Pandonia Improved Uncertainty Estimation

Ilias Bougoudis, Leonie Haunold, Manuel Gebetsberger, Martin Tiefengraber

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Outlook

Goals if this WP

1. Determine the common (=systematic) uncertainty of total O_3 when a literature reference is used.
2. Comparison of retrieved O_3 effective temperature and column with external datasets
   - MERRA-2 assimilations
   - O_3 sondes (extrapolated with MERRA-2)
   - Brewer V2 data
3. First attempt to compare uncertainties for total O_3 based on
   - Pandora using upcoming processor.
   - Brewer using V2 data.

O_3 Common Uncertainty Determination

Currently **no common uncertainty** for total O_3 given when **literature reference** is used!

Total O_3 based on literature reference uses O_3 temperature climatology.
→ **$O3_{lit}$**

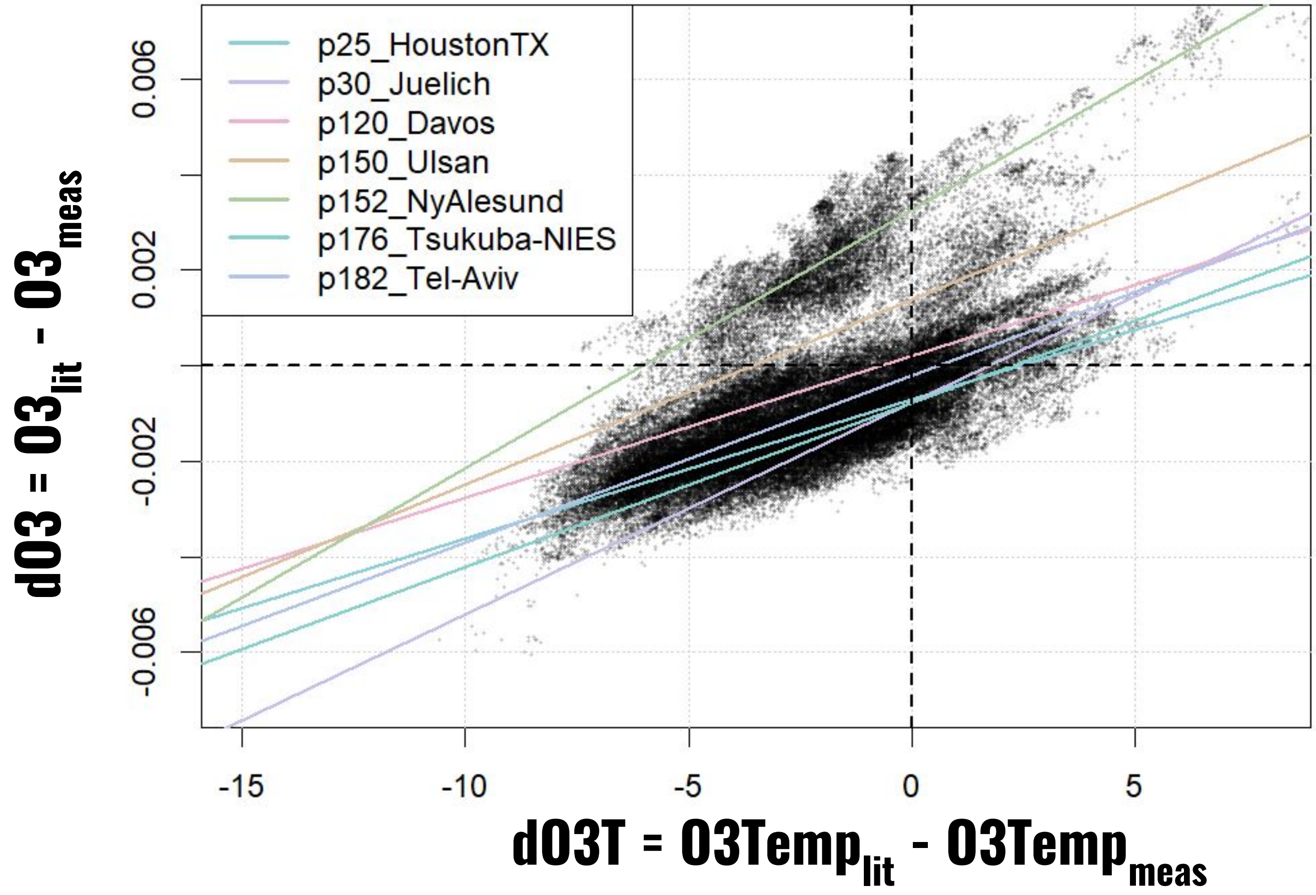
Total O_3 based on measured reference fits O_3 temperature.
→ **$O3_{meas}$**

Assumption:
Difference between $O3_{lit}$ and $O3_{meas}$ is driven by temperature difference.
→ **good estimate for common uncertainty**.

We ignore station specific differences, like

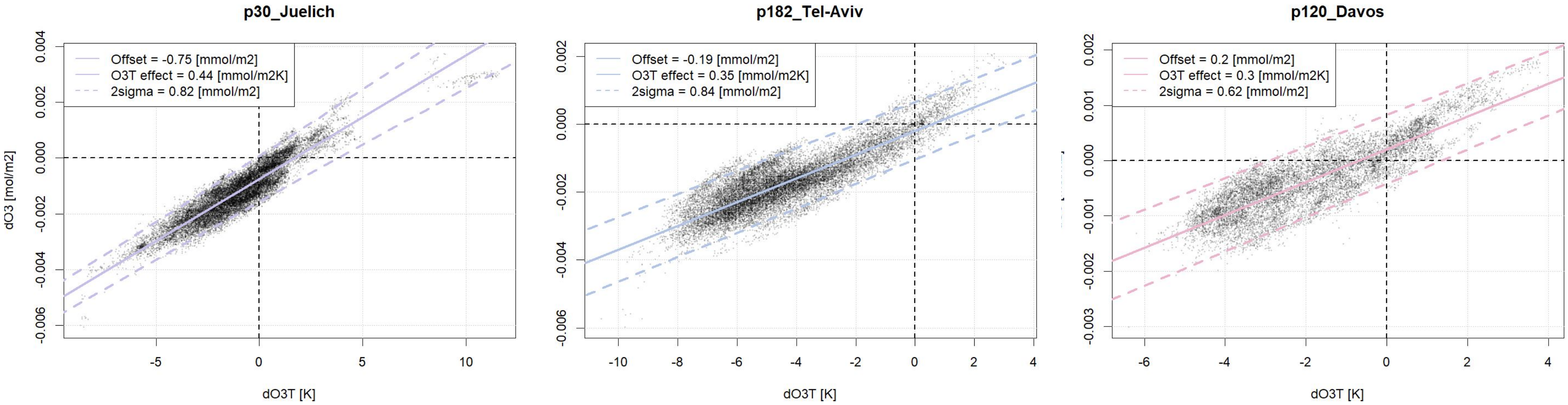
- bias in O_3 temperature climatology
- imperfect calibration of O_3 and O_3T

O_3 Common Uncertainty Determination



Common uncertainty to be evaluated as the standard deviation of the residuals of individual stations fit.

O_3 Common Uncertainty Determination



Median values (standard deviation) among instrument specific evaluation:

Offset [mmol/m2]	O_3T effect [mmol/K]	Common uncertainty [mmol/m2]
-0.19 (+/- 1.5)	0.35 (+/- 0.09)	0.43 (+/- 0.16)

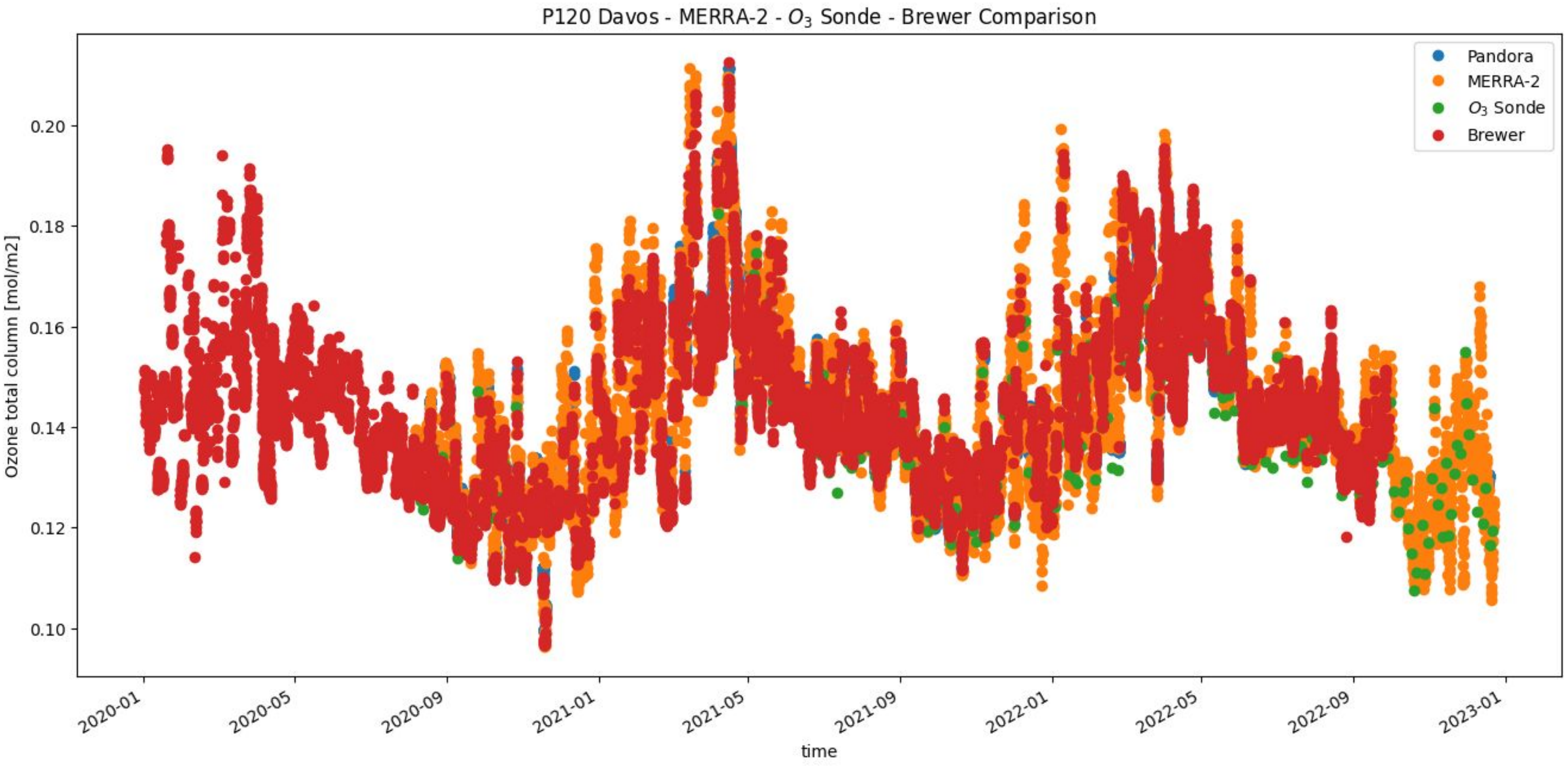
Comparisons of retrieved O_3 temperature with External Datasets

- MERRA-2 (Modern-Era Retrospective analysis for Research and Applications), is a NASA atmospheric reanalysis, based on the Goddard Earth Observing System Model, Version 5 (GEOS-5) data assimilation system

- O_3 sondes are lightweight, balloon-borne instruments that are mated to a conventional meteorological radiosonde. It transmits O_3 related data as the balloon ascents.
  - O_3 sondes were extrapolated with MERRA-2 data

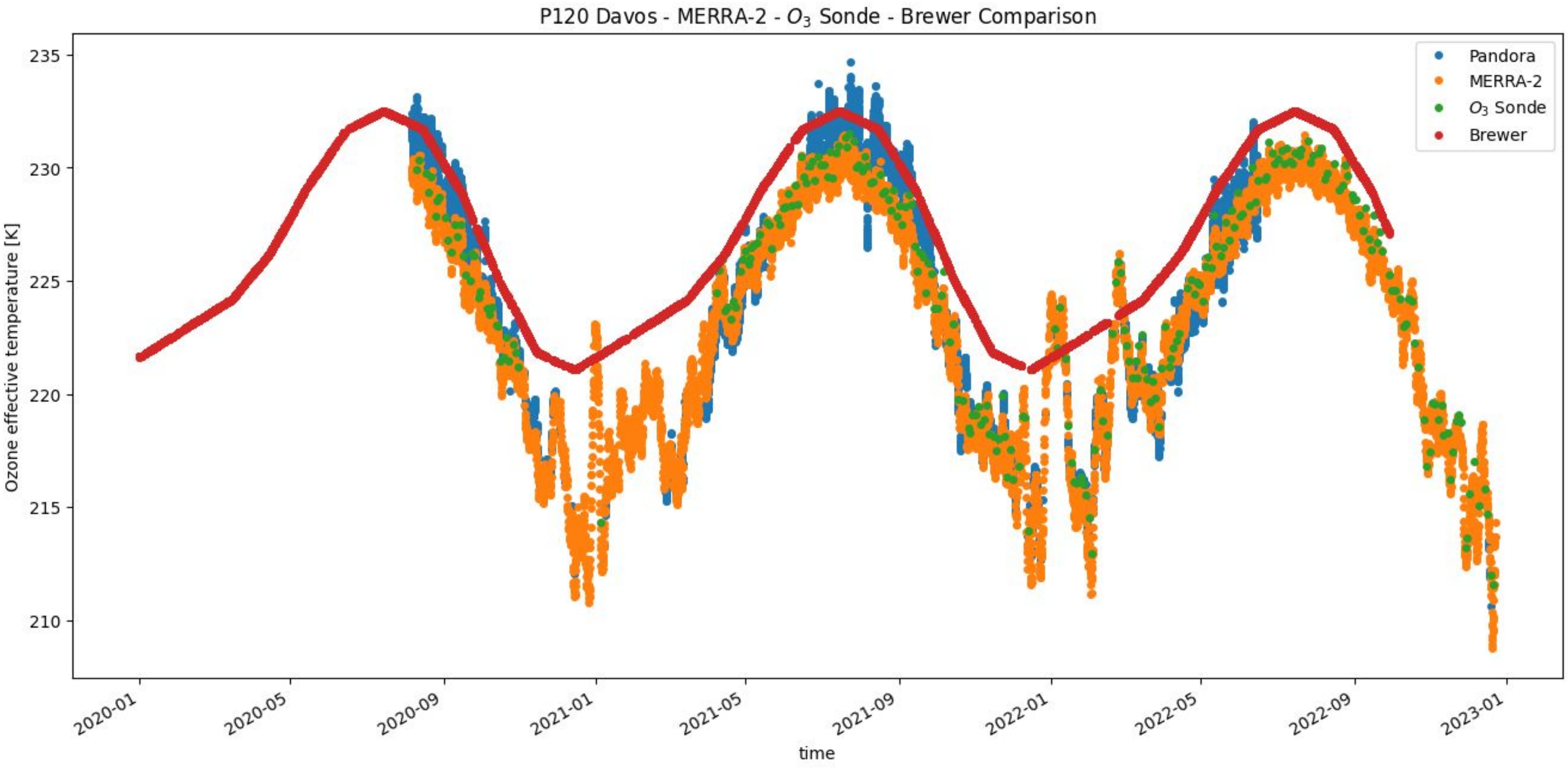
- EUBREWNET is a coherent network of European Brewer Spectrophotometer monitoring stations in order to harmonise operations and develop approaches, practices and protocols to achieve consistency in quality control, quality assurance and coordinated operations.
  - One co-located station used (Davos)

- Results will be shown per station; All Pandora data are quality and AMF filtered

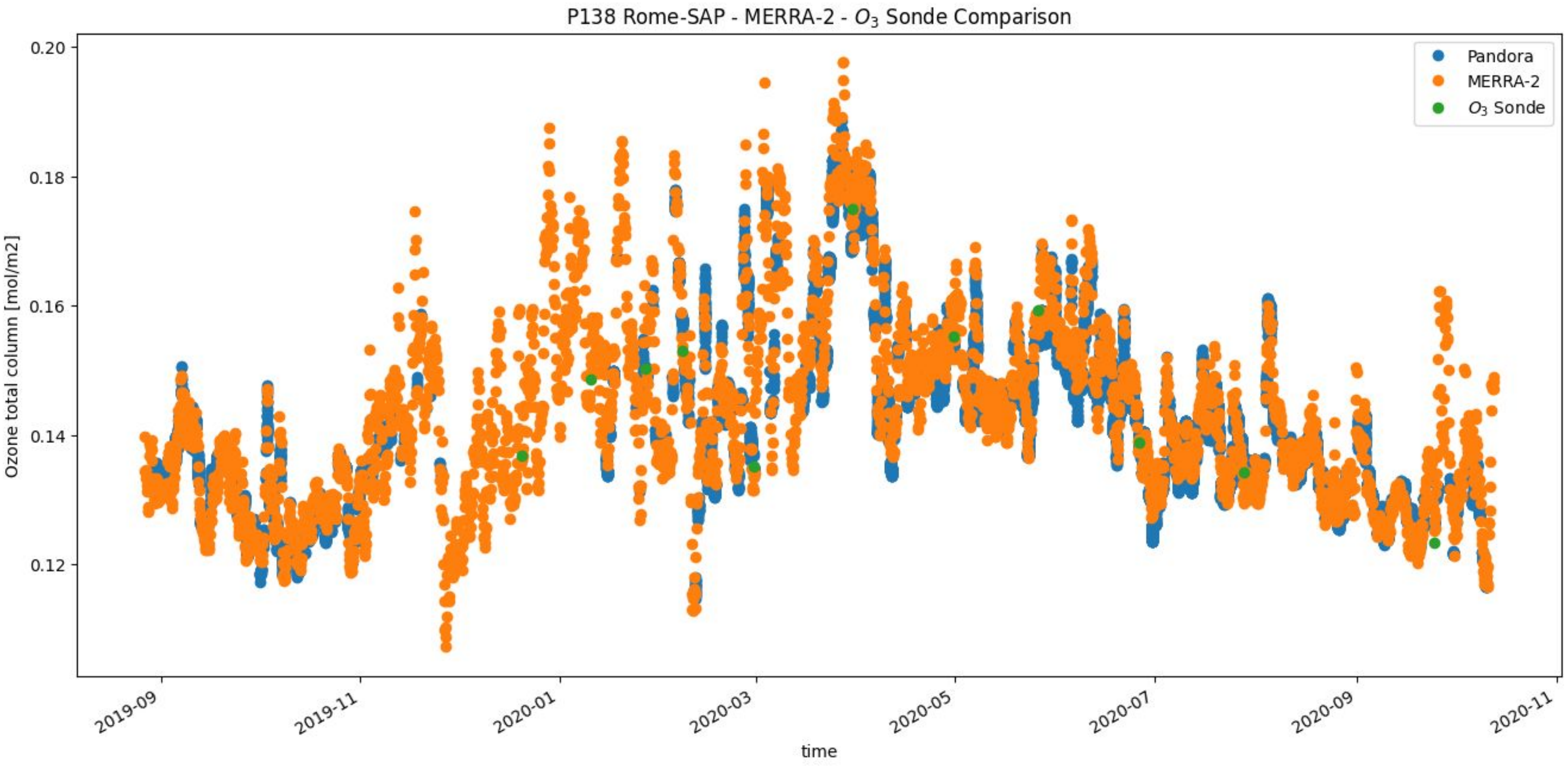


P120 Davos - MERRA-2 - O_3 Sonde - Brewer Comparison
Pandora
MERRA-2
O_3 Sonde
Brewer
Ozone total column [mol/m2]
0.10
0.12
0.14
0.16
0.18
0.20
2020-01
2020-05
2020-09
2021-01
2021-05
2021-09
2022-01
2022-05
2022-09
2023-01
time

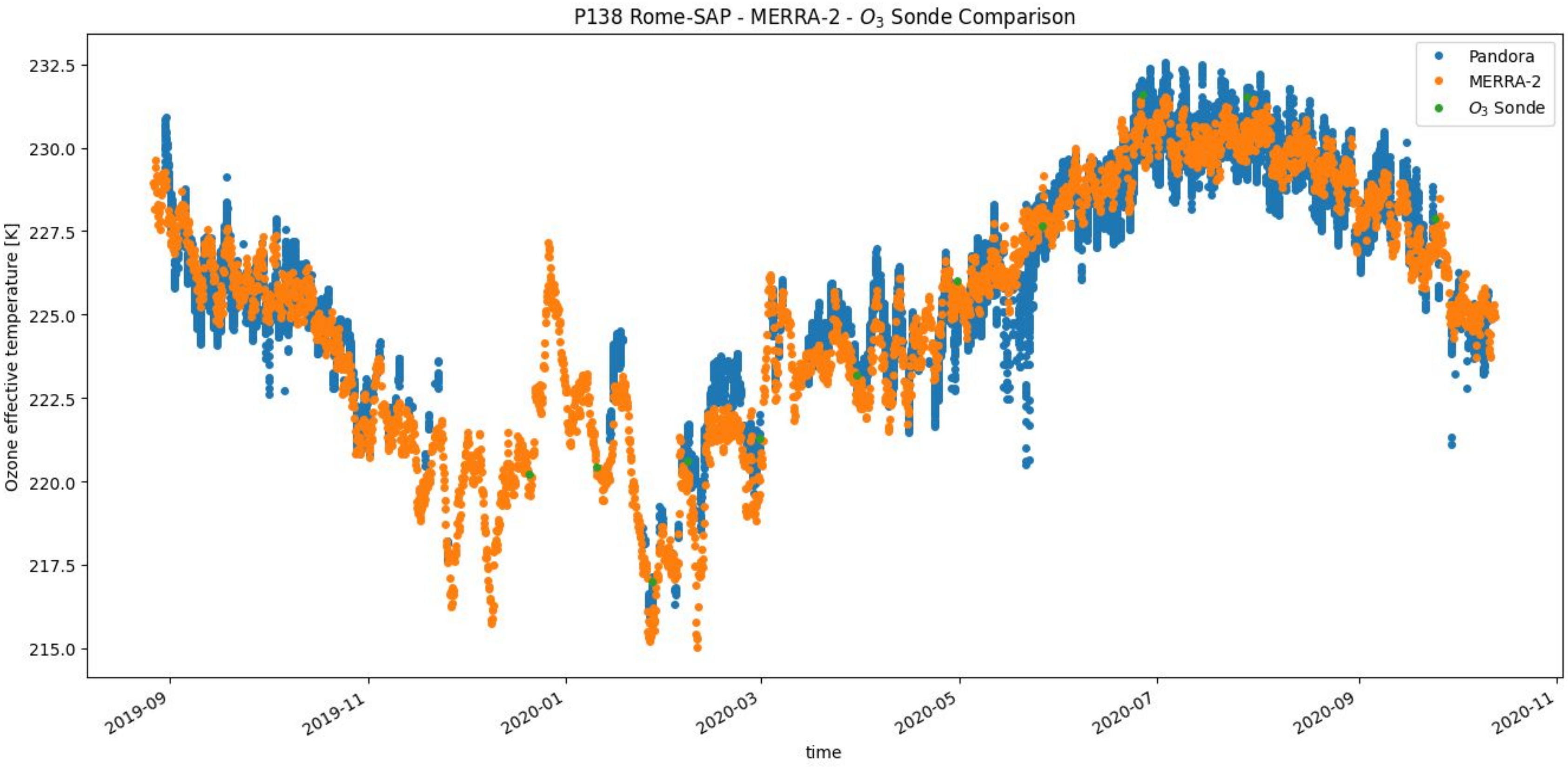
Comparisons with External Datasets - Davos



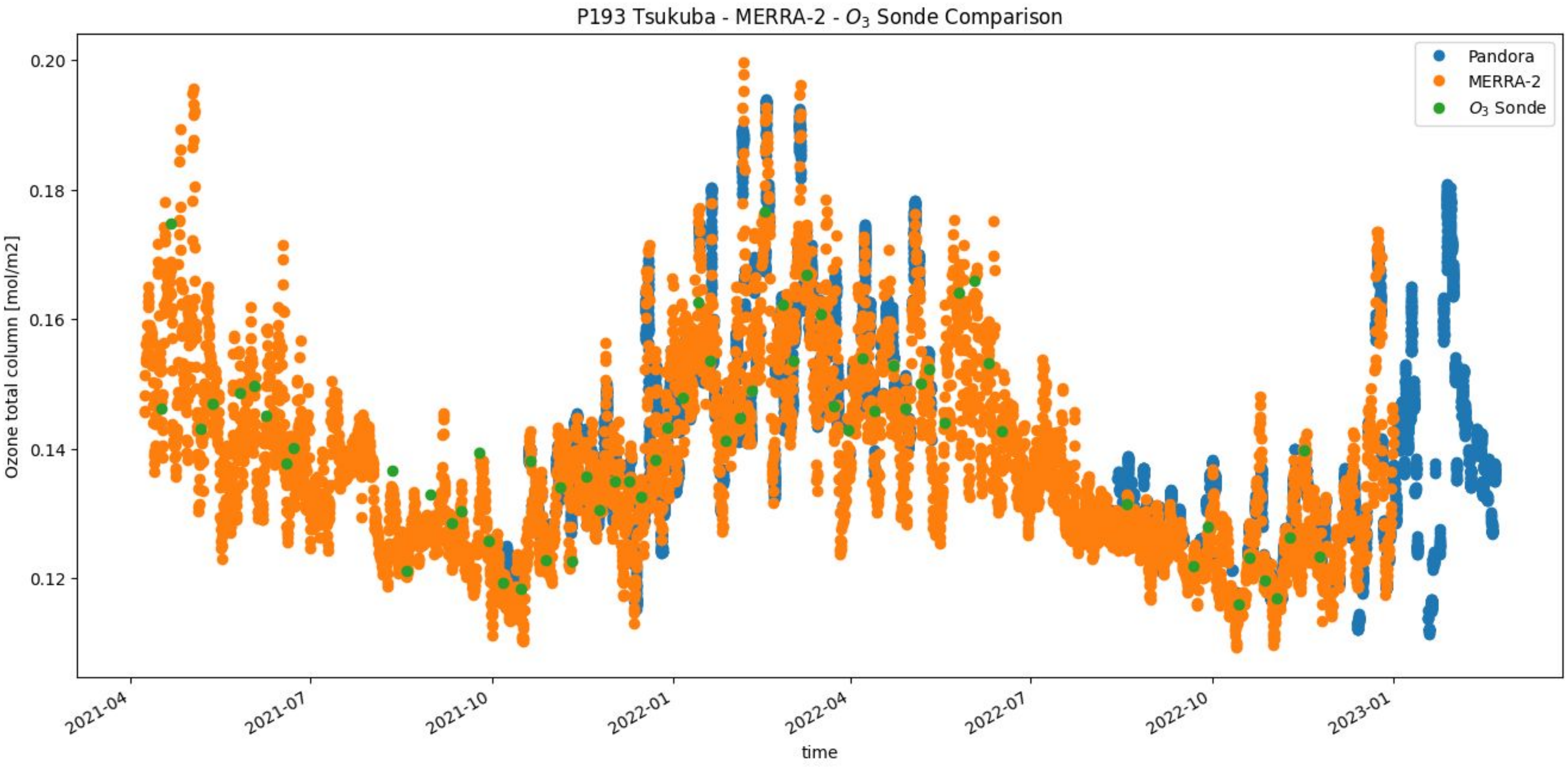
Comparisons with External Datasets - Rome



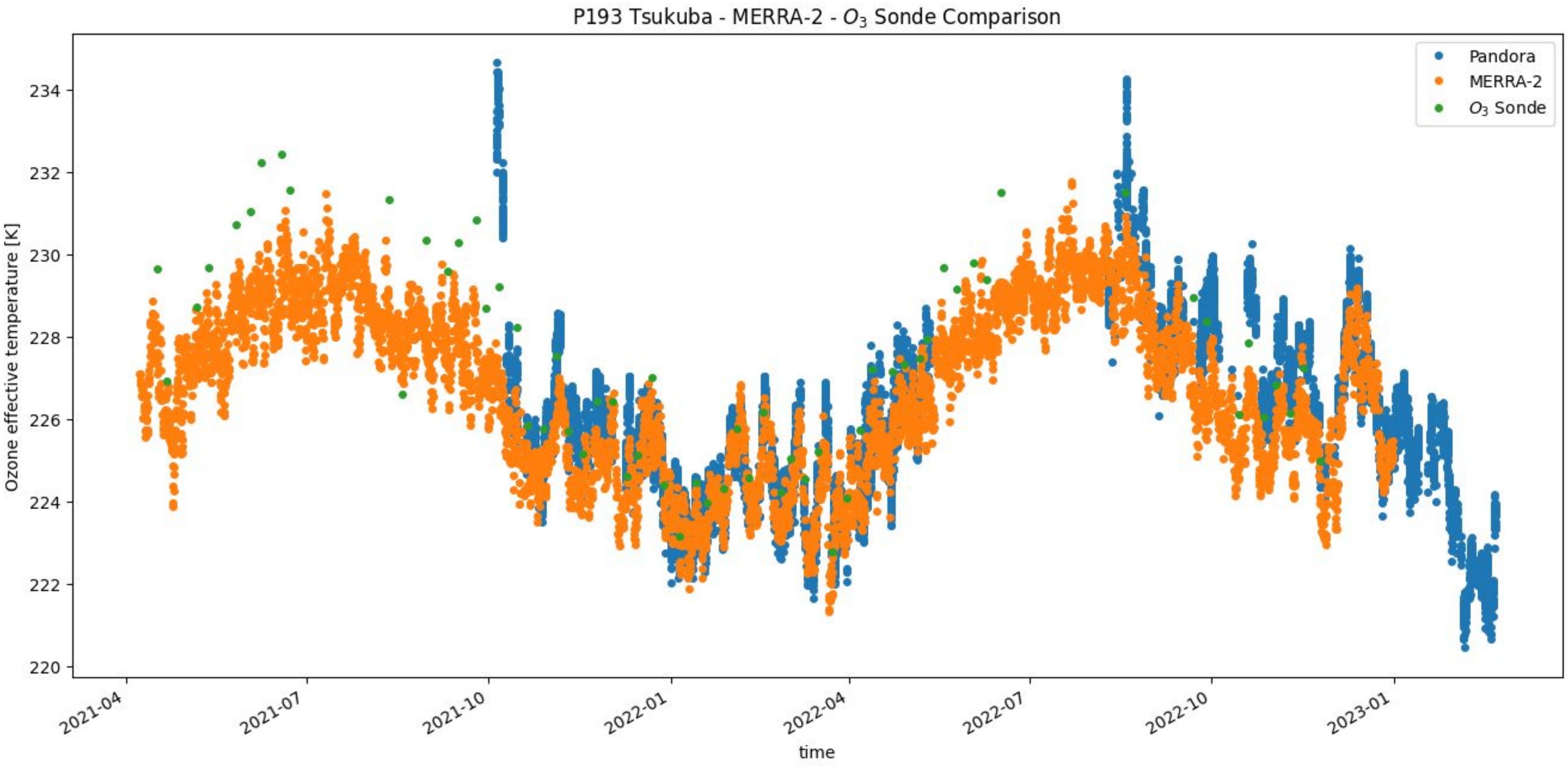
Comparisons with External Datasets - Rome



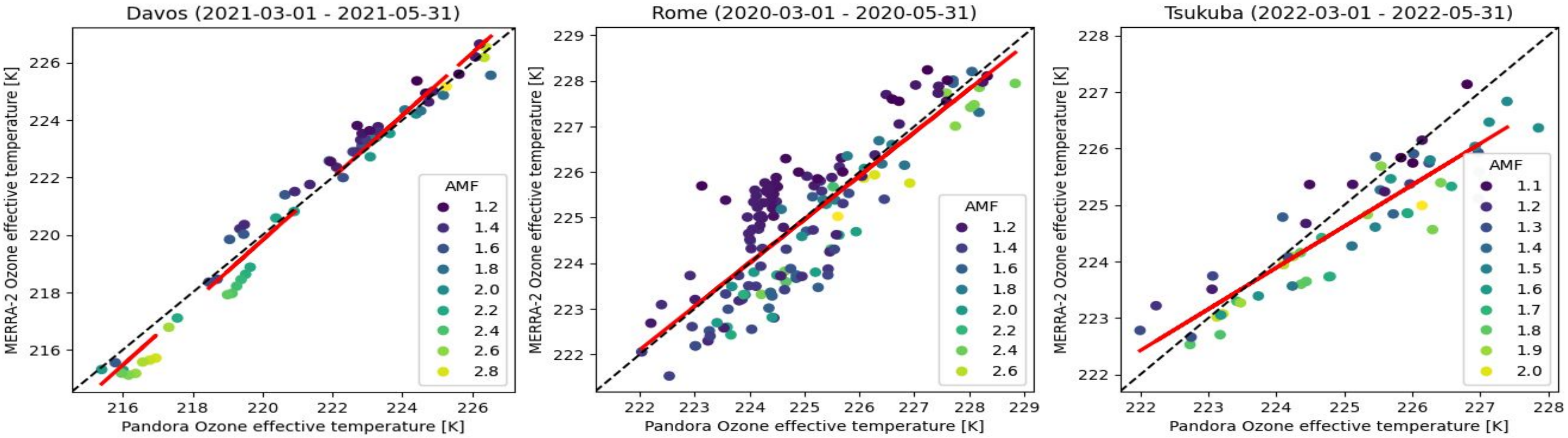
Comparisons with External Datasets - Tsukuba



Comparisons with External Datasets - Tsukuba



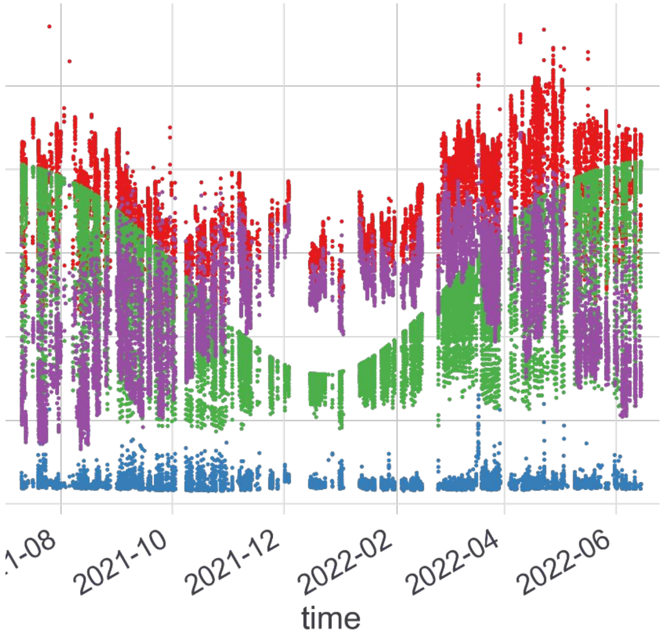
Comparisons with External Datasets - Davos



	Correlation	RMSE	Slope
Davos	0.98	0.63	1.08
Rome	0.84	0.88	0.95
Tsukuba	0.90	0.74	0.73

Uncertainty components

combined (total)



random (independent)
correlation length in time = 0
... measurement noise

Usually highest for high integration times.

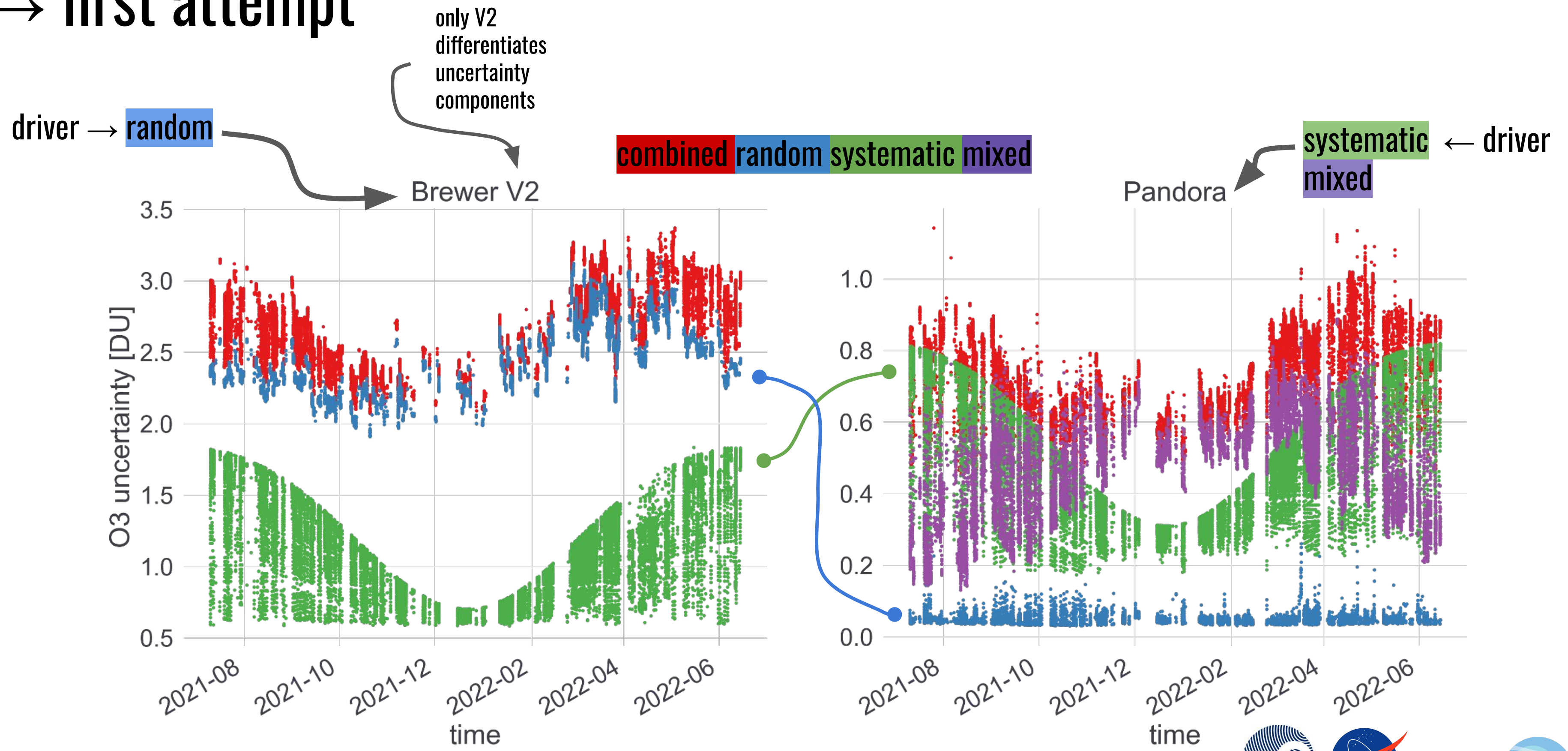
systematic (common)
correlation length in time = ∞
... calibration error

Highest for low AMFs (VC=SC/AMF)

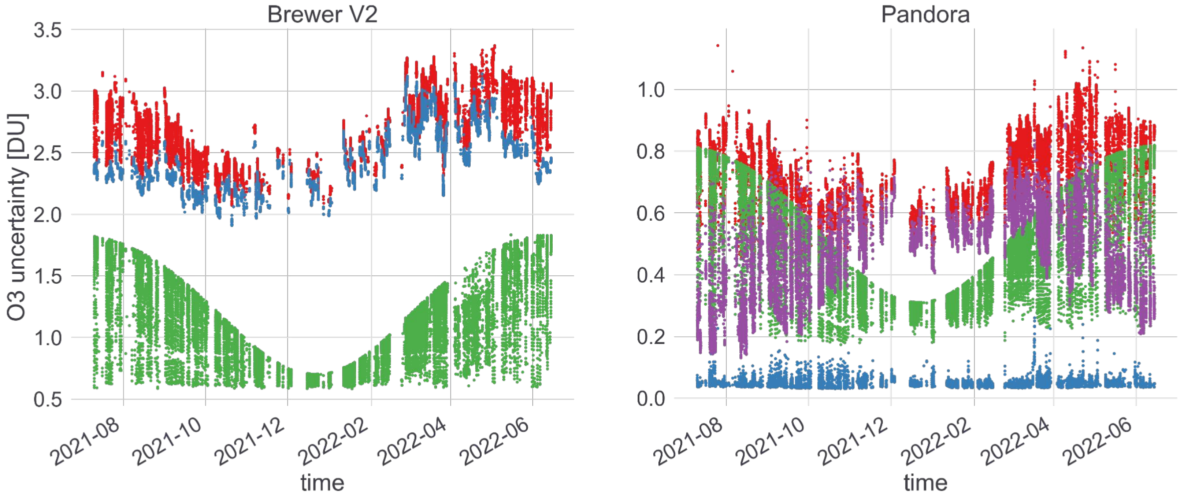
mixed (structured)
correlation length between 0 and ∞
... algorithm error
... cross section (effective) temperature

Highest for highest fitting RMS

Uncertainty component comparison for total O_3 in Davos → first attempt



Uncertainty component comparison for total O_3 in Davos → first attempt



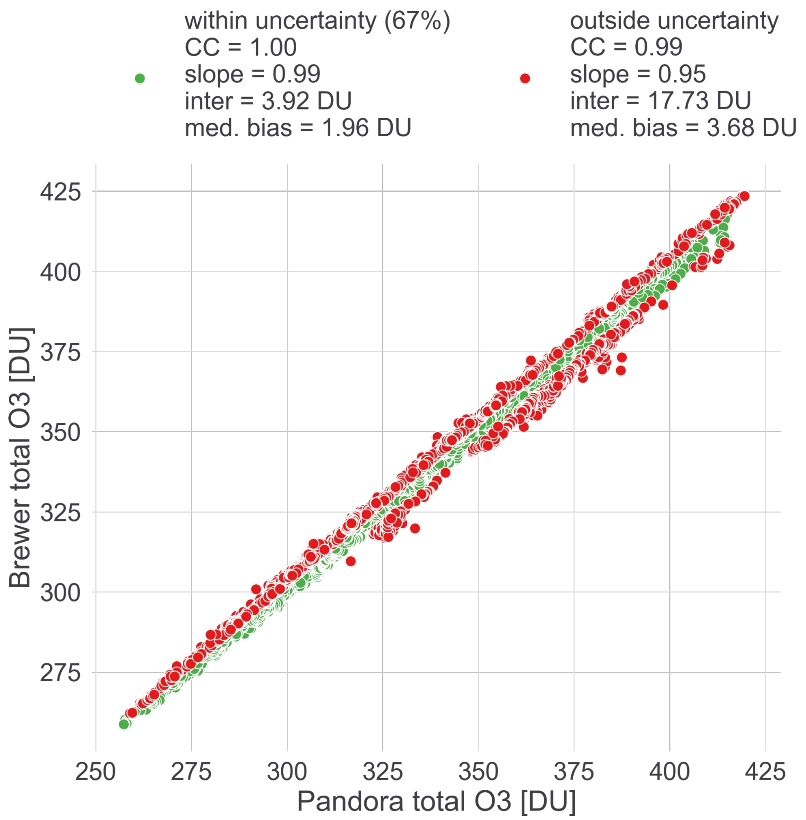
What drives the differences?

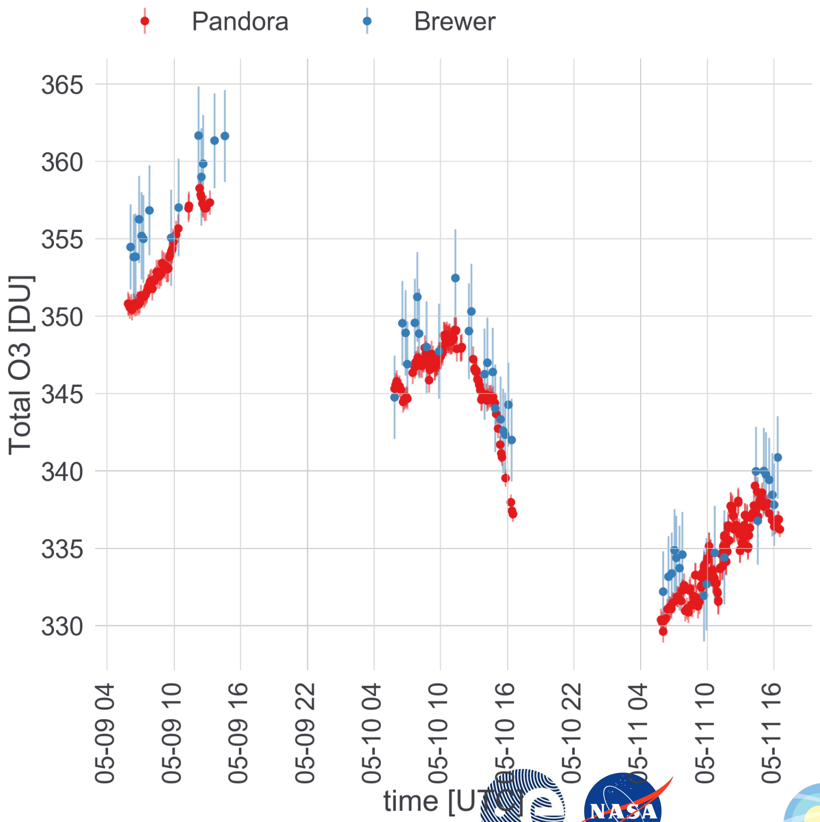
random
wavelengths: 200 (Pandora) vs 5 (Brewer)
Pandora much less noise
Brewer considers more than noise (seasonality)?

systematic
Pandora does not yet considers L1 uncertainty

mixed
only for Pandora.
For Brewer redistribution to random and systematic?

Uncertainty component comparison for total O_3 in Davos → first attempt



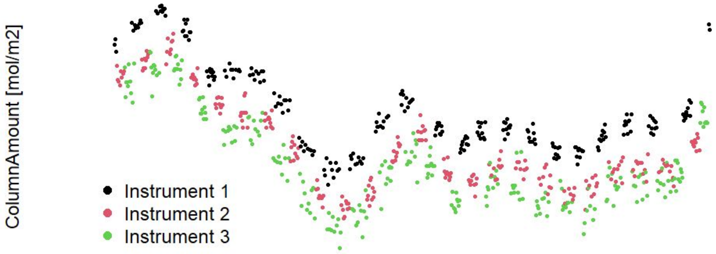


Suggested WP extension

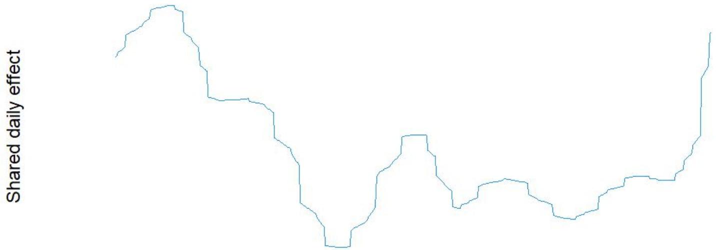
- **Include** the **newly developed** version **1.9 uncertainty** in the PGN **instrument calibration procedures** in order to prepare the move from version 1.8 to 1.9 as the official PGN retrieval software.
- With the exception of O_3, there is **hardly any external** (non PGN) **direct sun data** available **for uncertainty comparison** → **extent** the **validation** of PGN data uncertainties using the results of **collocated PGN instruments** using a statistical framework using **Generalized Additive Regression Models** (GAMs).

Suggested WP extension

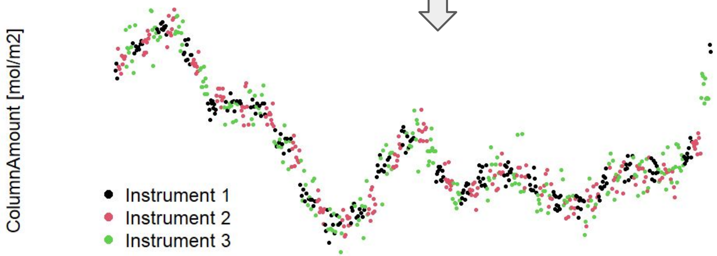
Uncertainty-component-validation using co-located Pandoras and Generalized Additive Models (GAM)



A



B

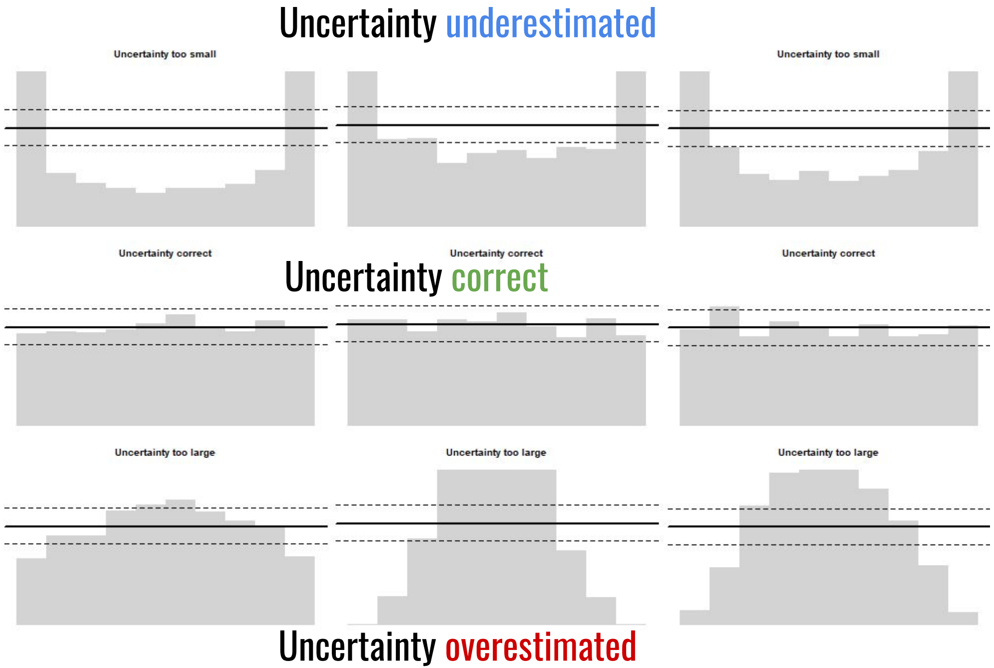


A) Obtain a **shared daily effect** among instruments:
   Evaluate instrument-specific offset to a baseline amount, which describes common (=systematic) uncertainty (~ calibration error)

B) Correct for offsets
   If there are no other error sources the remaining variation around the baseline should be attributed to the independent (=random) uncertainty solely that can be quantified in terms of statistical consistency

Suggested WP extension

Uncertainty-component-validation using co-located Pandoras and Generalized Additive Models (GAM)



The obtained baseline amount must be randomly distributed within the reported independent uncertainty. This results in uniformly distributed frequencies within equi-distant probability-bins to full-fill statistical consistency.

Correct Uncertainty -> Uniform
Low Uncertainty -> U-shape
High Uncertainty -> inverse U-shape

Anderson, J. L., 1996: A method for producing and evaluating probabilistic forecast from ensemble model integration. *J. Climate*, **9**, 1518–1530
Hamill, T. M., and S. J. Colucci, 1998: Evaluation of Eta RSM ensemble probabilistic precipitation forecasts. *Mon. Wea. Rev.*, **126**, 711–724

Thank you for your attention!!

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