QA4EO-IDEAS Cal/Val Workshop#2, webex, 2 December 2020

Improved uncertainty estimation in support to Pandonia Global Network (PGN)

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WP2125 - "Qualitative accuracy assessment of operational PGN data products"

- Goal (1) - Analyze the maturity level of the Pandonia Global Network (PGN) at the beginning and the end of phase 1 of this project.
- 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.
- Goal (3) - Determine the impact of uncertainties in the laboratory calibration on the official PGN data products total ozone (O3) and total nitrogen dioxide (NO2) column amounts.
  This task consumed the majority of the time and manpower effort in this project as it involved a lot of testing, variation, calculations, etc.

Goal (1) - Maturity level of PGN at the beginning and end of phase 1 of QA4EO-IDEAS

MM assessment for PGN for October 2019 - status at the start of QA4EO

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

- Maturity matrix (MM) approach is used to assess various features of a measurement network (Thorne et al., 2017).
- 7 categories (columns) with several sub-categories which are assigned a score from 1 to 6 (see legend).
- The maturity is considered in 3 broad categories that provide information on the scientific grade and sustainability of the measurements being assessed:

Score **1** & **2**: comprehensive measurement capability

Score **3** & **4**: baseline measurement capability

Score **5** & **6**: reference measurement capability

Goal (1) - Maturity level of PGN at the beginning and end of phase 1 of QA4EO-IDEAS

MM assessment for PGN for October 2020 - status at the end of phase 1 of QA4EO

Metadata	Documentation	Uncertainty characterization	Public access, feedback and update	Usage	Sustainability	Software (optional)
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Legend						
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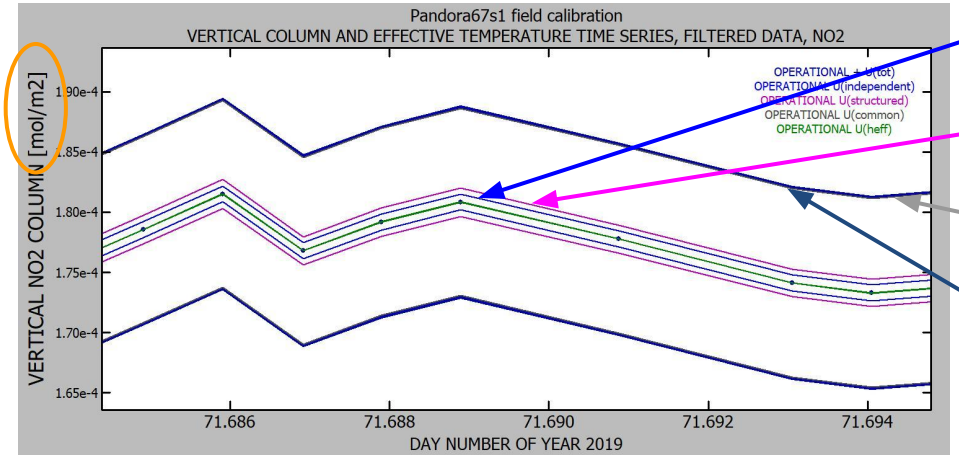
- Change in the ‘Uncertainty Quantification’ & ‘Long term data preservation’ panels compared to the assessment made for the previous year.

Goal (2) - Nomenclature and usage of the uncertainty output in the PGN data products

- Current version V1.7 of the Blick Software Suite (software to process all PGN data) will be soon replaced by V1.8.
- V1.8 extensively restructured and updated taking into account the correct nomenclature and usage of data uncertainties as recommended by NPL/Emma Woolliams.
- Error sources not “captured” by the uncertainty are included in the data quality flags:
  DQ0=high quality, DQ1=medium quality, DQ2=low quality
  DQ10, DQ11, DQ12: as above but data still not quality assured



Independent uncertainty

Structured uncertainty

Common uncertainty

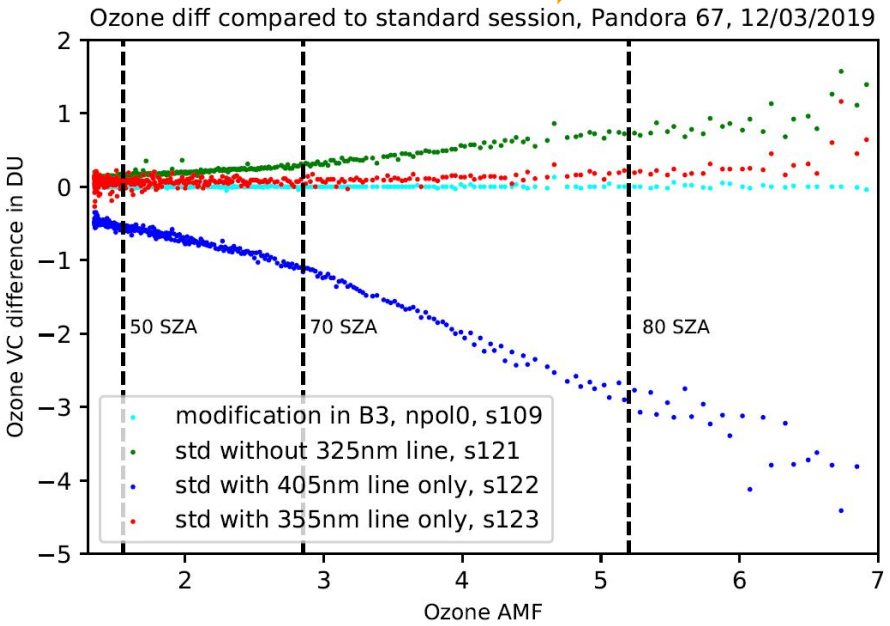
Total uncertainty

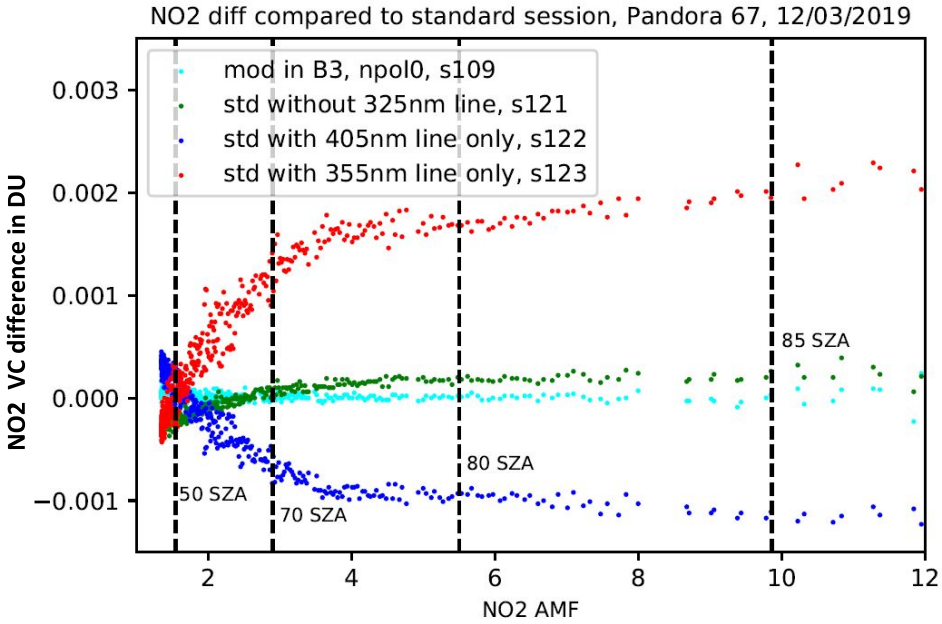
Goal (3) - Determine the impact of uncertainties in the laboratory calibration on ozone and NO_2 columns

- Case study using direct sun measurements made with Pandora #67 located at Greenbelt/USA on 12 March 2019.
- Analysis and calibration processing steps (or actions) using the Blick Calibration Software (BlickC) were done by introducing 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 following calibration steps were investigated:
  - Dark correction
  - Non-linearity correction
  - Latency correction
  - Flat field correction
  - Temperature correction
  - Stray light correction
  - Sensitivity correction
  - Wavelength correction

Example of impact for calibration step “Analyze stray light”

Difference to “reference” session for session with modified evaluation of the laboratory stray light measurements for **ozone** and **NO_2**.





Summary of the qualitative impact of the L1 correction steps on the retrieved total ozone and total NO_2 column amounts, sorted by decreasing impact

Note: 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 caused by different ways to calibrate the instrument.

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%

Conclusions of WP2125

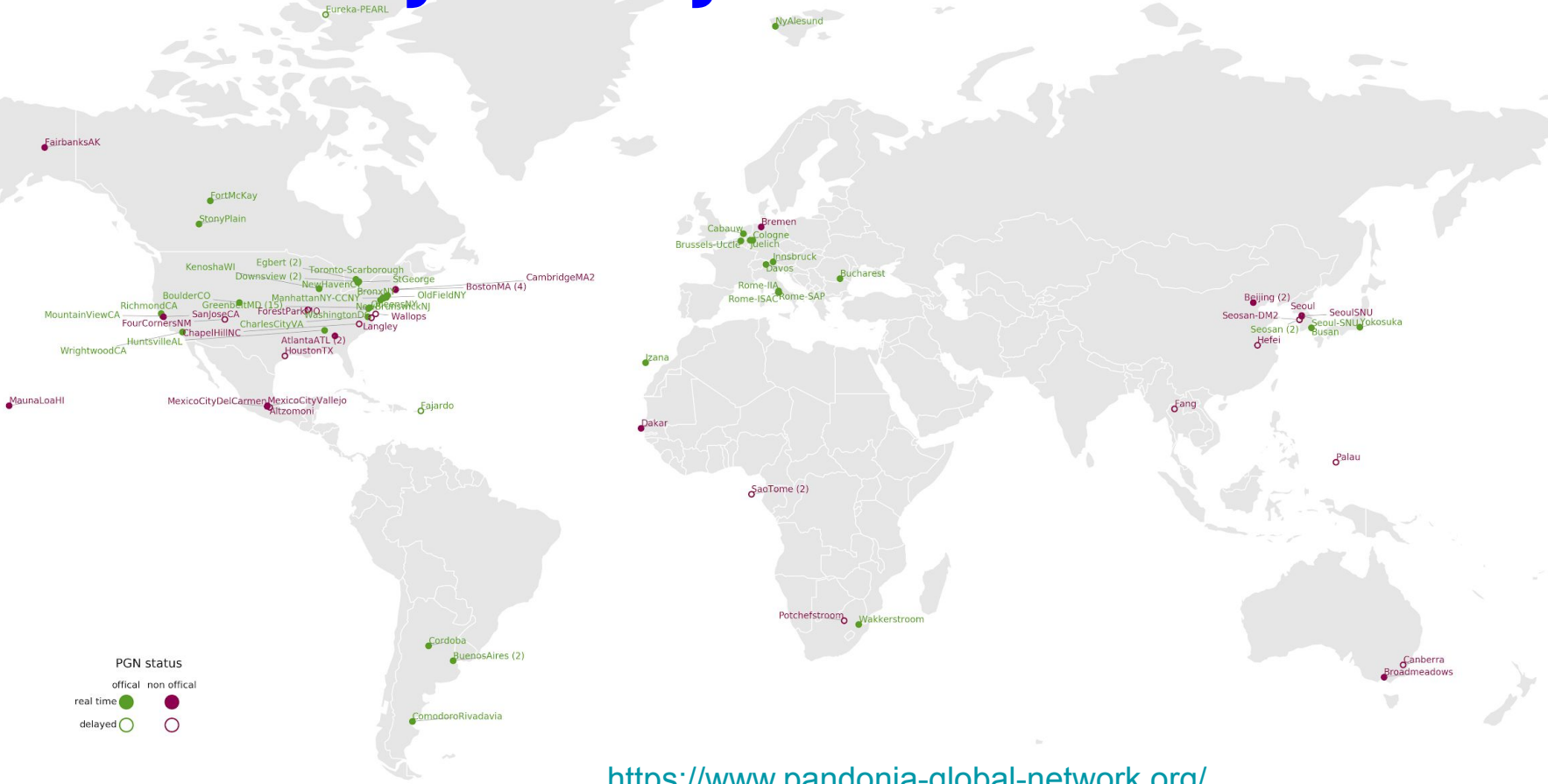
List of suggested improvements based on the outcome of the PGN uncertainty study to further reduce the uncertainty in the PGN products:

- The spectral coverage of the lasers with respect to the stray light calibration needs to be improved. Currently only the lab at NASA/Goddard Space Flight Center, in Greenbelt, MD, USA, has a sufficient number of lasers. Hence a major step to reduce the PGN data uncertainty is to improve the stray light calibration equipment in the PGN laboratories.

- The impact of laboratory uncertainties on the L1 data in the Blick processing software (BlickP) needs to be included as an additional (common) uncertainty, which totals the sum of all effects analyzed in this project. This will be developed during the next phase of this project.

- 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). This task is also included in the next phase of this project.

Thank you for your attention!



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