reference measurement capability*
Public access, feedback and update	Long term data preservation	4 / Metadata is not archived at a recognised data repository such as a National Meteorological Service, national archive or international repository.	*Matured to reference measurement capability*	
	User feedback mechanism	4 / Missing established feedback mechanism and no international data quality assessment results are considered.		*Matured to reference measurement capability*
Usage	Public and commercial exploitation	4 / Societal and economical benefits not yet demonstrated.		*Matured to reference measurement capability*
(optional) Software	Coding standards	3 / Compliance is not systematically checked in all code and not compliant to the standards.	4 / Measurement provider has not identified departures from the standards and no actions are planned to achieve full compliance.	*Matured to reference measurement capability (which includes actions planned to achieve full compliance.)*
	Security	Not applicable since the software package is open source and can therefore be changed by any user.		