Comparison of Ozone, Nitrogen Dioxide, and Formaldehyde Columns Retrieved By TEMPO and Pandora – ASDC Tools and Results

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Motivation and Description of Instruments

ASDC store data from various satellite, aerial, and ground-based missions. Along with providing access to the data, ASDC also provides user support. One of the user support activities is development of programmatic tools downloading, reading, and handling the data. Python notebooks comparing satellite and ground-based gas columns retrievals have been recently created.

The Tropospheric Emissions: Monitoring of Pollution (**TEMPO**) instrument is a grating spectrometer, sensitive to VIS and UV light within spectral ranges of 290-490 nm and 540-740 nm. The TEMPO instrument is aboard a commercial telecommunications satellite (Intelsat 40e) in GEO orbit over 91˚ W. The TEMPO completes an east-to-west scan of the field of regard in an hour. High resolution radiance measurements enable retrievals of atmospheric columns of O_3, NO_2, and HCHO. TEMPO data can be found at https://search.earthdata.nasa.gov/search?q=TEMPO_. More information can be found at https://tempo.si.edu/overview.html.

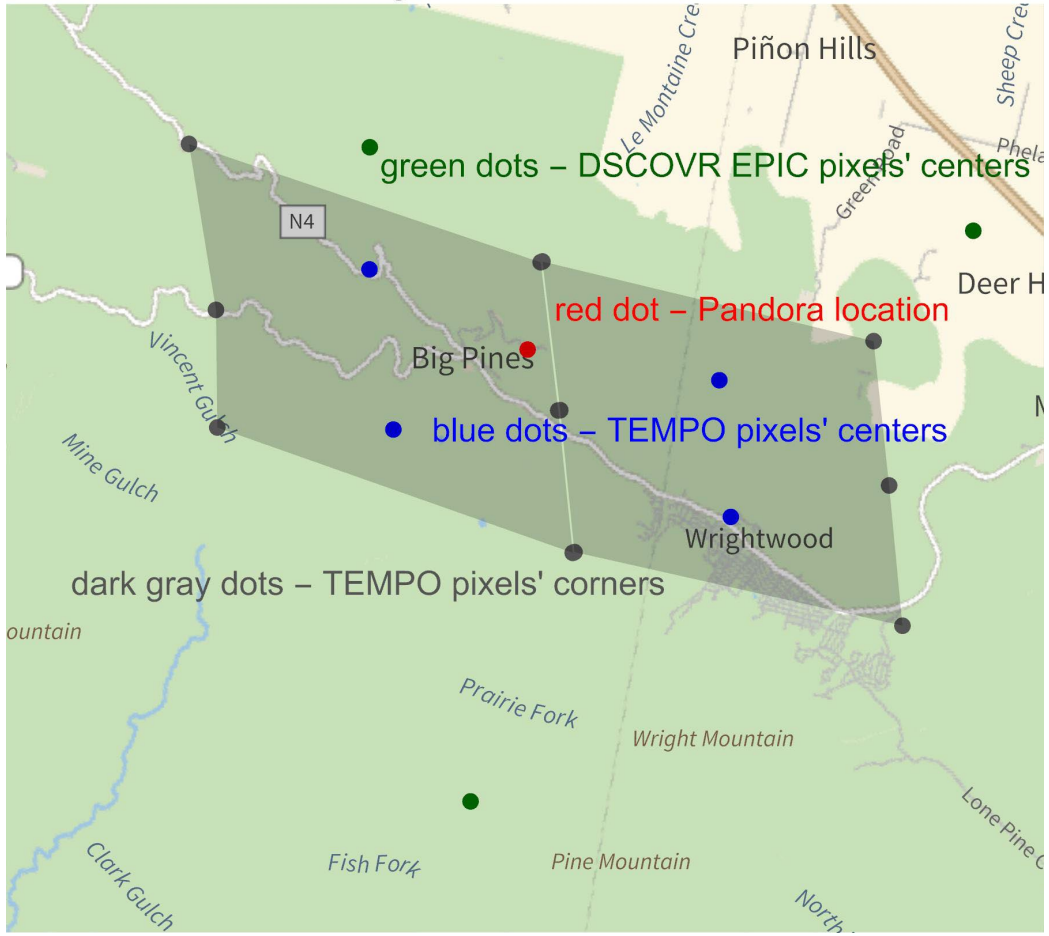
Direct Sun radiance measurements by **the Pandora** spectrometers are used to retrieve columnar amounts of trace gases (O_3, NO_2, HCHO) in the atmosphere. These retrievals are performed by means of differential optical absorption spectroscopy. See https://pandora.gsfc.nasa.gov/Instrument/ for more information. The Pandora data are available at https://data.pandonia-global-network.org/.

The NOAA's Deep Space Climate Observatory (**DSCOVR**) spacecraft is located at the Earth-Sun Lagrange-1 point giving the Earth Polychromatic Imaging Camera (**EPIC**) a unique angular perspective that is used in various science applications including ozone column retrievals. EPIC is a 10-channel spectroradiometer (317 – 780 nm) providing spectral images of the entire sunlit side of Earth using a 2048x2048 pixel CCD detector coupled to a 30-cm aperture Cassegrain telescope. DSCOVR EPIC O_3 product is derived from radiance measurements at 317.5 nm, 325 nm, and 340 nm, see https://epic.gsfc.nasa.gov/science/products/o3 for more information and https://search.earthdata.nasa.gov/search?q=dscovr_epic_l2_to3_03 for ozone data.

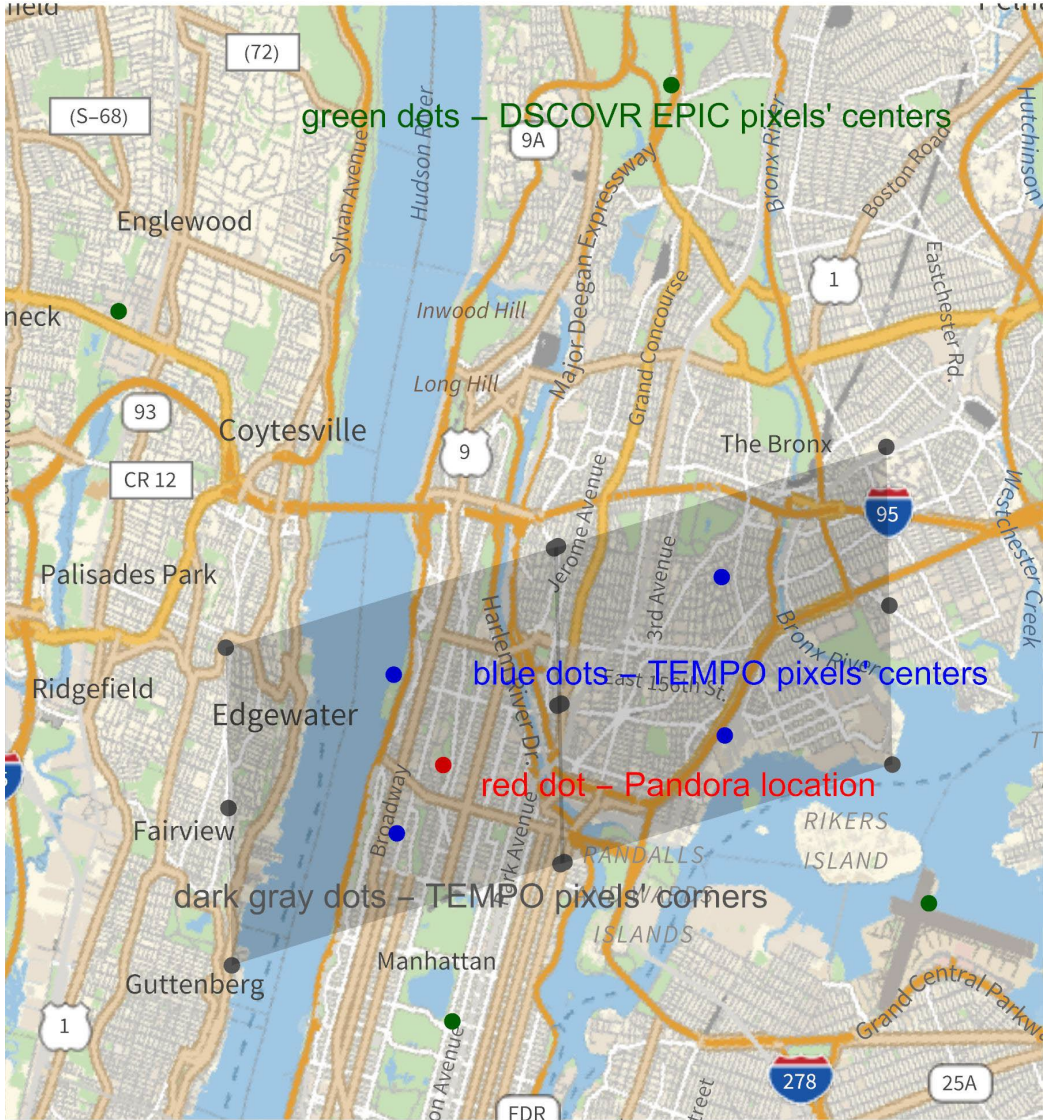
Co-locating Pandora stations and satellite pixels

Spatial extents of TEMPO pixels, gray shades, such that their centers, blue, enclose the position of Pandora, red; centers of DSCOVR EPIC pixels, green, within 0.1° deviation from the position of Pandora.

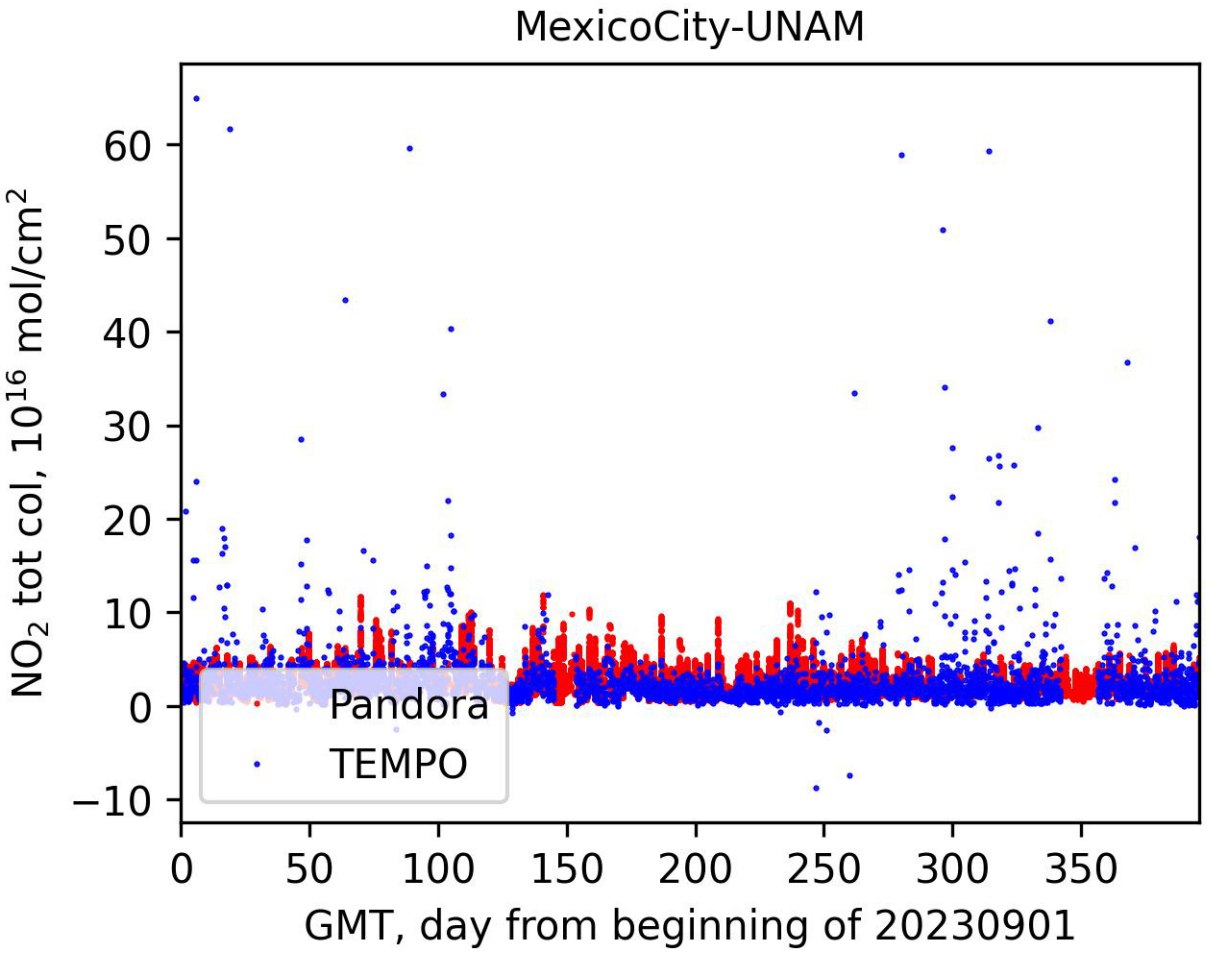
DSCOVR_EPIC_L2_TO3_03_20241003180857_03
TEMPO_O3TOT_L2_V03_20241003T181345Z_S009G08
over Pandora WrightwoodCA at 34.3819N 117.681W

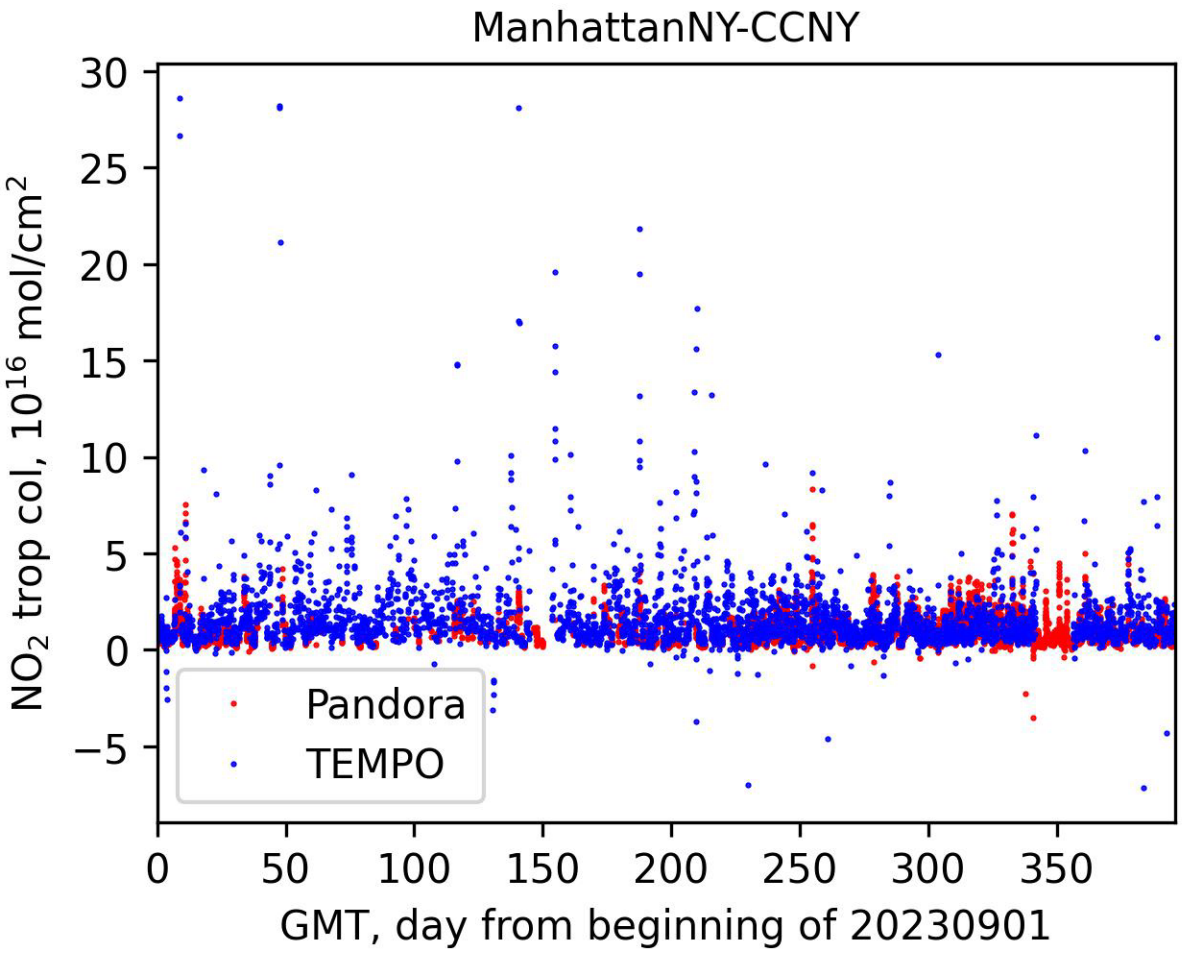


DSCOVR_EPIC_L2_TO3_03_20241003162055_03
TEMPO_O3TOT_L2_V03_20241003T164038Z_S008G03
over Pandora ManhattanNY−CCNY at 40.8153N 73.9505W



Timeseries





For long-term datasets, timeseries plots are not convenient for comparison. They are useful for gap detection.

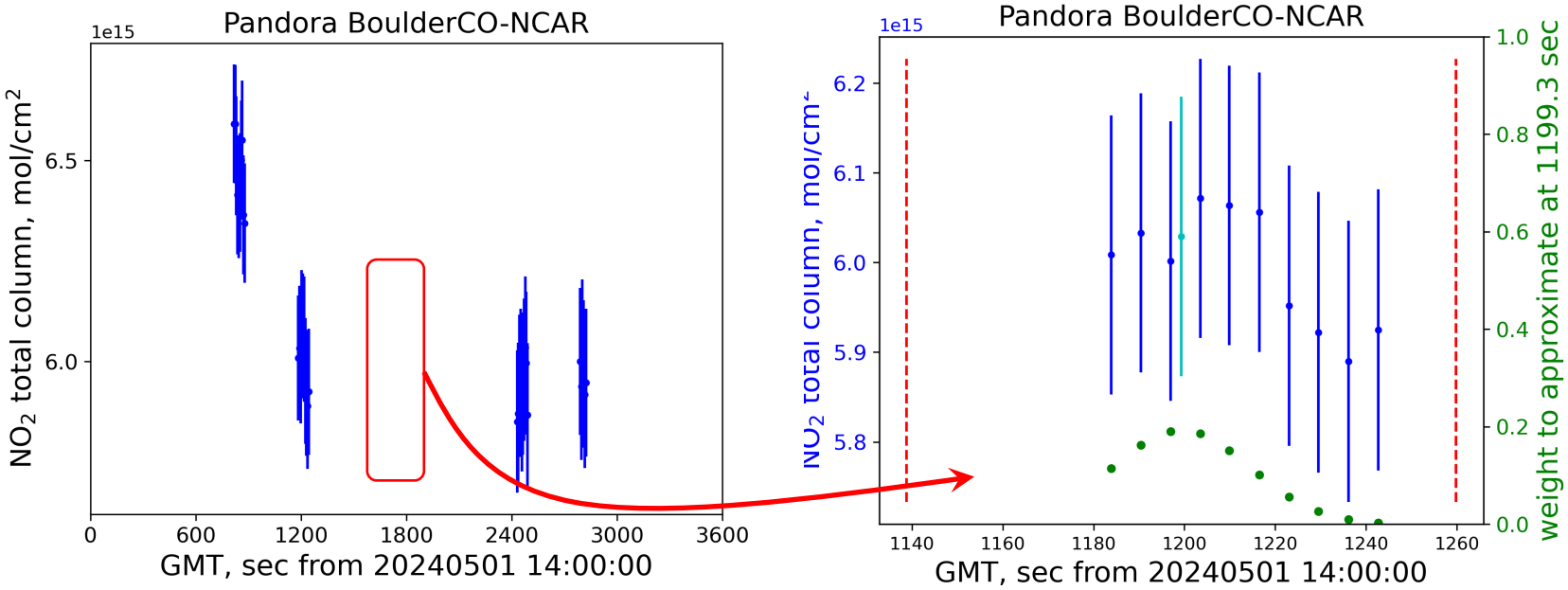
Temporal features of Pandora retrievals I

Temporal resolution of TEMPO varies with the rate of scanning; however, the nominal temporal resolution is 1 hour.

DSCOVR EPIC performs about 16 scans per day covering the entire planet.

From Pandora, there may be tens of measurements per hour with the frequency of measurements depending on the product. While direct comparisons of non-simultaneous measurements from TEMPO, DSCOVR EPIC, and Pandora give some qualitative understanding of their differences, it is highly desirable to bring them to the same times in a plausibly realistic way accounting for the volatile nature of the gas columns. Here we use "running window" averages with Gaussian-like weights:

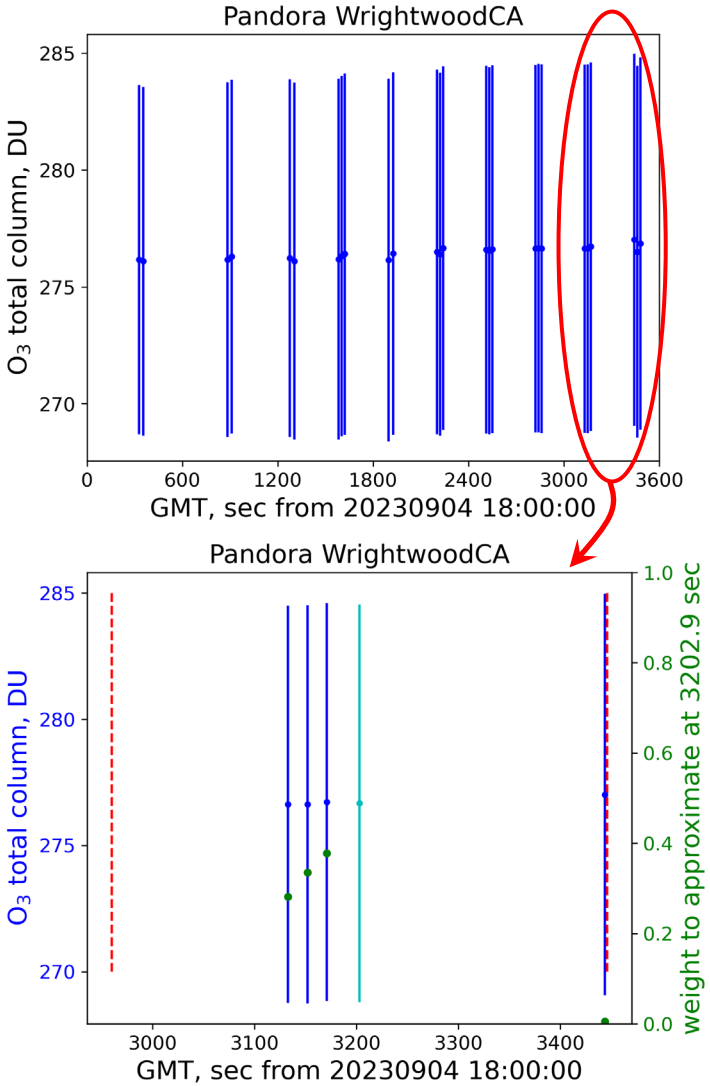
$$x_{int}(t) = \sum x(t_m) w(t_m, t), \quad w(t_m, t) = \exp\left[-\frac{(t - t_m)^2}{2\sigma^2}\right] \left(\sum \exp\left[-\frac{(t - t_m)^2}{2\sigma^2}\right]\right)^{-1}, \quad |t - t_m| \le \delta t_{max}$$



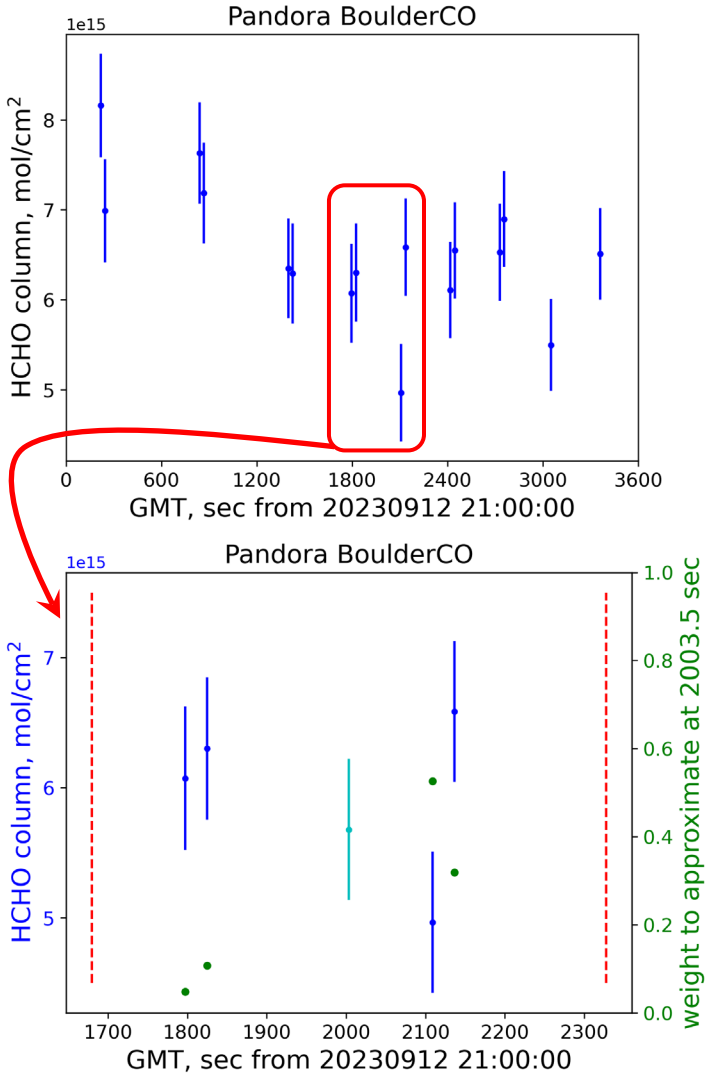
$\delta t_{max} = 60.48$ s $\sigma = 15.12$ s

Blue dots - actual Pandora retrievals with their uncertainties. Green dots – weights assigned to the retrievals. Red dashed lines – δt_{max} limits around time of interest, 1199.3 s, cyan dot – approximated value and uncertainty at the time of interest.

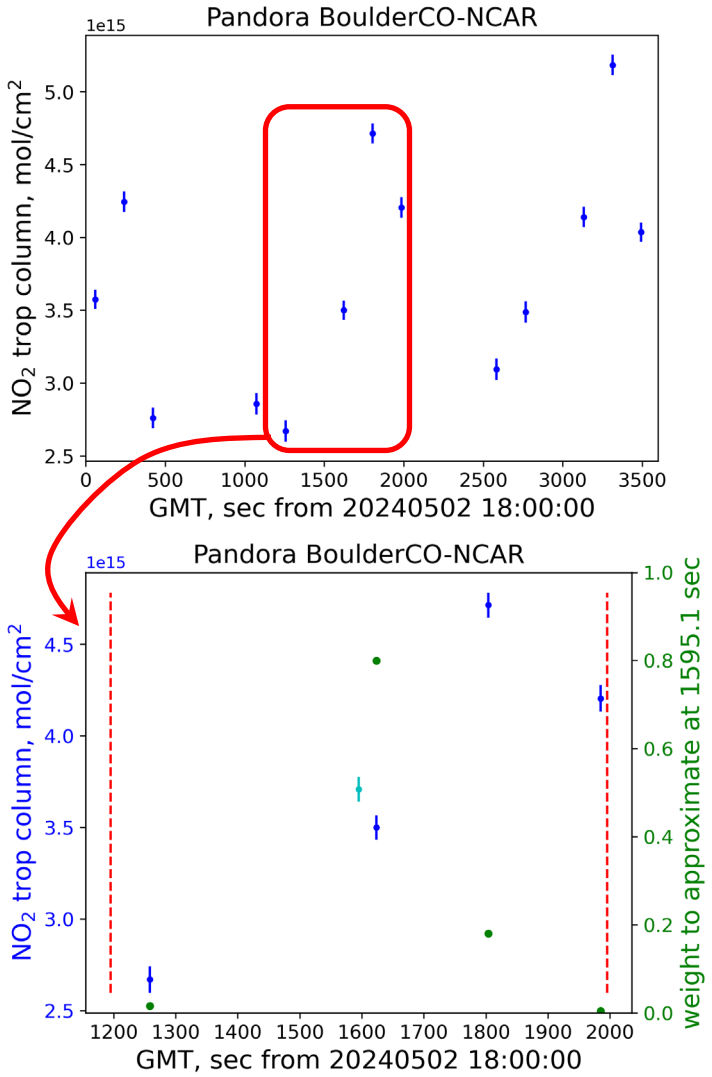
Temporal features of Pandora retrievals II



$\delta t_{max} = 243.0$ s
$\sigma = 81.00$ s



$\delta t_{max} = 324.0$ s
$\sigma = 81.00$ s



$\delta t_{max} = 405.0$ s
$\sigma = 121.5$ s

Python notebooks' structure and output

ASDC has created python notebooks comparing O_3 total, NO_2 total, HCHO total, and NO_2 tropospheric columns from corresponding TEMPO products against Pandora retrievals, O3 also compares DSCOVR EPIC total ozone column.

The notebooks perform the following steps:

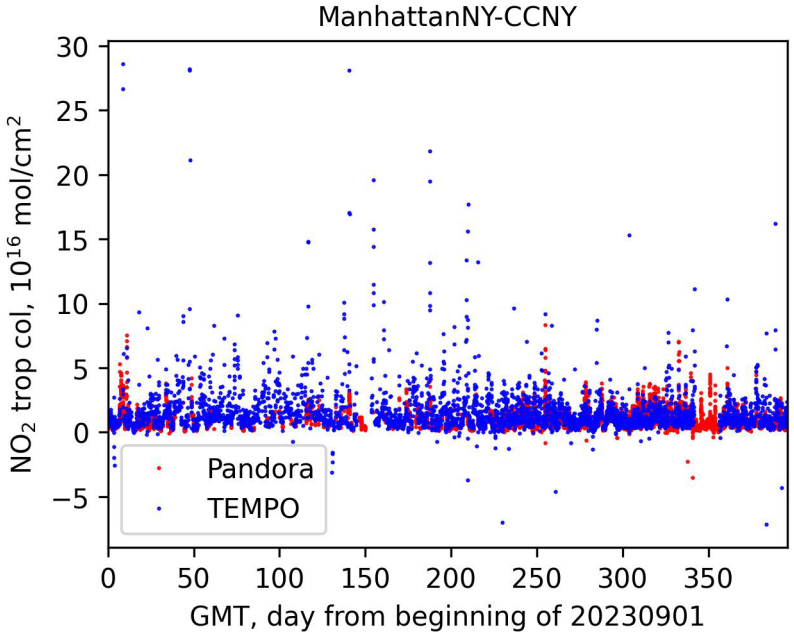
1) Available Pandora stations are listed, user is prompted to select one of them;
2) Appropriate Pandora data product is downloaded;
3) User is prompted to enter a timeframe of interest;
4) A timeseries of columnar retrievals with high quality flags within the timeframe is extracted from the Pandora data file;
5) TEMPO granules falling into the timeframe and covering the Pandora location are downloaded with the earthaccess library;
6) High quality TEMPO retrievals from the pixels surrounding the Pandora station are averaged;
7) Timeseries from both instruments are plotted and saved;
8) Pandora retrieved columns are averaged to the TEMPO times of observation;
9) Scatter plots showing Pandora vs TEMPO and a regression analysis are created and saved.

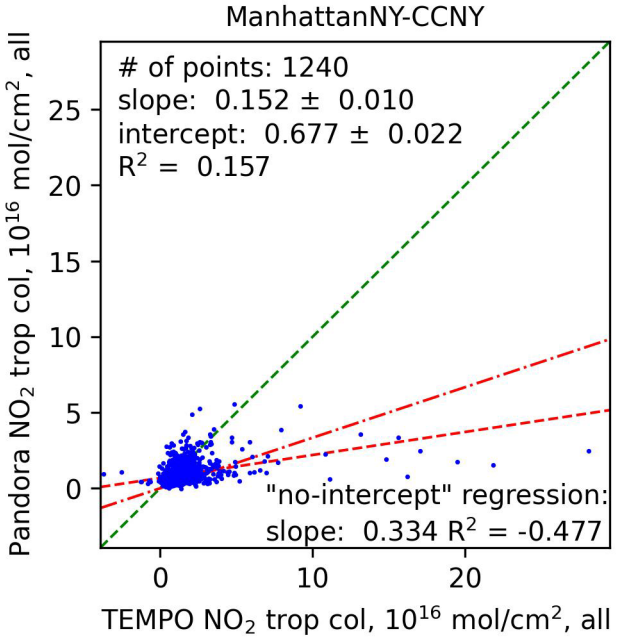
Note 1: Since TEMPO and Pandora retrievals (except O_3) can be negative, two sets of results are accumulated and analyzed:

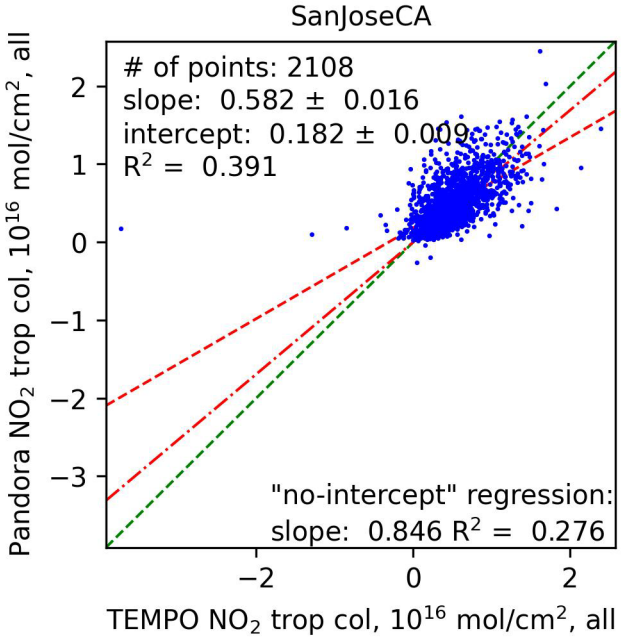
(1) all TEMPO retrievals of high quality;
(2) positive only retrievals of high quality.

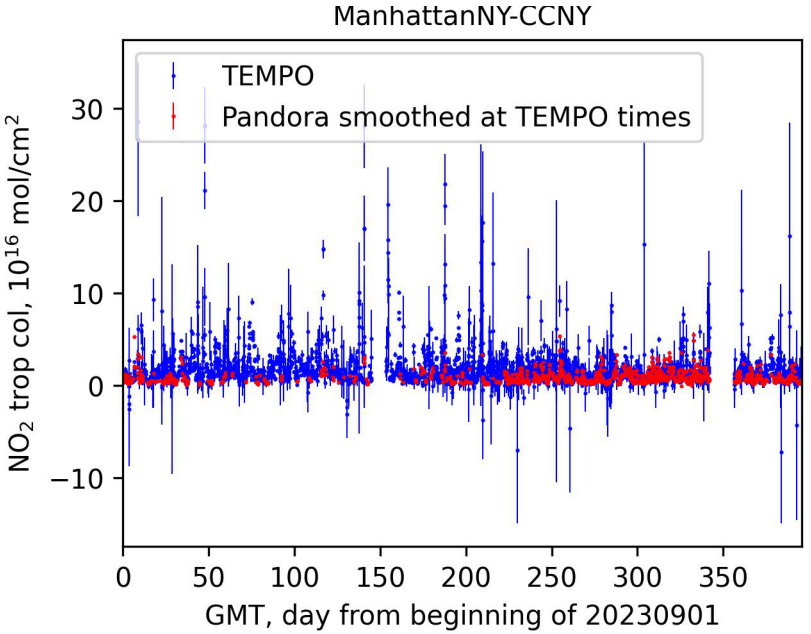
Note 2: notebook for ozone also creates a timeseries of DSCOVR EPIC retrievals of O3 total column.

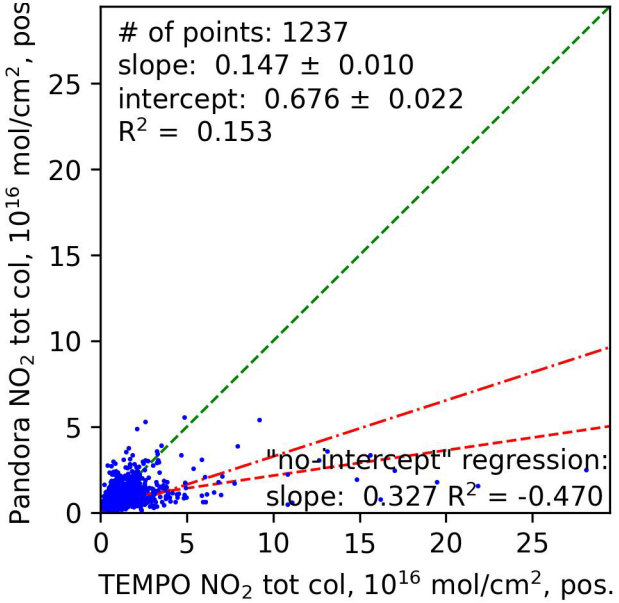
Nitrogen dioxide, tropospheric column

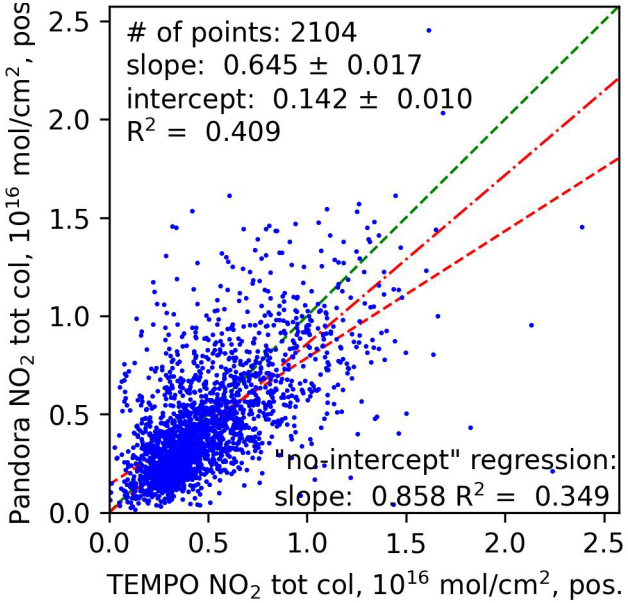










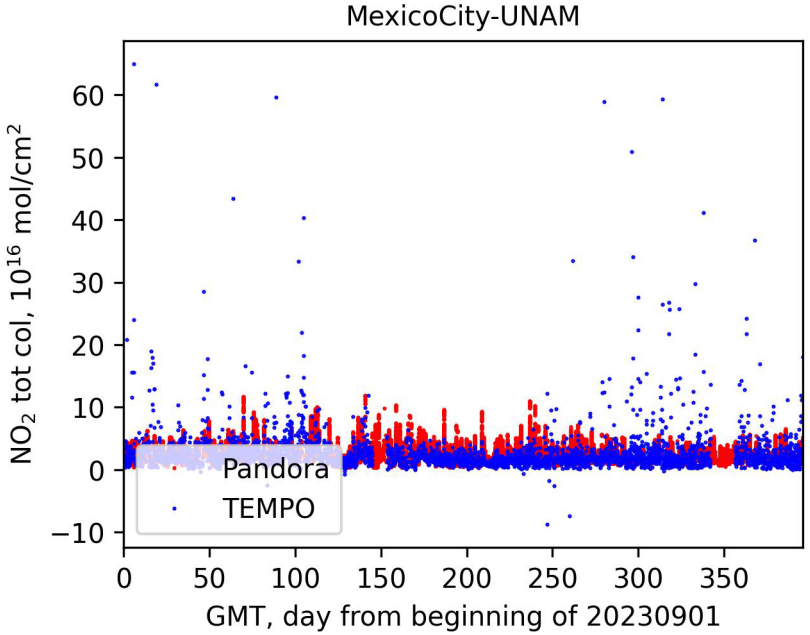


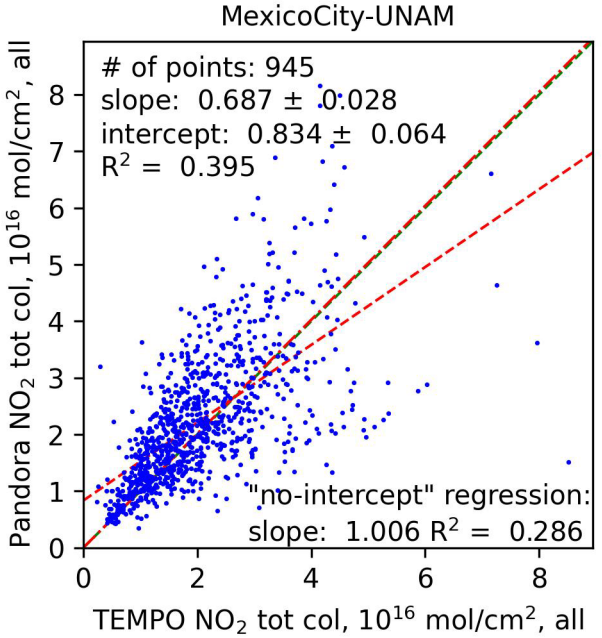
Green dashed – 1:1 reference

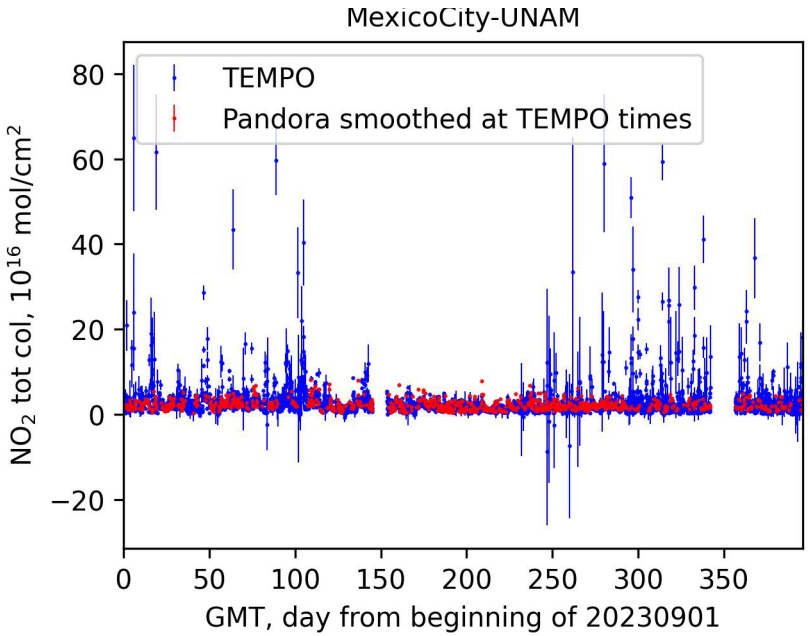
Red dashed – general line linear regression

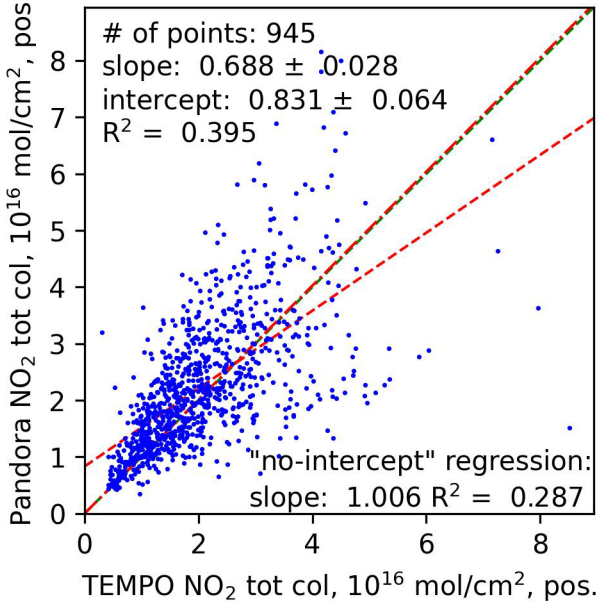
Red dash-dotted – $y = a \times x$ linear regression

Nitrogen dioxide, total column









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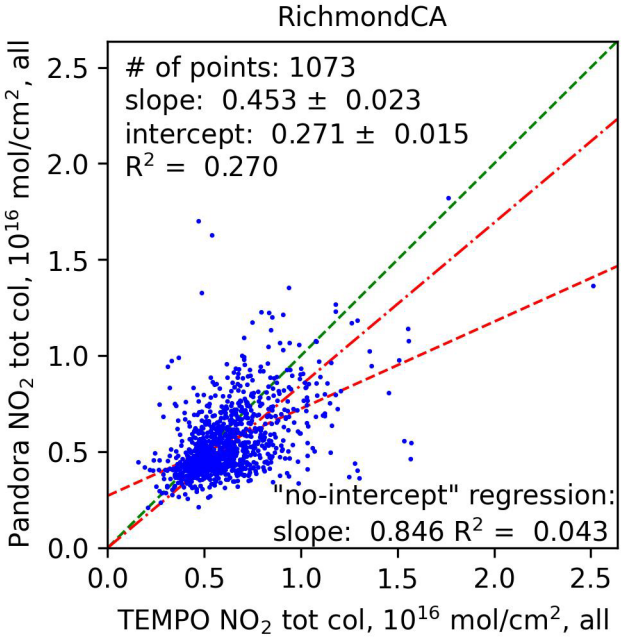
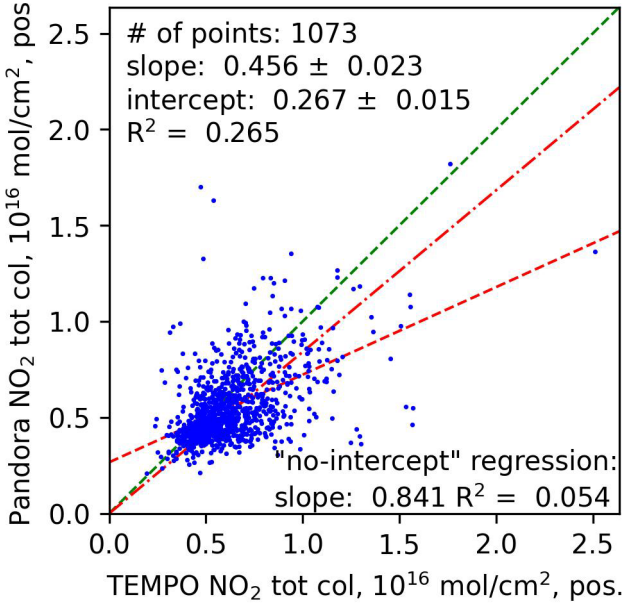
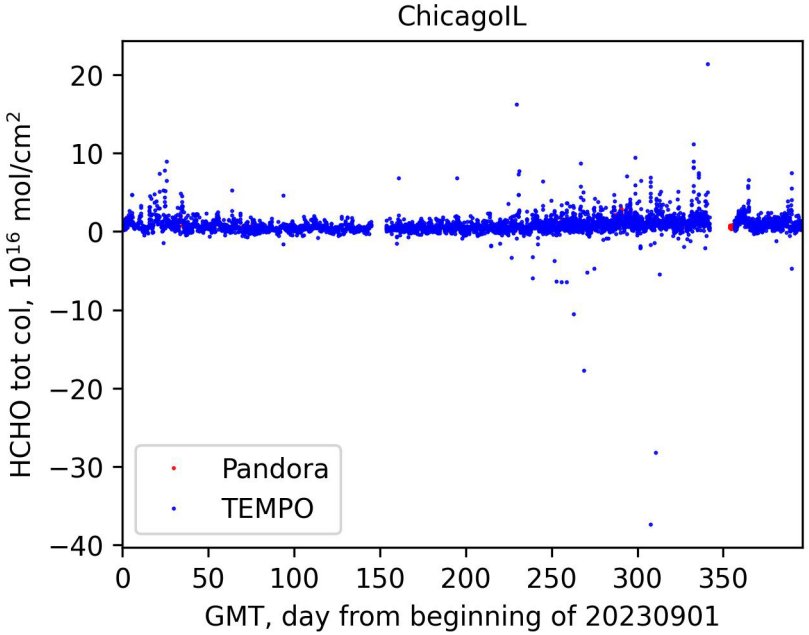
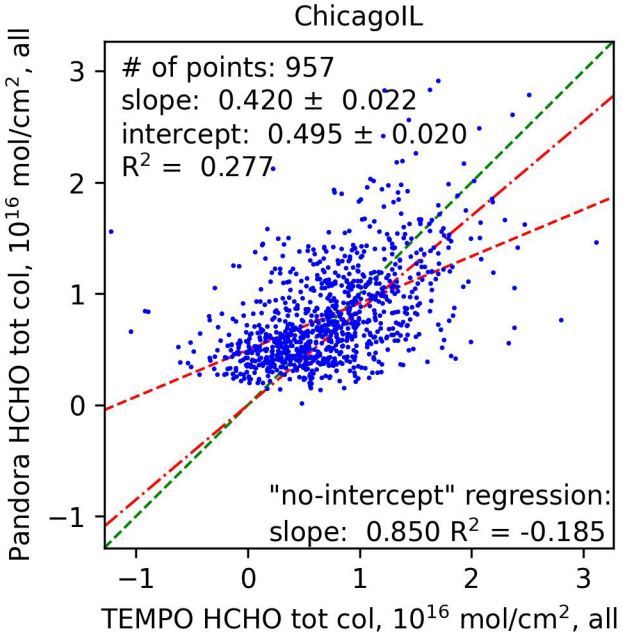
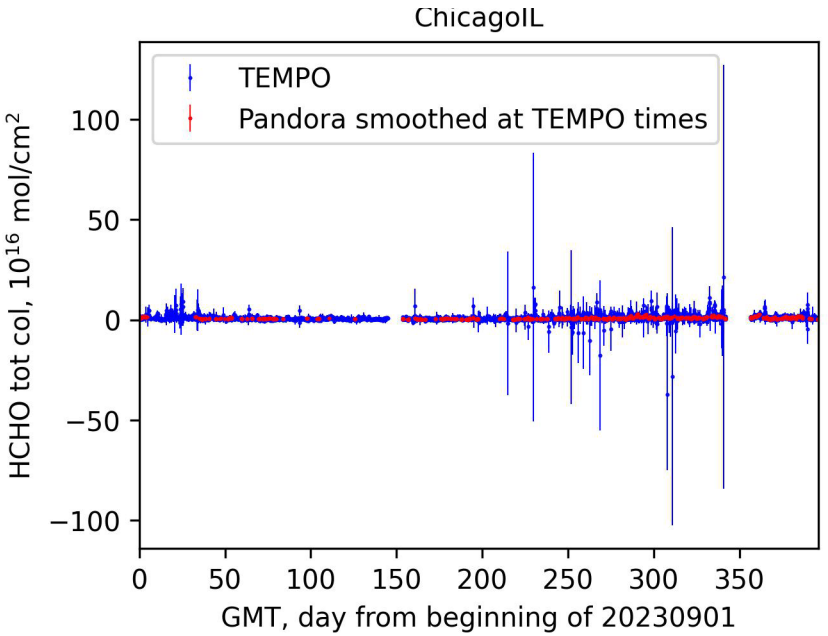


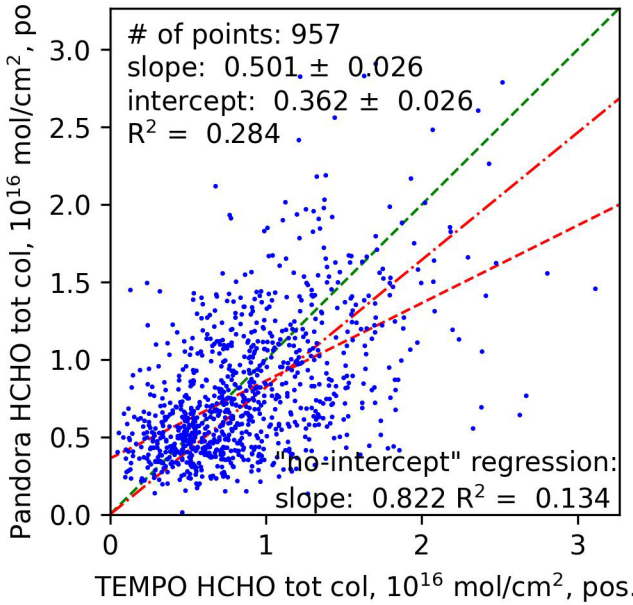


formaldehyde, total column









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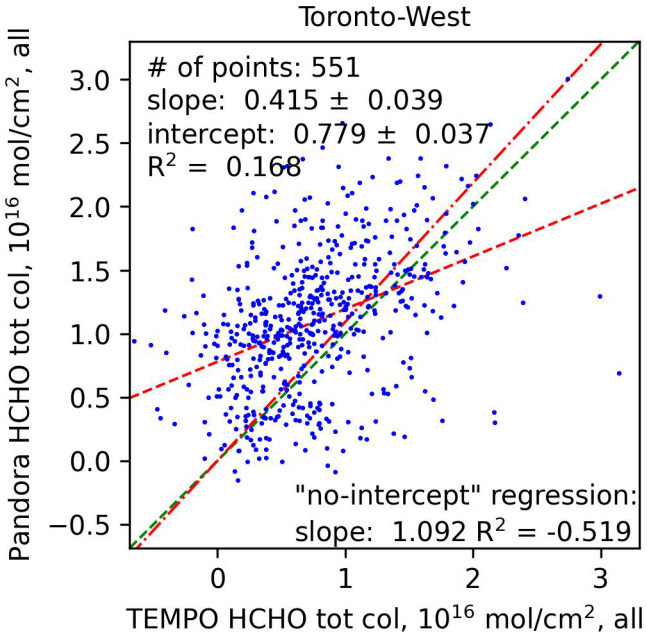
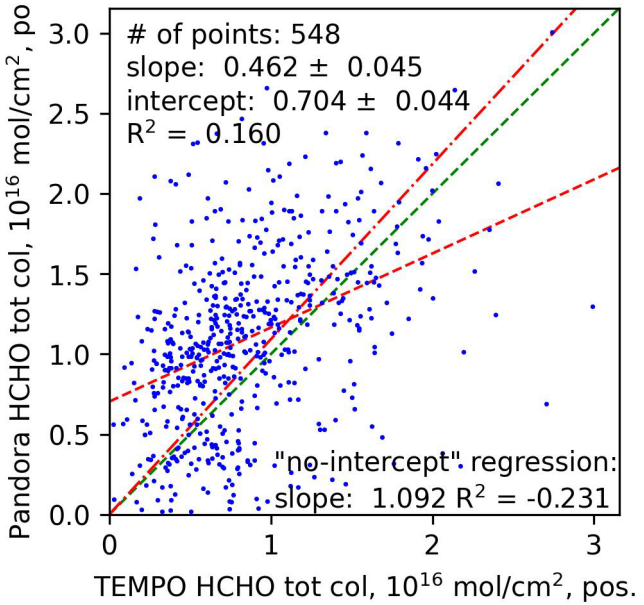
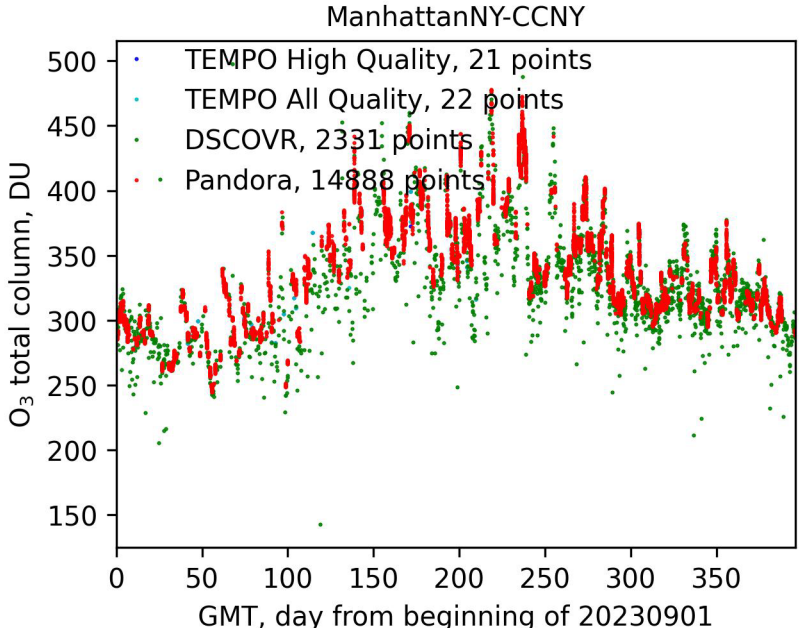
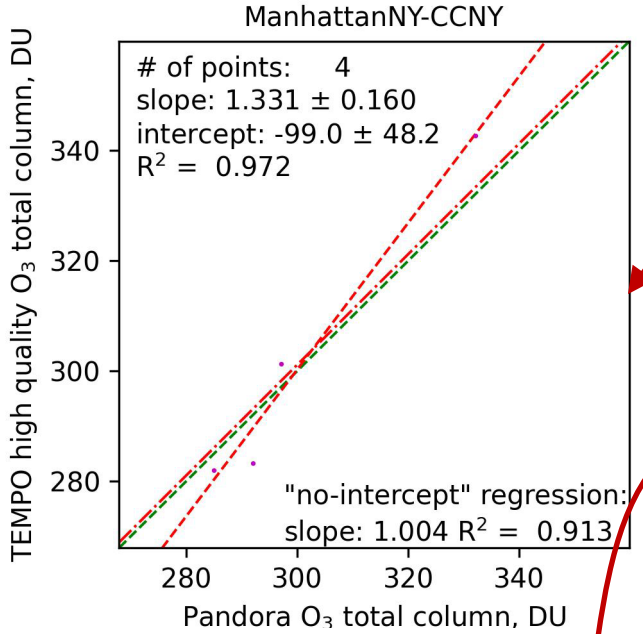


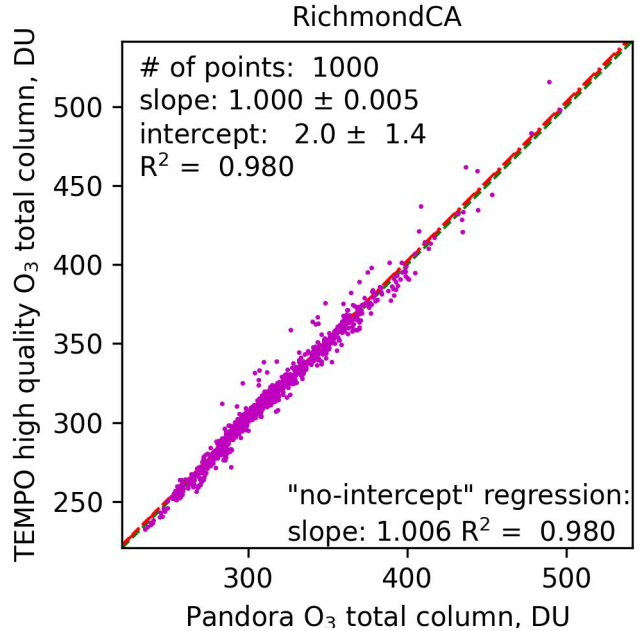


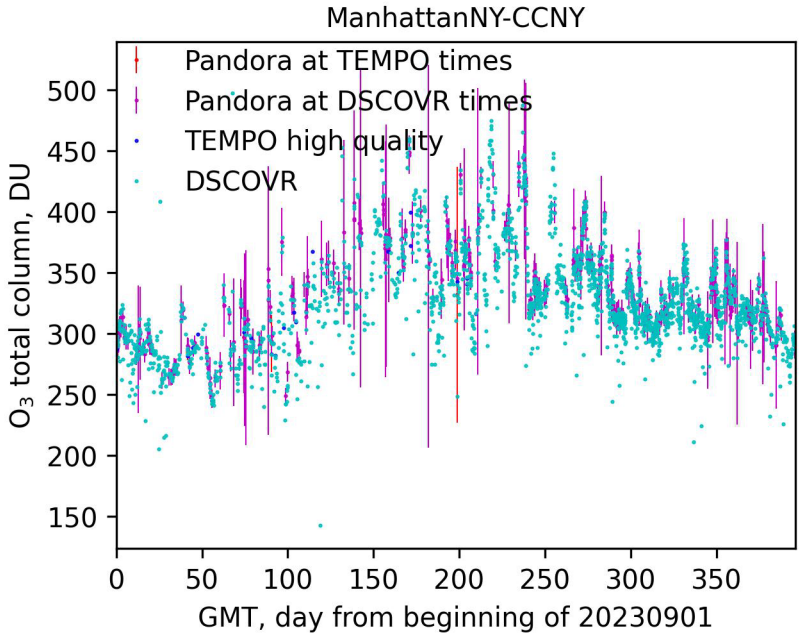
Ozone, total column

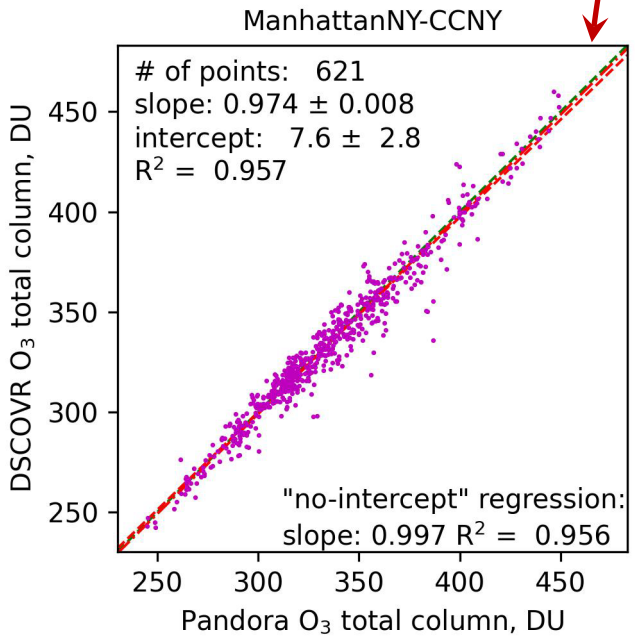




Why are there too few points here compare to DSCOVR EPIC retrievals?







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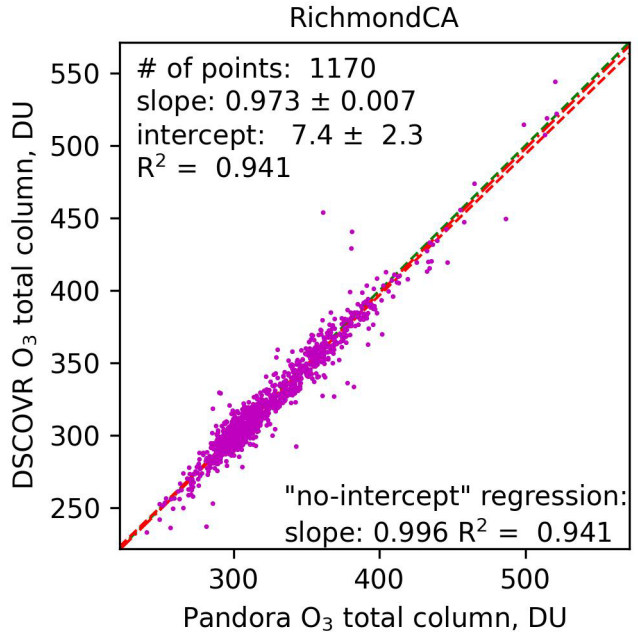
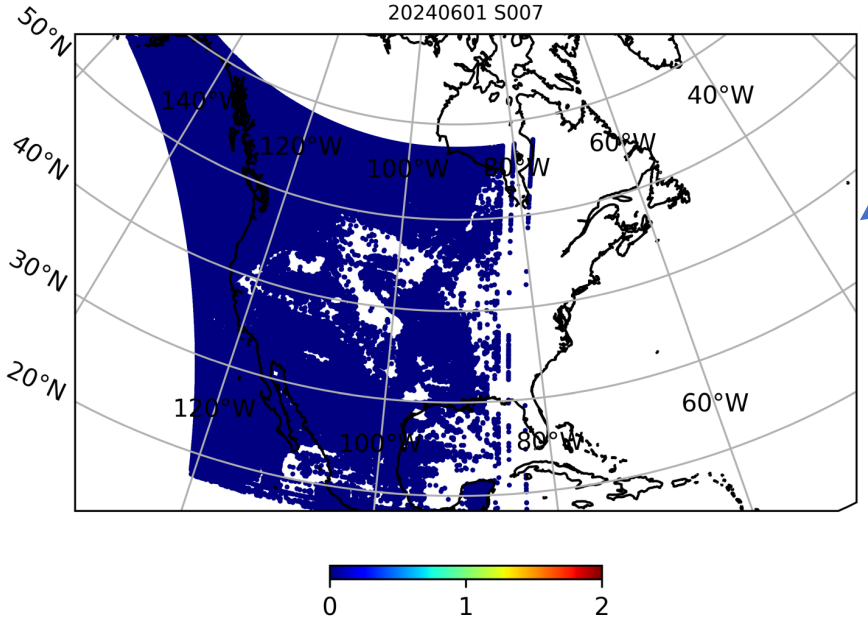
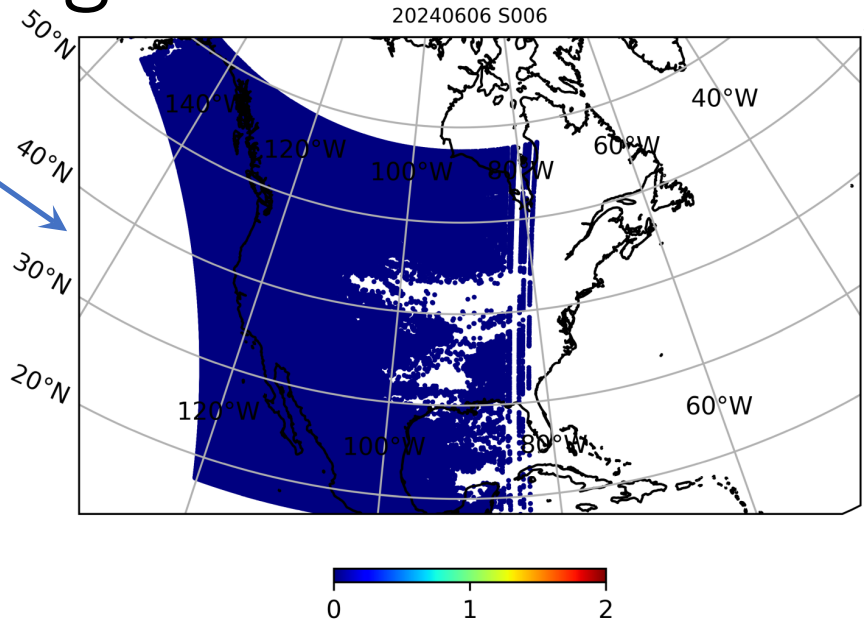


Distribution of Ozone High Quality Flag and Cloudiness



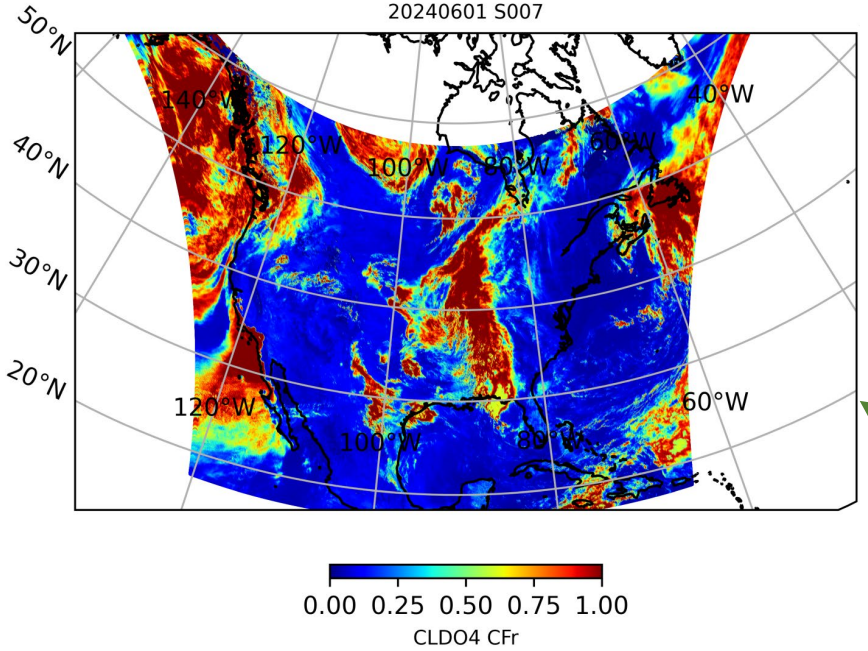


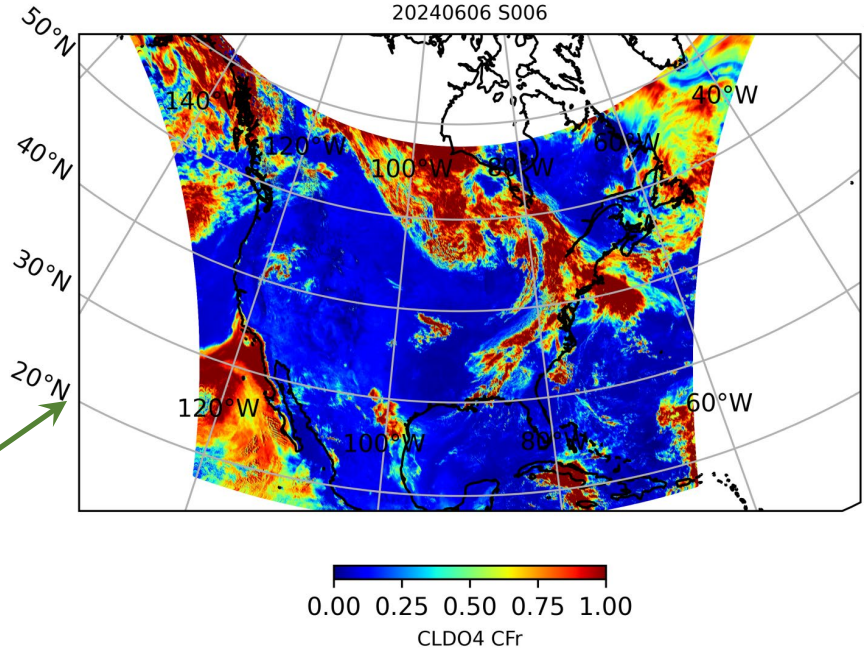
Quality flag 0 from TEMPO_O3TOT_L2_V03

Quality flag 0 recommended by the SAO TEMPO team in the User Guide does not occur over wide area of the USA and Canada East coast. Highest quality flag distribution hardly correlates with cloudiness, though it is hard to believe that ozone total column can be retrieved in the presence of dense clouds.

Seemingly, there are serious flaws in the algorithm assigning quality flags in TEMPO ozone product.

Cloud fraction from TEMPO_CLDO4_L2_V03





Conclusion

- Python notebooks enabling interactive comparison of TEMPO and Pandora retrievals of trace gases columns were created and made available via the NASA ASDC GitHub page, https://github.com/nasa/ASDC_Data_and_User_Services/tree/main/TEMPO/L2_validation_codes.
- Limited results included in this presentation show only qualitative match between TEMPO and Pandora retrievals of NO_2 total and tropospheric columns and HCHO total column. Significant intercept of the general linear regression and low coefficient of determination confirm the visually apparent shapelessness of clouds of data points in the retrieval scatter plots.
- Removal of physically meaningless negative retrievals from consideration does significantly change regression statistics.
- Due to the synthetic nature of NO_2 total column in TEMPO data, it would be interesting to derive NO_2 stratospheric column from Pandora total and tropospheric columns and then compare it directly with the TEMPO counterpart. This constitutes future work along with further optimization of the notebooks.
- Ozone total columns retrieved by both TEMPO and DSCOVR EPIC show reasonable match with Pandora retrievals.
- A problem with QF assignment algorithm in TEMPO ozone product leads to insufficient statistics over the East coast.
- Differences between satellite and ground-based retrievals are site dependent which may indicate to quality control issues with Pandora. Discussion on Pandora quality flags can be found in Rawat, P. et al., Atmos. Meas. Tech. Discuss., in review, 2024, https://doi.org/10.5194/amt-2024-114.