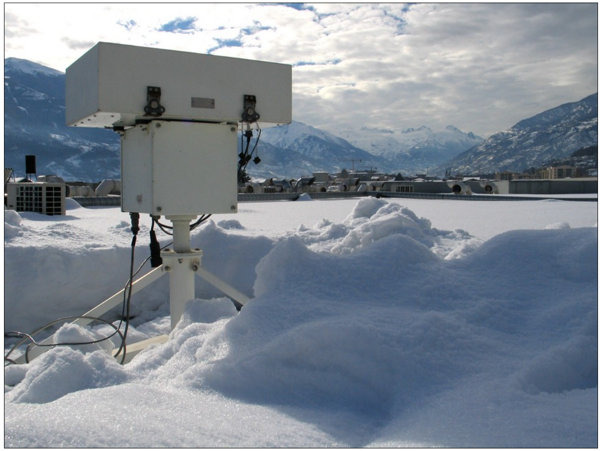
Nighttime ground-based observations for trace gas retrievals with the Brewer spectrophotometer

WP 2324



Henri Diémoz - ARPA Valle d'Aosta

IDEAS QA4EO Cal/Val WS#5, Thessaloniki

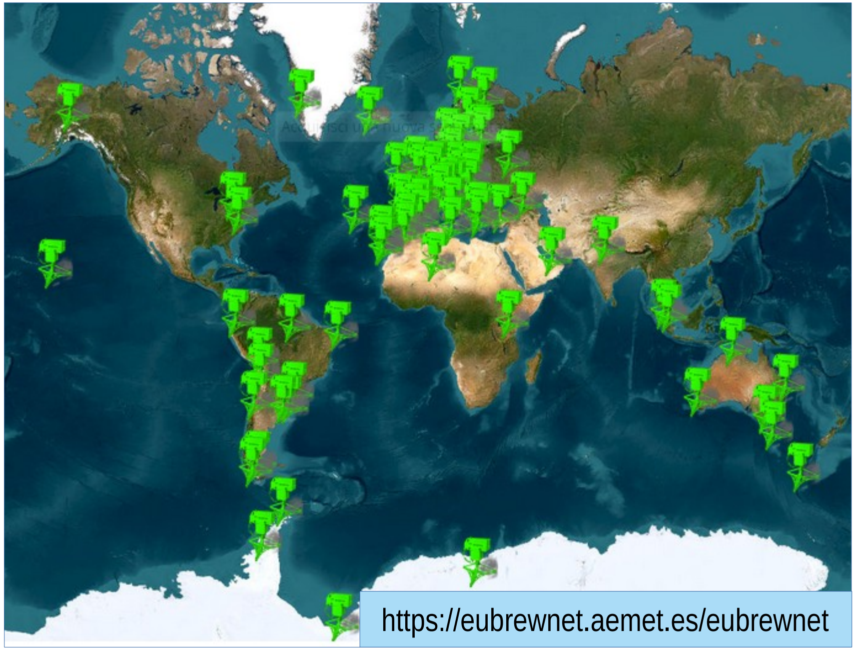
Goals

Development of an algorithm for **nighttime NO_2** retrievals from Brewer spectrophotometers (BAQUNIN – Sapienza and Aosta)

Evaluation of O_3 and NO_2 nighttime retrievals

Characterisation and correction of **spectral straylight** in single monochromator Brewers

The Brewer network



About 200 instruments measuring O_3 (UV)

~80 of them (MkIV) also able to measure NO_2 (visible)

The measurement/retrieval technique

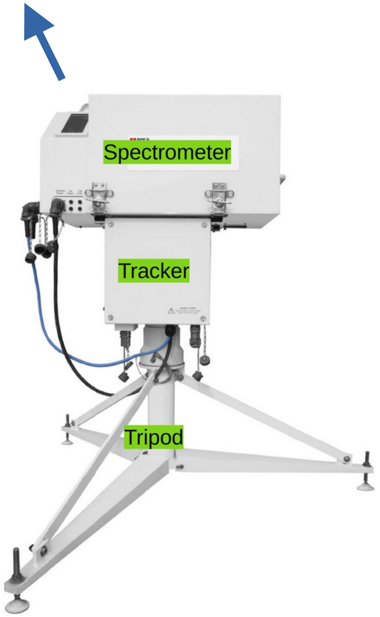
Reference instrument for **total O_3** retrievals from the **sun**. Direct-sun technique well validated (>40 years).

Recent improvements of **NO_2 retrievals** (using the **sun** as the source).

Not much work on **nighttime O_3** retrievals (focused moon).

No study on **nighttime NO_2** retrievals with Brewers so far.

Moon image projected on entrance slit without diffusers. Brewer pointing is fixed while the moon drifts accross the slit.



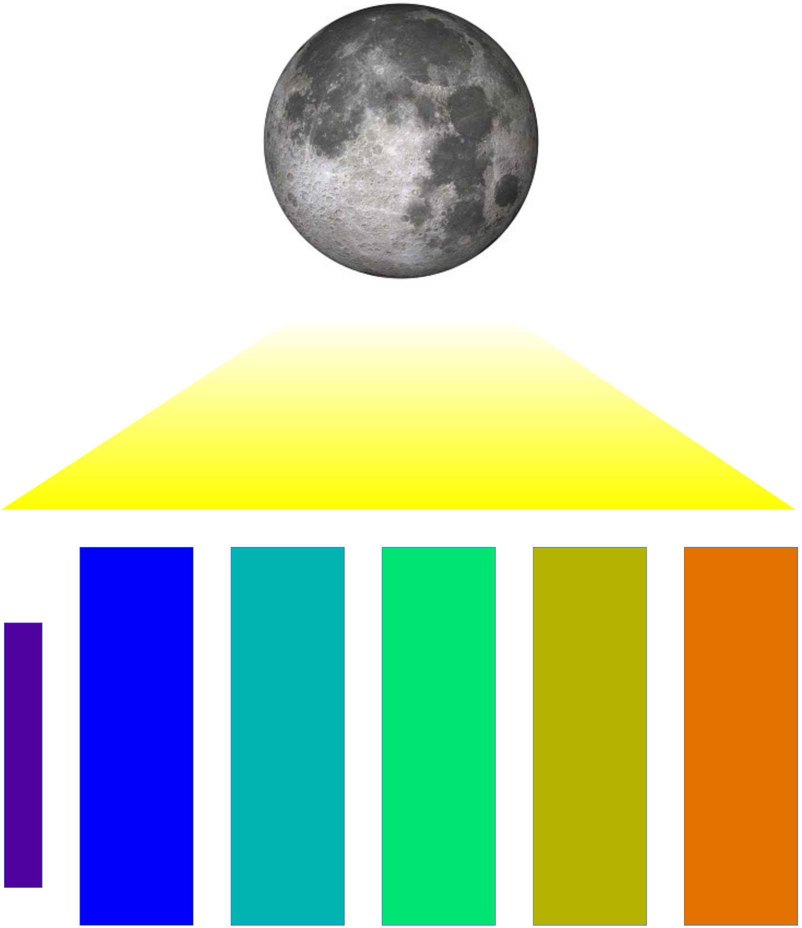
Previous phases

Assessment of **Brewer ephemeris** algorithm accuracy (against NASA's SPICE)

Daytime NO_2 retrieval algorithm

Nighttime NO_2 retrieval algorithm (using 5 wavelengths to reduce instabilities)

First nighttime O_3 and NO_2 datasets at Sapienza University in Rome – **BAQUNIN supersite**



Previous phases

Published

V. Savastiouk, H. Diémoz, C. T. McElroy, *A physically based correction for stray light in Brewer spectrophotometer data analysis*, Atmos. Meas. Tech., 2023

Atmos. Meas. Tech., 16, 4785–4806, 2023
https://doi.org/10.5194/amt-16-4785-2023

Atmospheric Measurement Techniques
Open Access
EGU

A physically based correction for stray light in Brewer spectrophotometer data analysis

Vladimir Savastiouk[1,★], Henri Diémoz[2,★], and C. Thomas McElroy[3]

[1]International Ozone Services Inc., Toronto, Ontario, Canada
[2]Regional Environmental Protection Agency (ARPA) of the Aosta Valley, Saint-Christophe, Italy
[3]Department of Earth and Space Science and Engineering, York University, Toronto, Ontario, Canada
[★]These authors contributed equally to this work.

Correspondence: Vladimir Savastiouk (vl@dimir.ca)

Received: 30 June 2023 – Discussion started: 6 July 2023
Revised: 31 August 2023 – Accepted: 4 September 2023 – Published: 20 October 2023

Abstract. Brewer ozone spectrophotometers have become an integral part of the global ground-based ozone monitoring network collecting data since the early 1980s. The double-monochromator Brewer version (MkIII) was introduced in 1992. With the Brewer hardware being so robust, both single- and double-monochromator instruments are still in use. The main difference between the single Brewers and the double Brewers is the much lower stray light in the double instrument. Laser scans estimate the rejection level of the single Brewers to be $10^{-4.5}$, while the doubles improve this to 10^{-8}, virtually eliminating the effects of stray light. For a typical single-monochromator Brewer, stray light leads to an underestimation of ozone of approximately 1 % at 1000 DU ozone slant column density (SCD) and can exceed 5 % at 2000 DU, while underestimation of sulfur dioxide reaches 30 DU when no sulfur dioxide is present. This is because even a small additional stray light contribution at shorter wavelengths significantly reduces the calculated SCD at large values. An algorithm for stray light correction based on the physics of the instrument response to stray light (PHYCS) has been developed. The simple assumption is that count rates measured at any wavelength have a contribution from stray light from longer, and thus brighter, wavelengths because of the ozone cross-section gradient leading to a rapid change in intensity as a function of wavelength. Using the longest measured wavelength (320 nm) as a proxy for the overall brightness provides an estimate of this contribution. The sole parameter, on the order of 0.2 % to 0.6 %, that describes the percentage of light at the longest wavelength to be subtracted from all channels is determined by comparing ozone calculations from single- and double-monochromator Brewers making measurements side-by-side. Removing this additional count rate from the signal mathematically before deriving ozone corrects for the extra photons scattering within the instrument that produce the stray light effect. Analyzing historical data from co-located single- and double-monochromator Brewers provides an estimate of how the stray light contribution changes over time in an instrument. The corrected count rates of the measured wavelengths can also be used to improve other calculations: the sulfur dioxide column and the aerosol optical depth, the effective temperature of the ozone layer, or any other products. A multi-platform implementation of PHYCS, `rmstray`, to correct the count rates for stray light and save the corrected values in a new B-file for use with any existing Brewer data analysis software is available to the global Brewer user community at https://doi.org/10.5281/zenodo.8097038 (Savastiouk and Diémoz, 2023).

1 Introduction

Developed in the late 1970s at what is now known as Environment and Climate Change Canada (ECCC), the Brewer spectrophotometer has become an important research and monitoring ground-based instrument to determine, among other quantities, the amount of ozone in the atmosphere and the solar ultraviolet (UV) irradiance reaching the surface (Kerr et al., 1985). As an essential component of

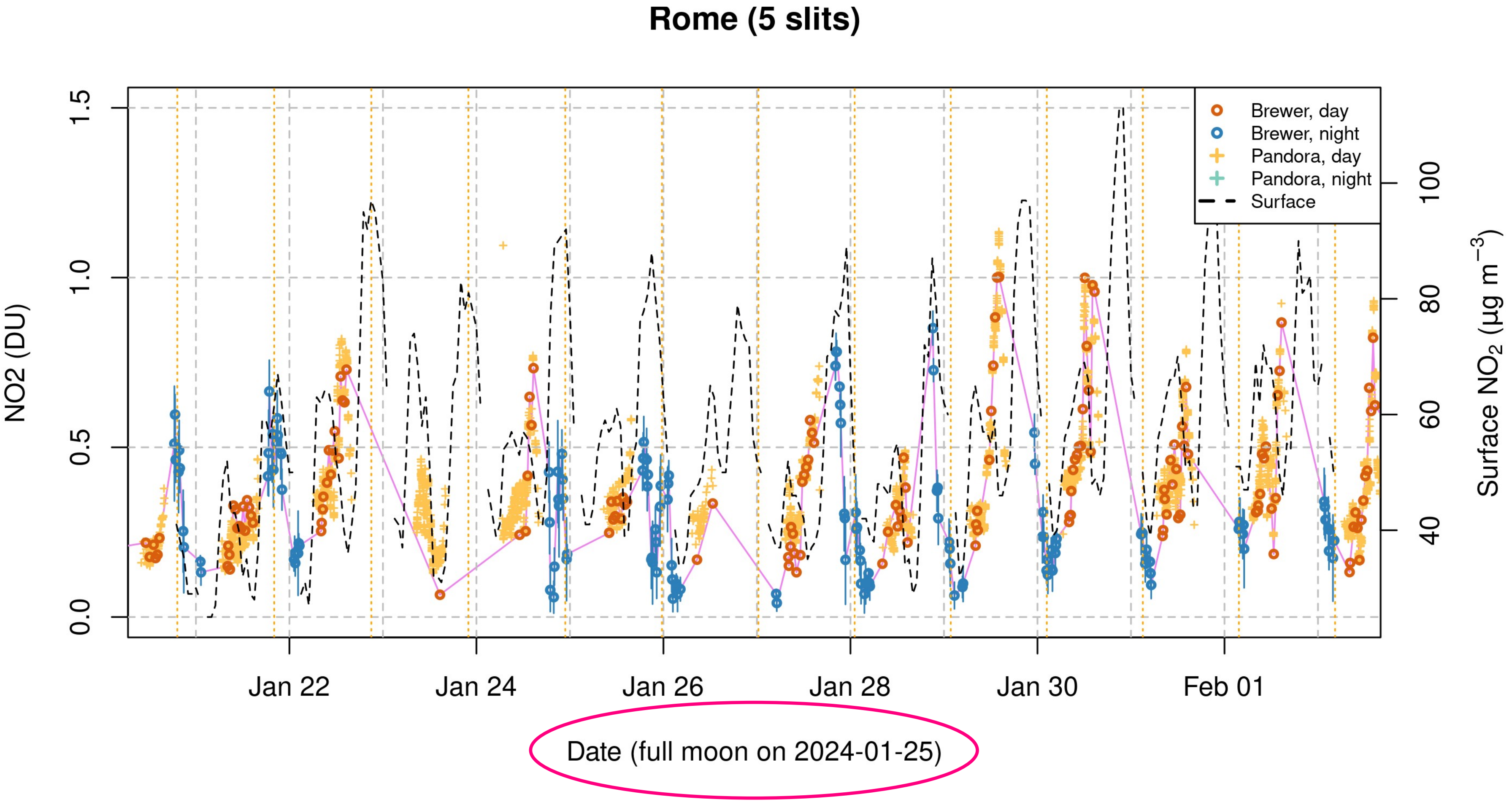
Current phase

Same measurement schedule in **Rome** (Sapienza University, #067) and **Aosta** (ARPA, #066):

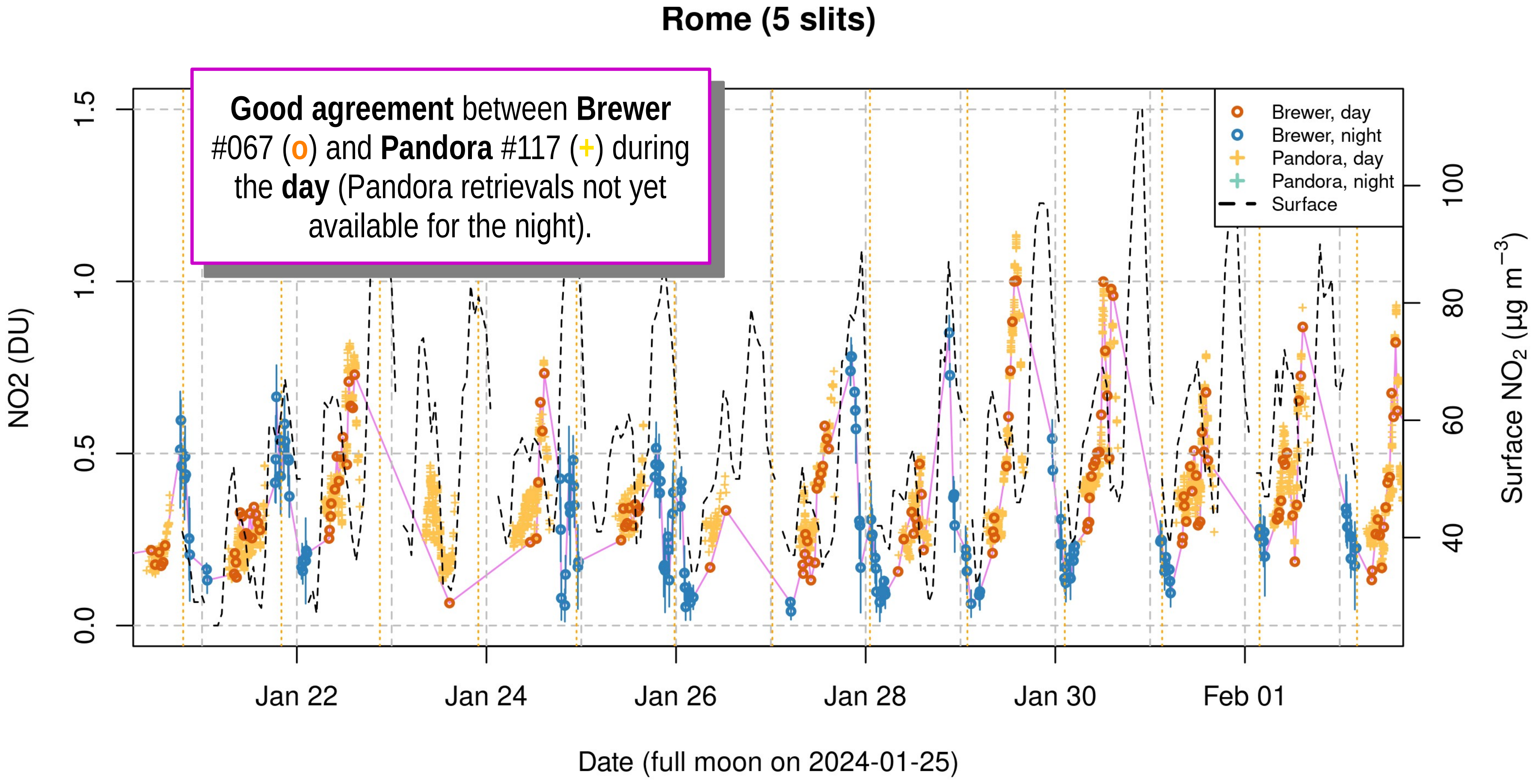
- including O_3 and NO_2 retrievals
- during both the day and the night.

The Aosta station will serve as a ground truth for comparison/validation exercises of spaceborne retrievals over **complex orography**.

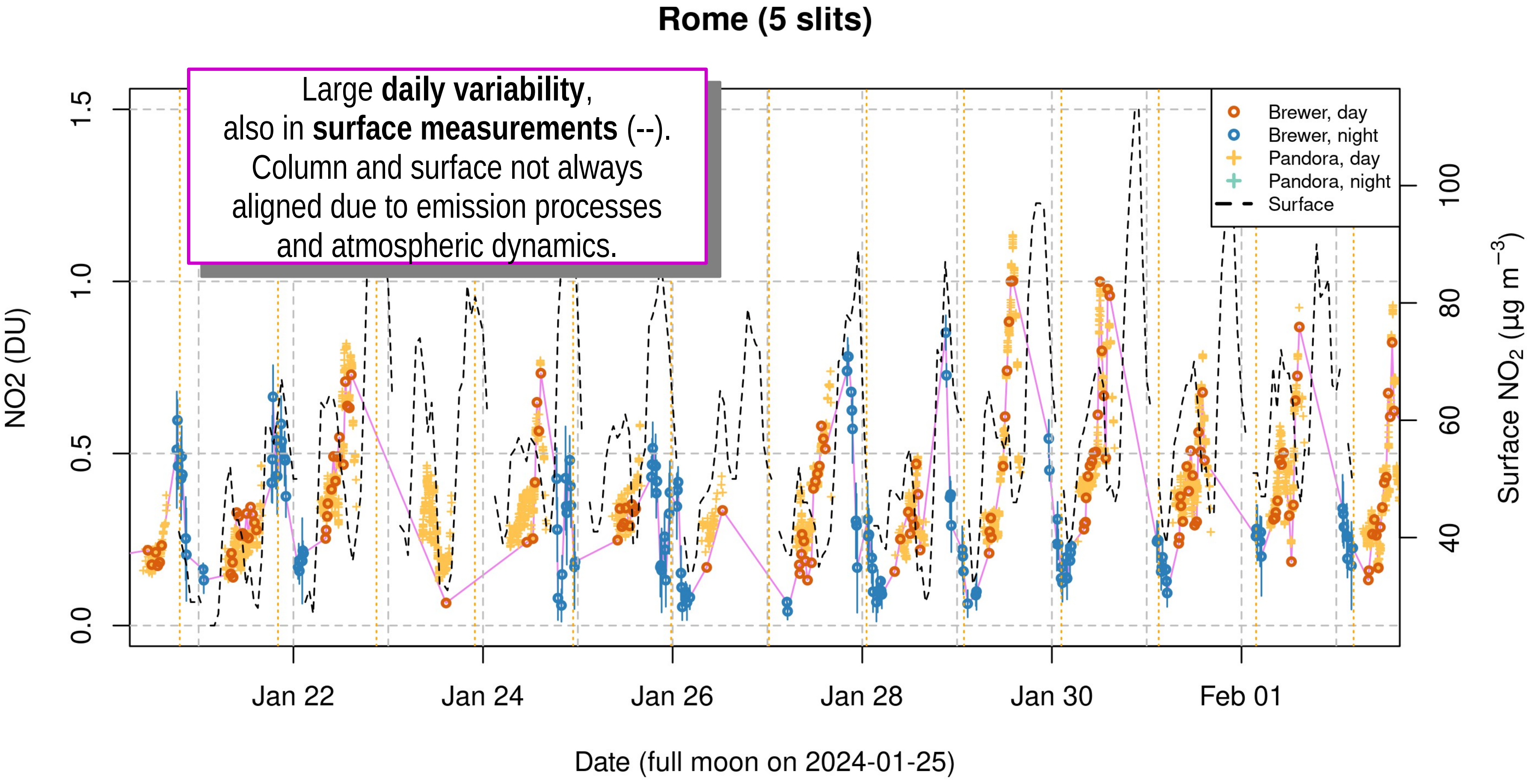
NO_2, daytime and nighttime



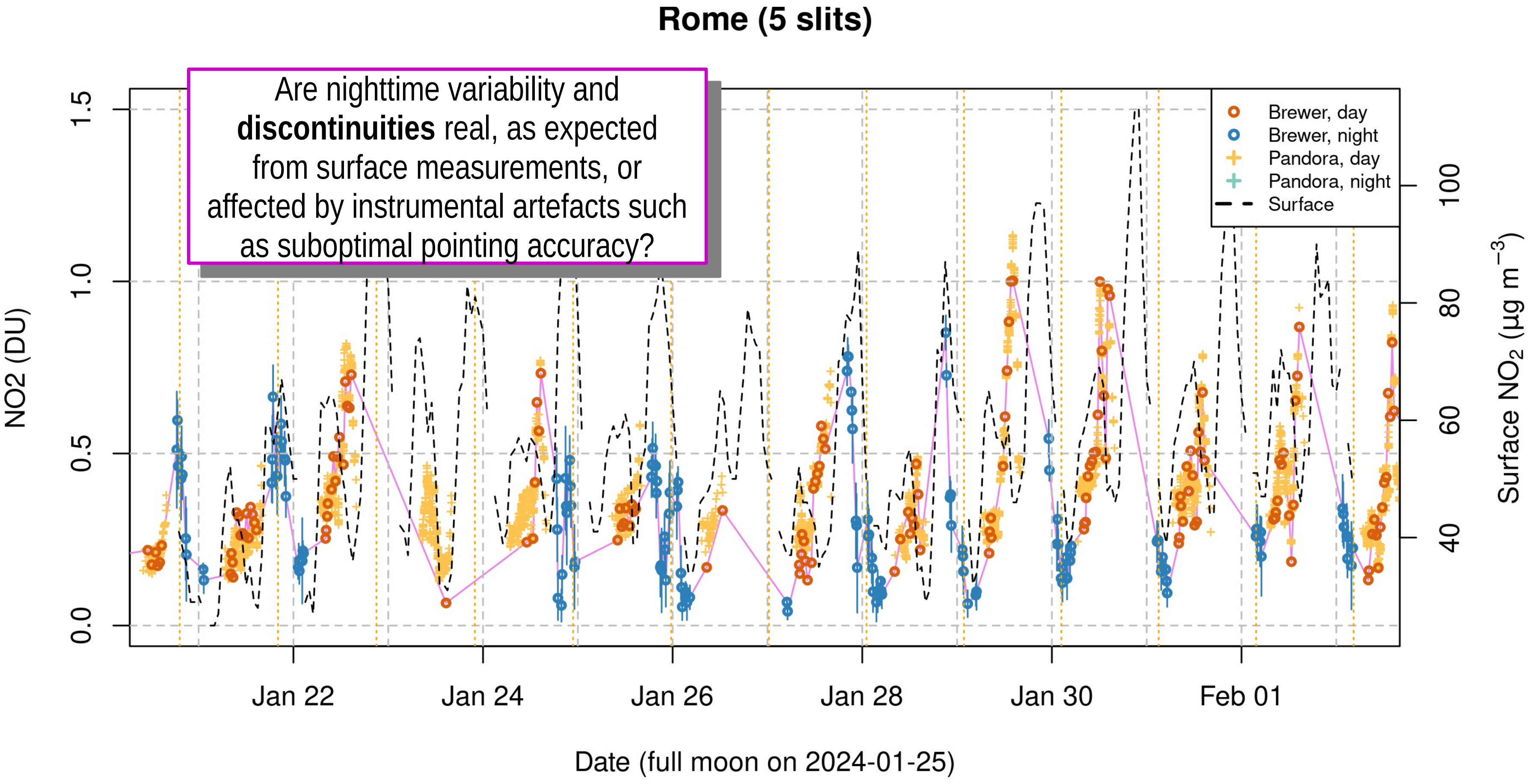
NO_2, daytime and nighttime



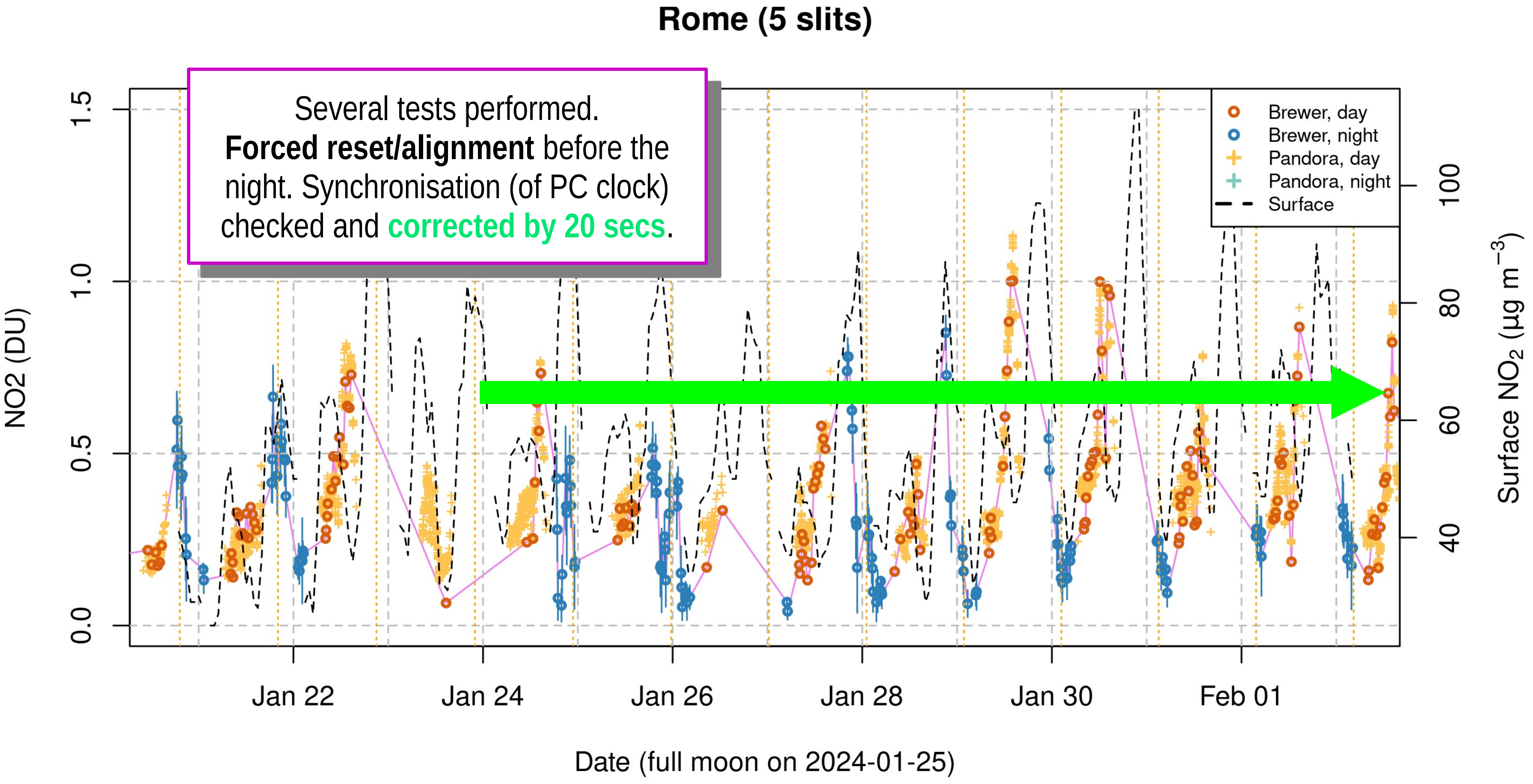
NO_2, daytime and nighttime



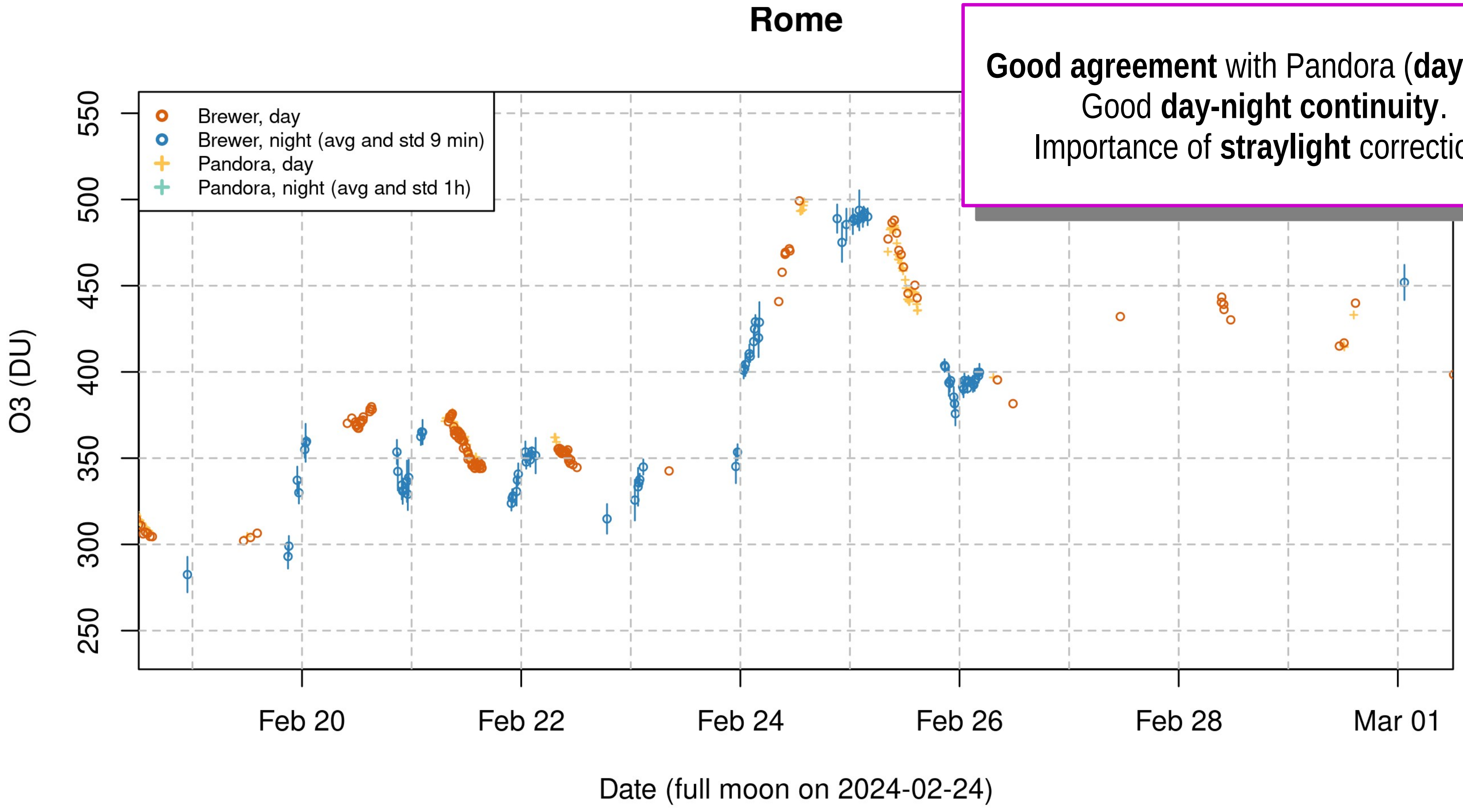
NO_2, daytime and nighttime



NO_2, daytime and nighttime

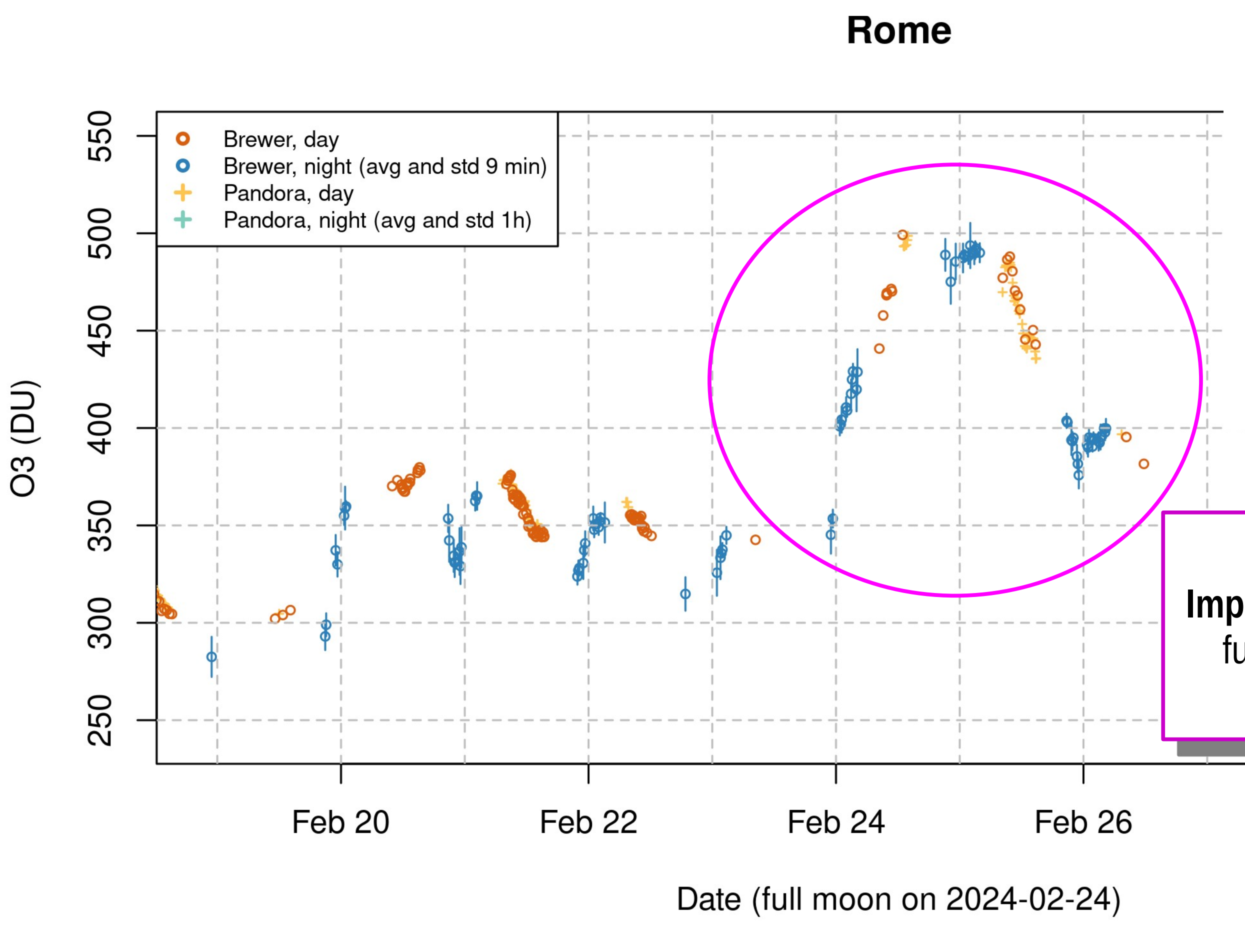


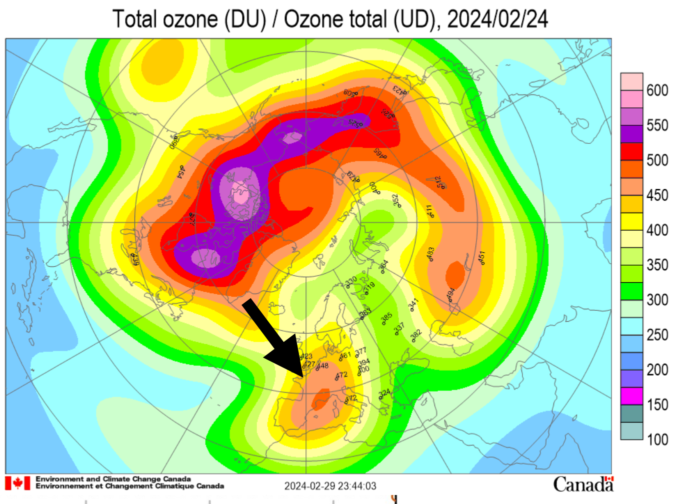
O_3, daytime and nighttime



Good agreement with Pandora (**day** only).
Good **day-night continuity**.
Importance of **straylight** correction.

O_3, daytime and nighttime





Importance of **nighttime** measurements to fully understand the **ozone dynamics**.

Deliverables

1/ Datasets in harmonised data format (**GEOMS**)

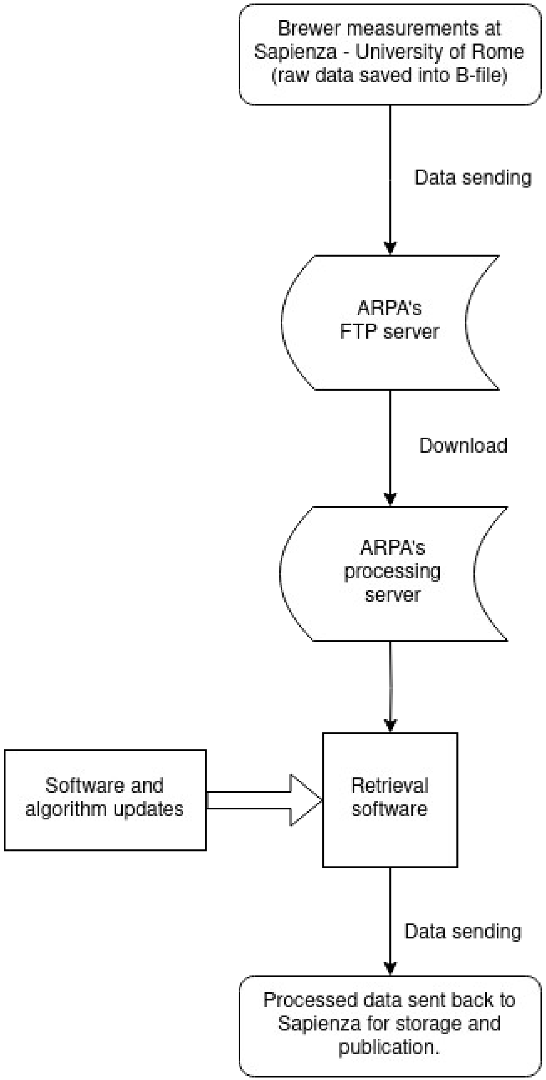
```
File GEOMS_solar_NO2.nc (NC_FORMAT_NETCDF4):

     12 variables (excluding dimension variables):
        float LATITUDE.INSTRUMENT[]   (Contiguous storage)
            VAR_SIZE: 1
            VAR_NAME: LATITUDE.INSTRUMENT
            VAR_DESCRIPTION: Inst. geolocation. Latitude north (decimal degrees)
            VAR_NOTES:
            VAR_DEPEND: CONSTANT
            VAR_DATA_TYPE: REAL
            VAR_UNITS: deg
            VAR_SI_CONVERSION: 0.0;1.74533E-2;rad
            VAR_VALID_MIN: -90
            VAR_VALID_MAX: 90
            VAR_FILL_VALUE: -90000
        float LONGITUDE.INSTRUMENT[]   (Contiguous storage)
            VAR_SIZE: 1
            VAR_NAME: LONGITUDE.INSTRUMENT
            VAR_DESCRIPTION: Inst. geolocation. Longitude east (decimal degrees)
            VAR_NOTES:
            VAR_DEPEND: CONSTANT
            VAR_DATA_TYPE: REAL
            VAR_UNITS: deg
            VAR_SI_CONVERSION: 0.0;1.74533E-2;rad
            VAR_VALID_MIN: -180
            VAR_VALID_MAX: 180
            VAR_FILL_VALUE: -90000
        float ALTITUDE.INSTRUMENT[]   (Contiguous storage)
            VAR_SIZE: 1
            VAR_NAME: ALTITUDE.INSTRUMENT
            VAR_DESCRIPTION: Inst. geolocation. Altitude of the instrument relat
            VAR_NOTES:
            VAR_DEPEND: CONSTANT
            VAR_DATA_TYPE: REAL
            VAR_UNITS: m
            VAR_SI_CONVERSION: 0.0;1.0;m
            VAR_VALID_MIN: -1000
            VAR_VALID_MAX: 10000
            VAR_FILL_VALUE: -90000
        float INTERNAL.INSTRUMENT.TEMPERATURE[DATETIME]   (Contiguous storage)
            VAR_SIZE: 9055
            VAR_NAME: INTERNAL.INSTRUMENT.TEMPERATURE
            VAR_DESCRIPTION: Internal temperature sensor
            VAR_NOTES:
            VAR_DEPEND: DATETIME
            VAR_DATA_TYPE: REAL
            VAR_UNITS: degC
            VAR_SI_CONVERSION: 273.15;1;K
            VAR_VALID_MIN: -100
```

Deliverables

1/ Datasets in harmonised data format (**GEOMS**)

2/ Conceptualisation of a **real time processor** and documentation → based on transfer from Sapienza to ARPA

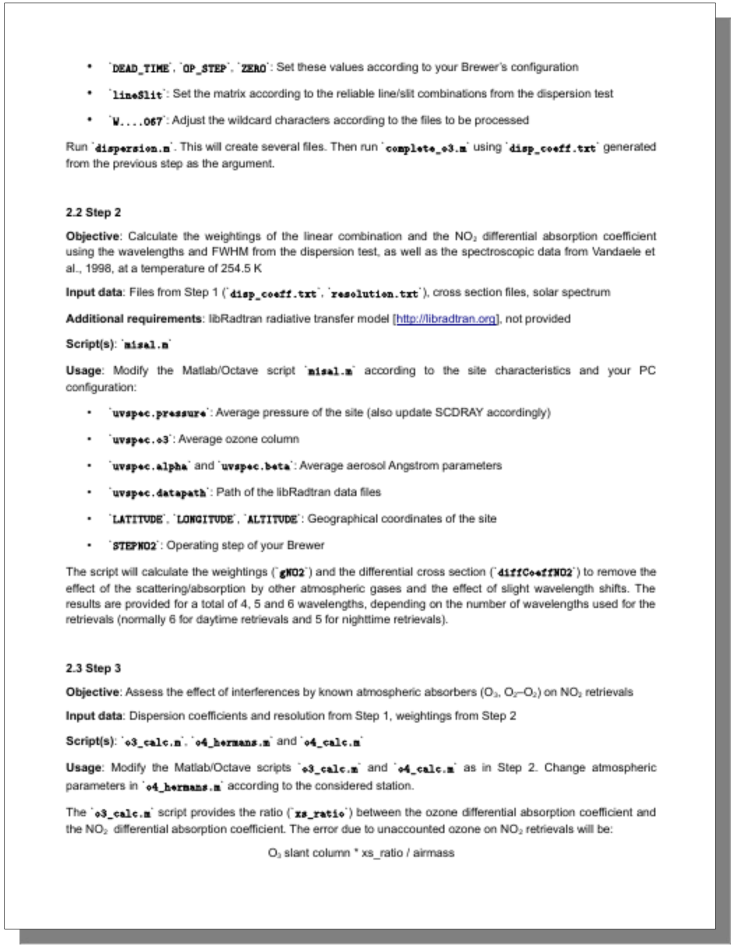


Deliverables

1/ Datasets in harmonised data format (**GEOMS**)

2/ Conceptualisation of a **real time processor** and documentation → based on transfer from Sapienza to ARPA

3/ Retrieval **software** with description



- `DEAD_TIME`, `OP_STEP`, `ZERO`: Set these values according to your Brewer's configuration
- `lineSlit`: Set the matrix according to the reliable line/slit combinations from the dispersion test
- `W....067`: Adjust the wildcard characters according to the files to be processed

Run `dispersion.m`. This will create several files. Then run `complete_o3.m` using `disp_coeff.txt` generated from the previous step as the argument.

2.2 Step 2

Objective: Calculate the weightings of the linear combination and the NO_2 differential absorption coefficient using the wavelengths and FWHM from the dispersion test, as well as the spectroscopic data from Vandaele et al., 1998, at a temperature of 254.5 K

Input data: Files from Step 1 (`disp_coeff.txt`, `resolution.txt`), cross section files, solar spectrum

Additional requirements: libRadtran radiative transfer model [http://libradtran.org], not provided

Script(s): `misal.m`

Usage: Modify the Matlab/Octave script `misal.m` according to the site characteristics and your PC configuration:

- `uvspec.pressure`: Average pressure of the site (also update SCDRAY accordingly)
- `uvspec.o3`: Average ozone column
- `uvspec.alpha` and `uvspec.beta`: Average aerosol Angstrom parameters
- `uvspec.datapath`: Path of the libRadtran data files
- `LATITUDE`, `LONGITUDE`, `ALTITUDE`: Geographical coordinates of the site
- `STEPNO2`: Operating step of your Brewer

The script will calculate the weightings (`gNO2`) and the differential cross section (`diffCoeffNO2`) to remove the effect of the scattering/absorption by other atmospheric gases and the effect of slight wavelength shifts. The results are provided for a total of 4, 5 and 6 wavelengths, depending on the number of wavelengths used for the retrievals (normally 6 for daytime retrievals and 5 for nighttime retrievals).

2.3 Step 3

Objective: Assess the effect of interferences by known atmospheric absorbers (O_3, O_2–O_2) on NO_2 retrievals

Input data: Dispersion coefficients and resolution from Step 1, weightings from Step 2

Script(s): `o3_calc.m`, `o4_hermans.m` and `o4_calc.m`

Usage: Modify the Matlab/Octave scripts `o3_calc.m` and `o4_calc.m` as in Step 2. Change atmospheric parameters in `o4_hermans.m` according to the considered station.

The `o3_calc.m` script provides the ratio (`xs_ratio`) between the ozone differential absorption coefficient and the NO_2 differential absorption coefficient. The error due to unaccounted ozone on NO_2 retrievals will be:

O_3 slant column * xs_ratio / airmass

Final remarks

Combined uncertainty estimation and **data quality** evaluation for **daytime** NO_2 and O_3 measurements have been provided by previous research, e.g. Diémoz et al., ESSD, 2021.

To be completed for nighttime NO_2 retrievals: comparison with **Pandora** during the night using recent data will be helpful to **identify possible systematic effects** that still need to be accounted for and corrected.

Plan to **implement stray light correction in EUBREWNET**.