



QA4EO Cal/Val Workshop # 1, 19-21 February 2020, Univ. La Sapienza, Rome, Italy

Uncertainty of PGN data products

- current status and planned improvements

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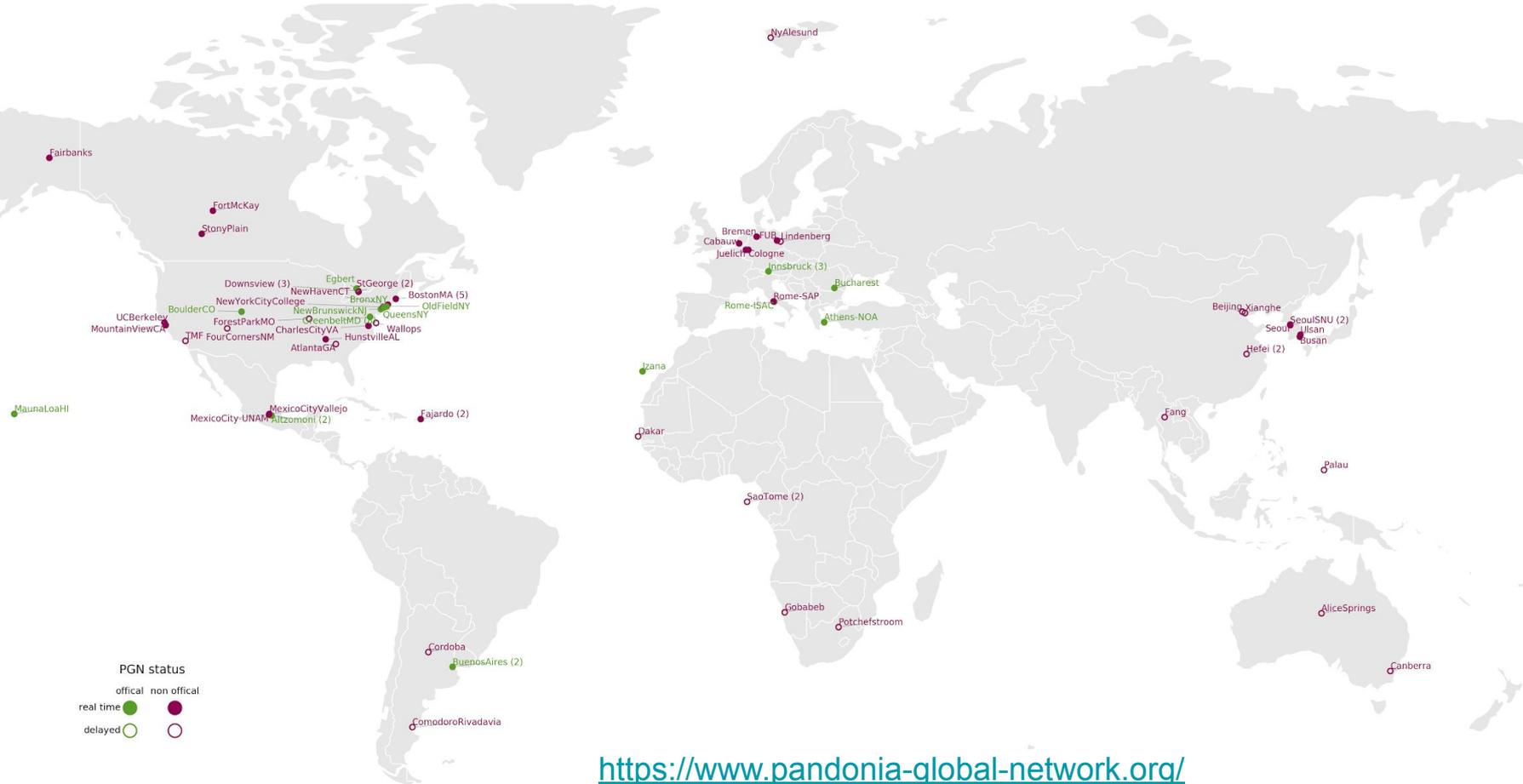
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Pandonia Global Network (Dec 2019)



<https://www.pandonia-global-network.org/>

Total columns (DU)



Tropospheric columns (DU)



Surface concentrations (ppb)



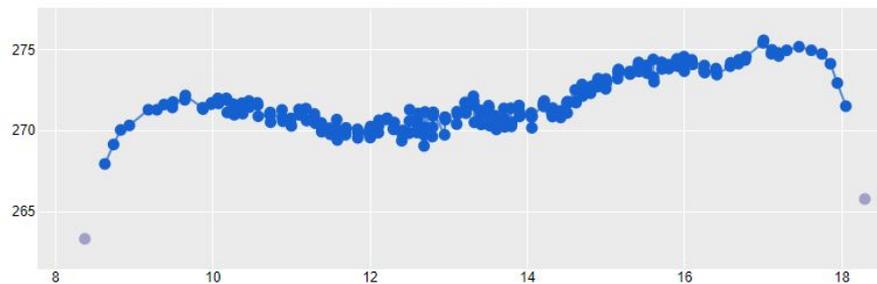
2020-02-19
x-axes are local time

Izana - 101

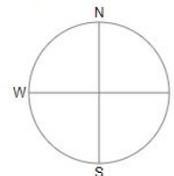


101: O3 - total column

2020-02-19



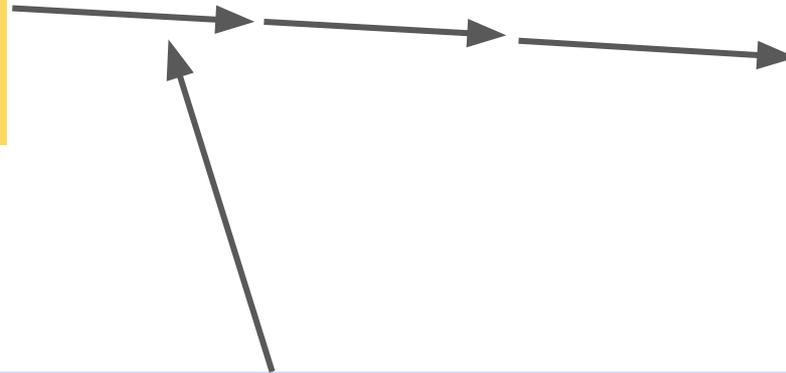
parameter	value	median
local time	-	-
total column	DU -	2.713e+2
uncertainty	DU -	8.662e-2
fit RMS	-	4.510e-3
wl. shift	nm -	4.573e-2
SZA	deg -	-
AMF	-	-
T int.	ms -	-
FW1	-	-
FW2	-	-



PGN Products Uncertainty

Currently given:

- Precision
- Data quality flags

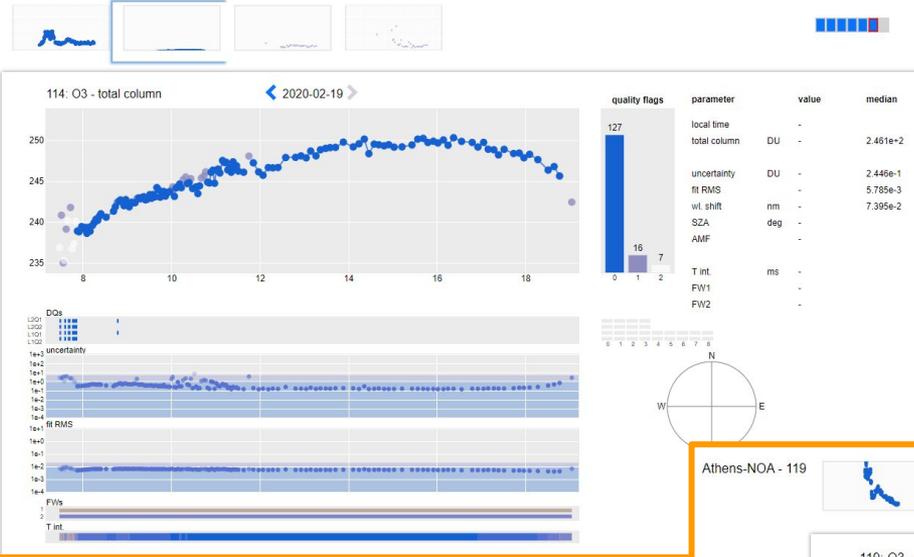


Final goal:

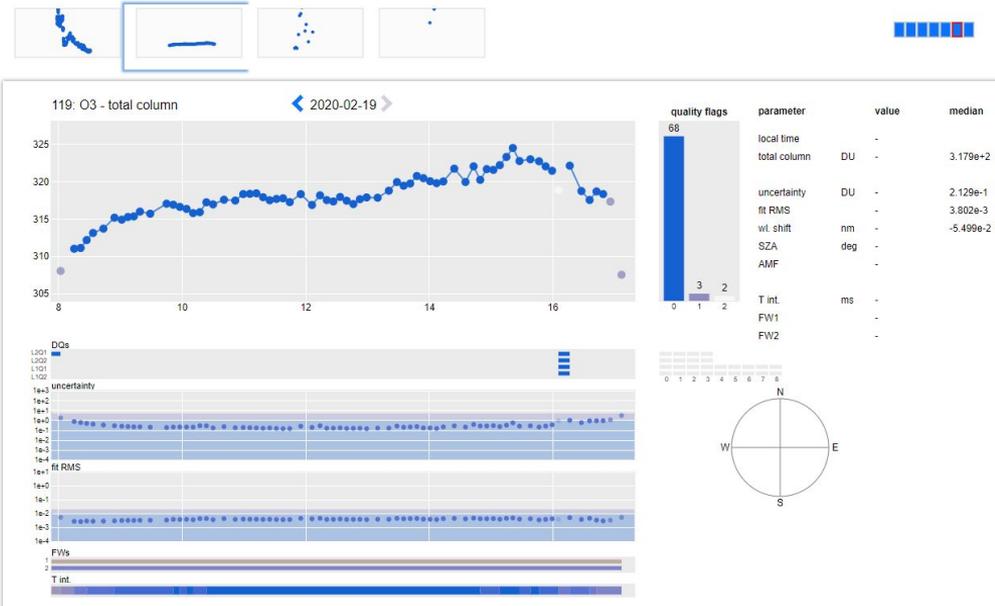
- Accuracy

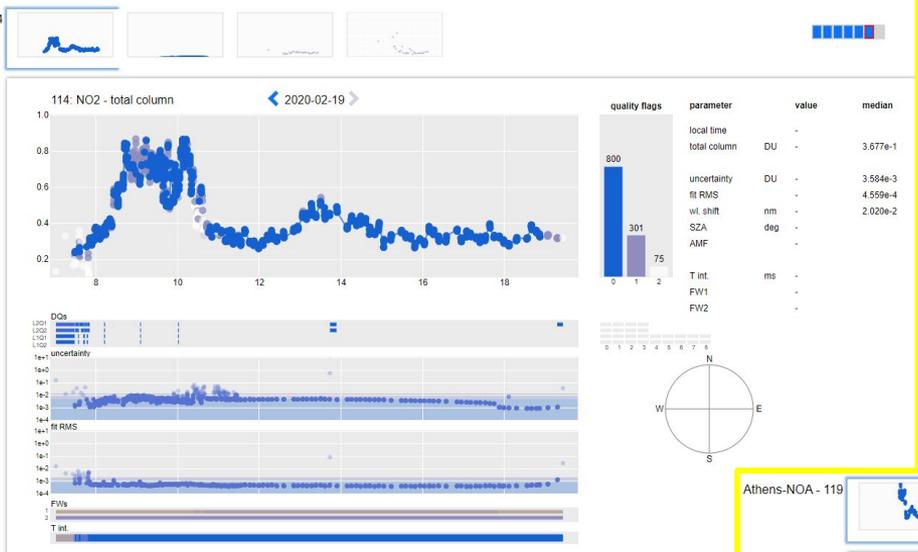
QA4EO - WP2125 = Phase 1 of this process

Qualitative study on the systematic uncertainties involved in all processing steps from raw data (Level 0, L0), over corrected spectra (Level 1, L1) to final products (Level 2, L2)

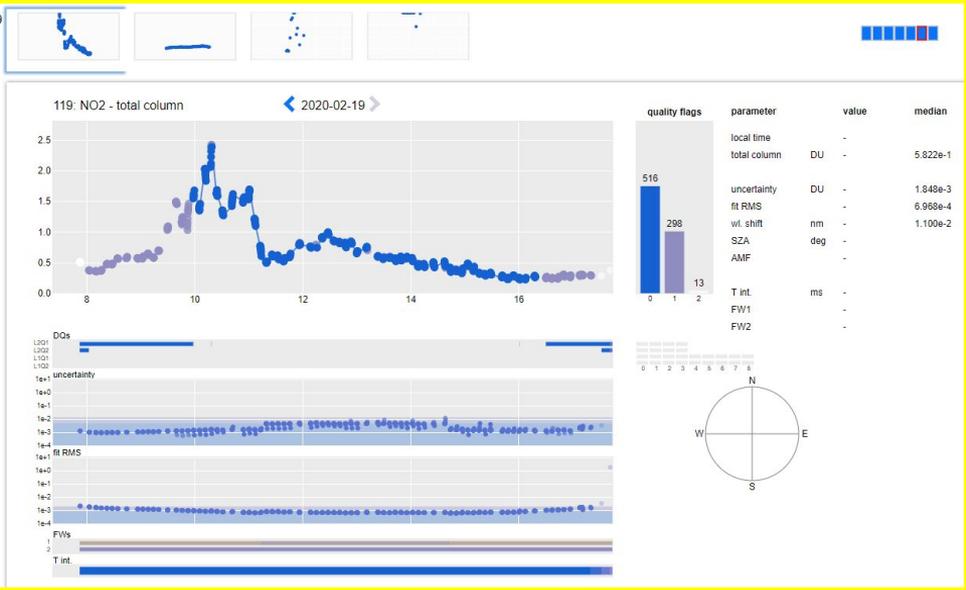


O₃





NO₂



Current uncertainty information: Precision

Raw data (L0)

- **“Measured uncertainty”**: This is the combination of instrumental noise and atmospheric variation over the measurements duration, based on the measured standard error of the raw data (over several cycles).
- **“Instrumental uncertainty”**: This is the instrumental noise over the measurements duration, based on the calculated instrumental noise of the raw data which is known from the calibration.

The “Measured uncertainty” and “Instrumental uncertainty” are propagated through all correction steps and reported in the L1 and L2 data.

Current uncertainty information: Data quality flags (DQF)

A combination of data quality indicators such as ...

- the uncertainties from the previous slide
- the rms of the spectral fitting residuals
- wavelength shifts
- ...

is used to produce the DQF:

- DQF 0 means assured high data quality. Those data can be used with high confidence.
- DQF 1 means assured medium data quality. Depending on the application, the user should decide whether to use these data.
- DQF 2 means assured low data quality. For most purposes, the user should not use these data. As for DQF 1, the low quality can origin from instrumental or atmospheric sources.

Outline for QA4EO - WP on Pandonia Products Uncertainty



Goal:

Do a study to determine the hierarchy and magnitude of each of the uncertainty estimates for all data processing steps and parameters involved in the data analysis.

Individual tasks:

- A. Perform a qualitative study on the systematic uncertainty of the L1 correction steps.
- B. Perform a qualitative study on the systematic uncertainty of the preparation of the data for the spectral fitting.
- C. Perform a qualitative study on the systematic uncertainty of the spectral fitting.
- D. Perform a qualitative study on the systematic uncertainty of the air mass factor.



Outline for QA4EO - WP on Pandora Products Uncertainty



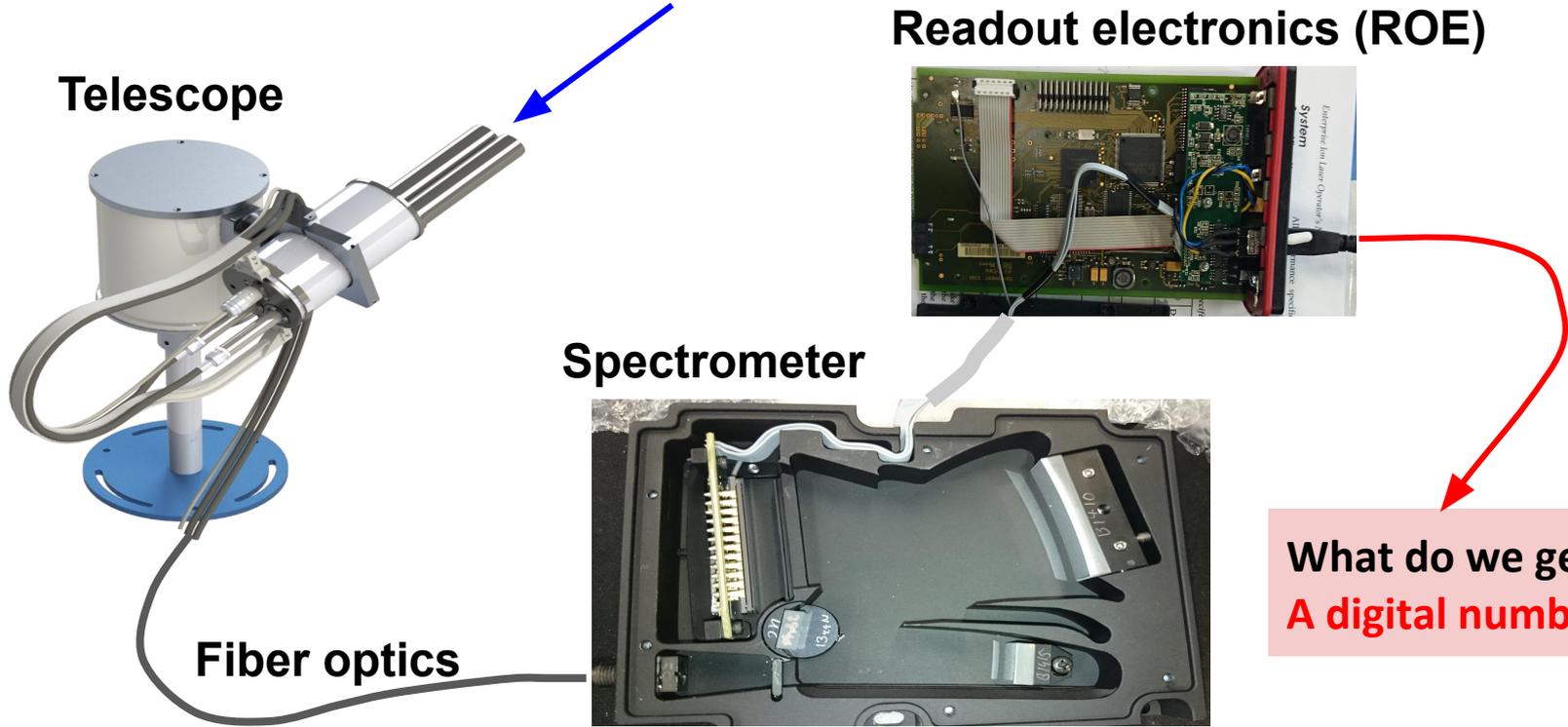
Method

- The relevant parameters for each of the processing steps are identified and - for the sensitivity study - each is changed individually within realistic limits to quantify the impact of that change.
- The data processing algorithm is then rerun many times with the parameter being slightly changed for each new run and the change in the corresponding uncertainty is logged and investigated.
- The following slides show examples for some of the L1 correction steps. However for these case the correction is not just modified, but “switched off” entirely.



What do we want to measure?

Spectral Irradiance $[W/m^2/nm]$ = Energy received per time interval $(J/s=W)$ per area (m^2) per wavelength interval (nm)



What do we get?
A digital number (DN)

Setup and operation of routines to perform a qualitative study on the systematic uncertainty of the **L1 correction steps**:

**From front (telescope)
to back (readout electronics)**



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

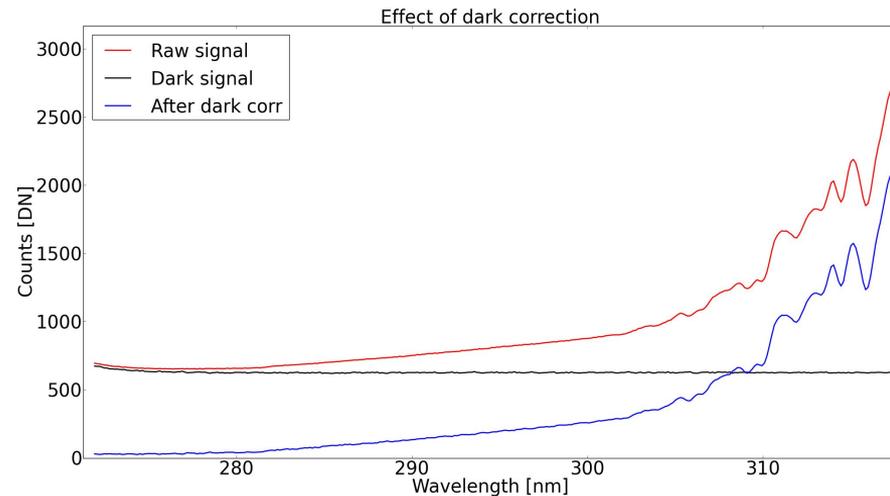
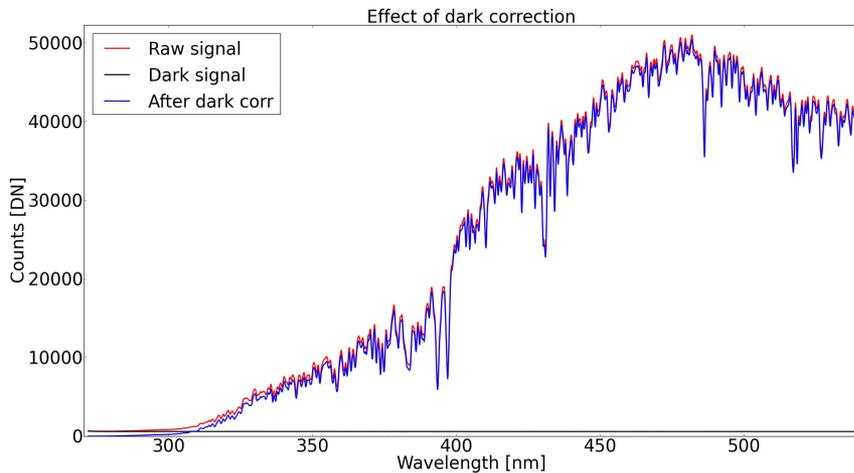
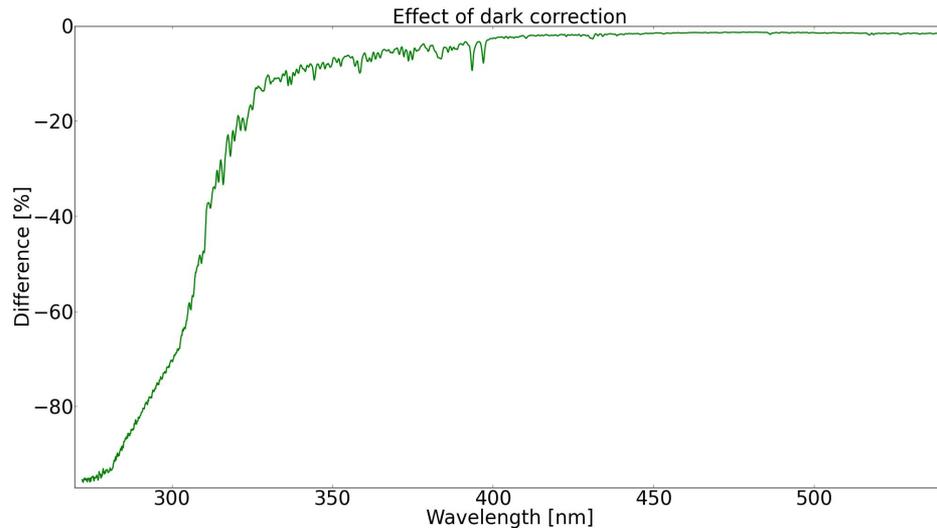


**From back (DN)
to front (Radiance)**

Sneak peek effects on L1

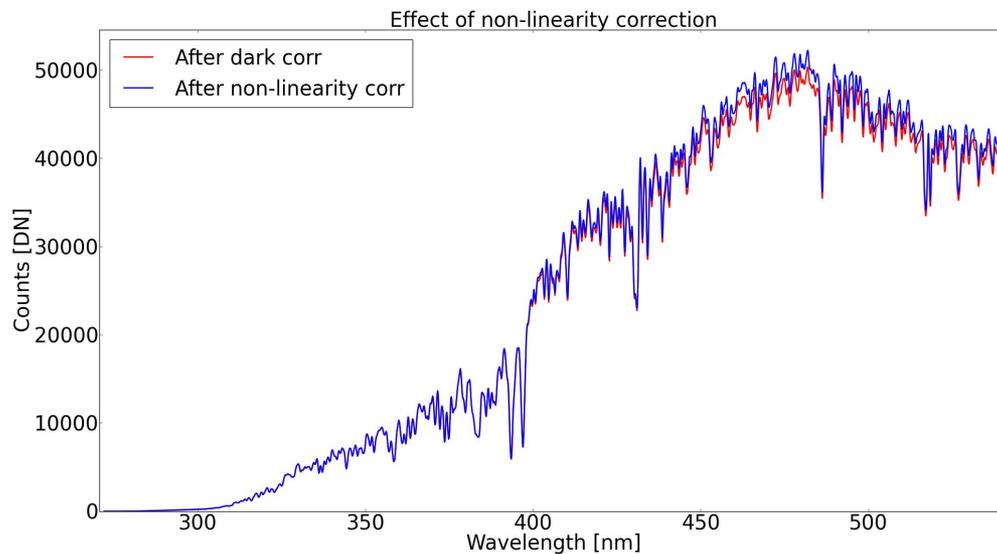
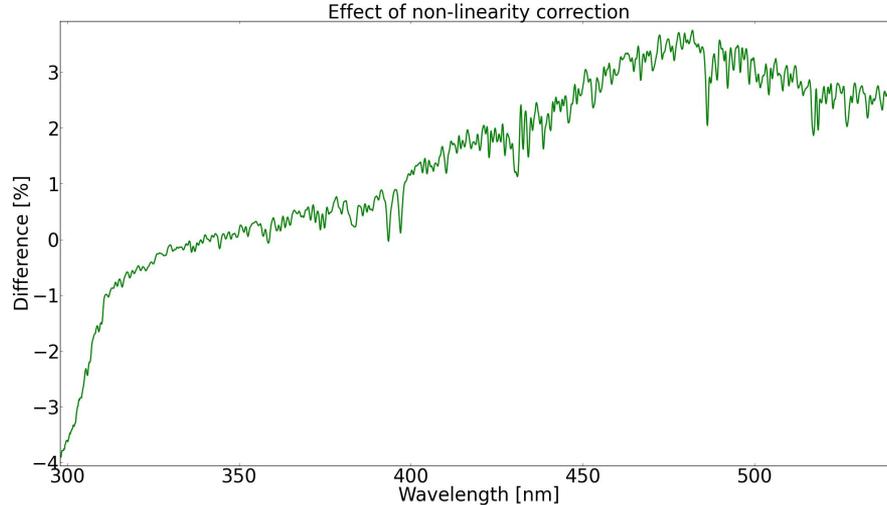
Effect of Dark correction

Spectra shown here are direct sun at noon (SZA=56°) on 17 Oct 2019 at Innsbruck.



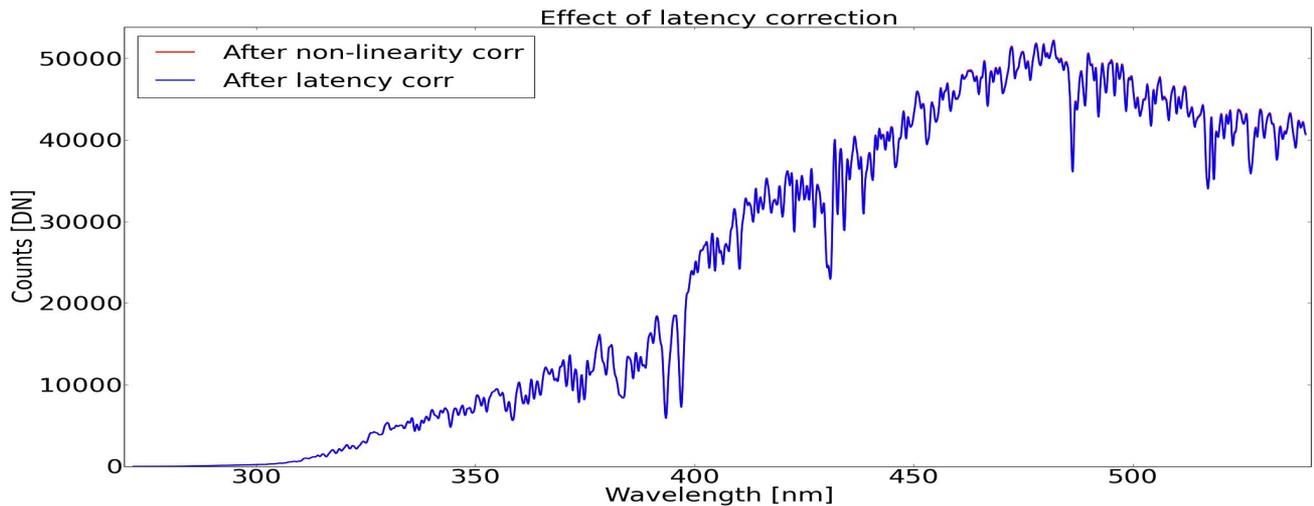
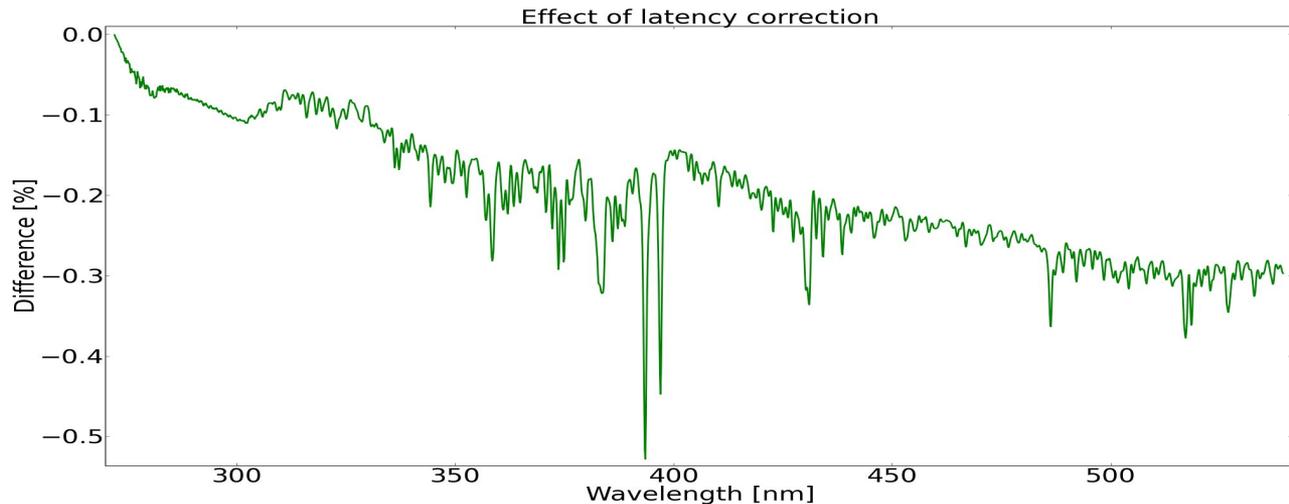
Sneak peek effects on L1

Effect of Non-linearity correction



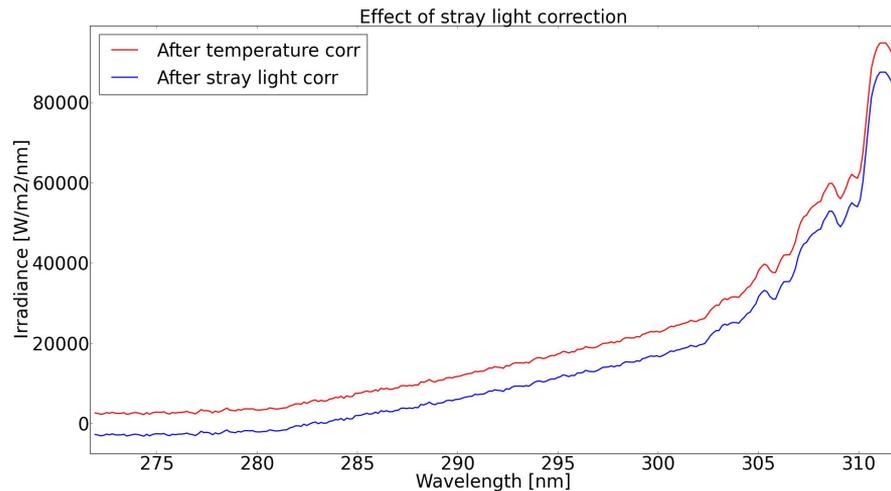
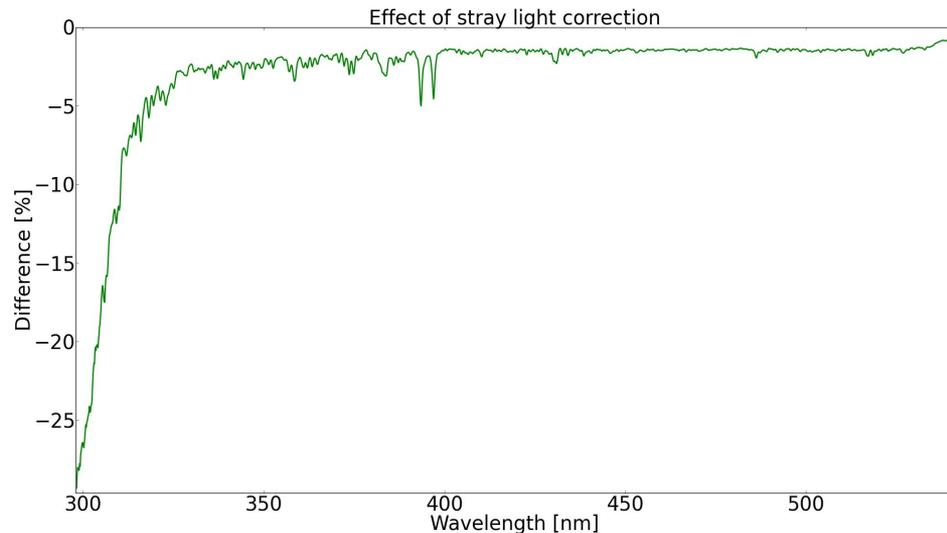
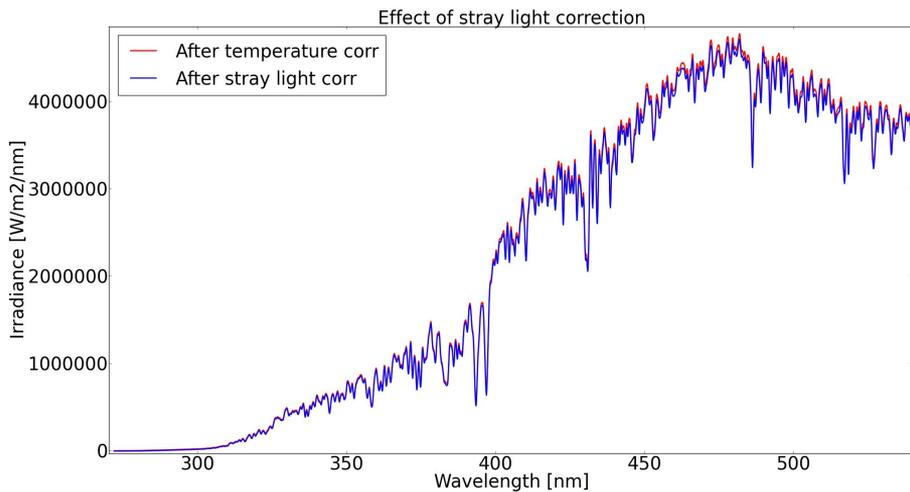
Sneak peek effects on L1

Effect of latency correction



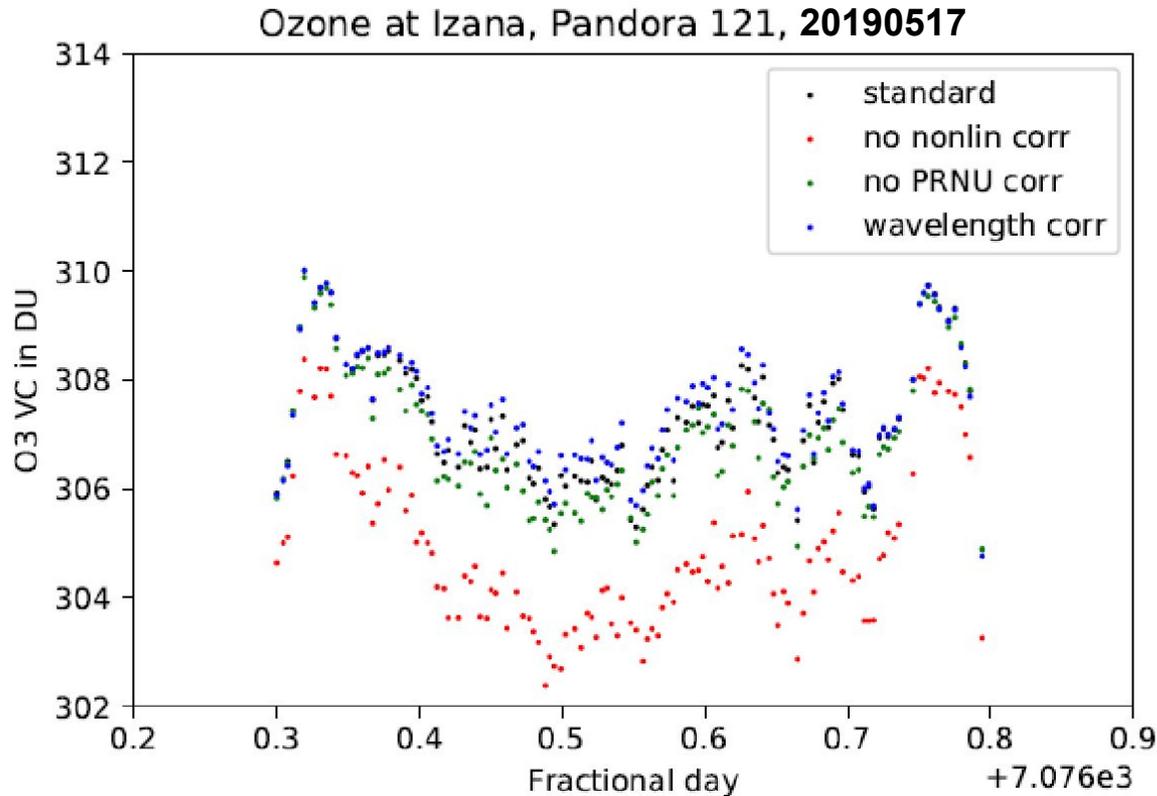
Sneak peek effects on L1

Effect of Stray light correction



Sneak peek effects on L2

Effects of Linearity,
PRNU, wavelength
correction



Thank you



Description of the NO₂ total column PGN data product

- Total NO₂ column amount between the surface and the top of the atmosphere
- Measured in direct sun mode (see Figure below) using the nvs1 retrieval code
- NO₂ amount is expressed in DU, 1 DU = 2.687e20 molecules/m³
- The precision of the NO₂ column is <0.005 DU for DQF 0 data
- The accuracy is approx. 0.05 DU for DQF 0 data at 1-sigma with data accuracy depending mostly on the quality of the calibration
- PGN NO₂ data is retrieved above 400 nm -> straylight not important
- NO₂ is extremely heterogeneous in time and space
-> comparison with e.g. surface in-situ data more complicated
- Difference in viewing geometry compared to satellite data
-> possible cause for differences to PGN data

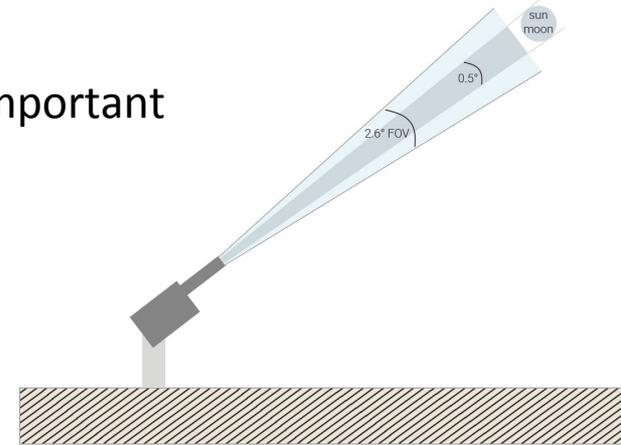


Figure: Direct sun observations

Direct sun observations and AMF

The air mass factor (AMF) in the PGN direct sun retrievals used to convert the measured slant columns into vertical columns can be estimated as follows:

$$\text{AMF}(Z A^*) = \sec(Z A')$$

Assumption: The vertical distribution of the trace gas is a delta function at h_{eff} .

The accuracy of AMF depends mostly on how well h_{eff} represents the "truth" but is in general better than 2% for $Z A < 80^\circ$.

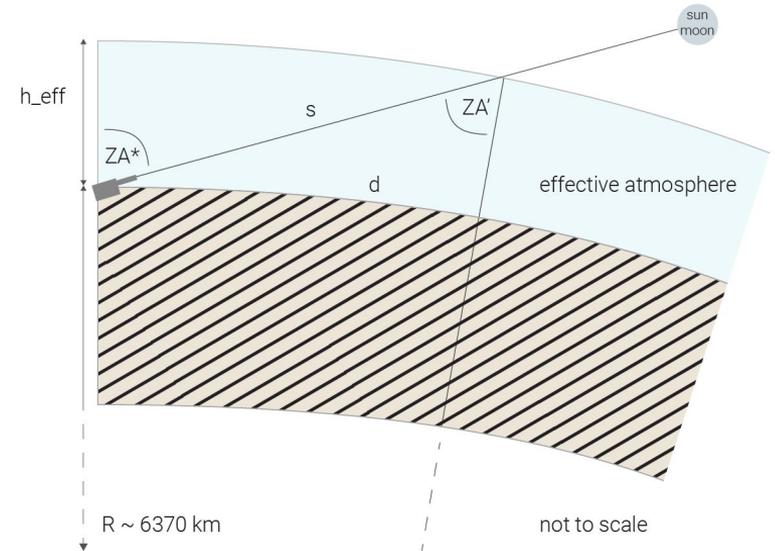


Figure: Direct sun geometry