Intercomparison of Pandora MAX-DOAS NO_2 retrievals with in-situ network measurements and airborne observations across the Eastern US

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Motivation

- MAX-DOAS retrievals of partial columns and surface concentrations across the Pandonia Global Network are a high potential dataset for TEMPO validation (See Figure 1)
- Evaluation of the pandora instrument MAX-DOAS measurements via comparisons with ground-based and airborne measurements can provide more information regarding the utility and limitations of the new measurements prior to use in satellite validation

Figure 1. Map of all active Pandora instruments within TEMPO's field of regard (FOR) over North America

MAX-DOAS retrievals

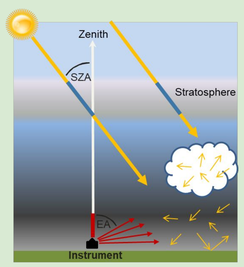


Figure 2. MAX-DOAS observation geometry highlighting scattering processes affecting measurements

Gas absorption depends on:

Wavelength
Rayleigh scattering
Aerosol profile and properties
Clouds
Scanning elevation angles
Solar zenith angle
Gas profiles
Surface albedo

Pandora instruments use a combined empirical/geometrical approach informed by optimal estimation to derive partial column and surface concentration retrievals:

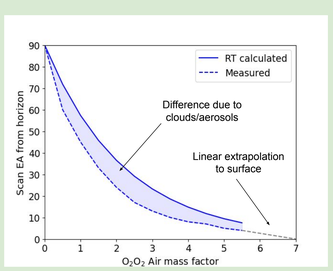


Figure 3. Conceptual illustration of MAX-DOAS O_2O_2 scattering correction algorithm

- Measured rayleigh scattering from O_2O_2 collision complex compared with radiative transfer model to correct for aerosol/cloud scattering
- Surface measurement is extrapolated down from largest elevation angle
- Both short and long scan modes with a fixed azimuth angle, measured down to horizon and back up to zenith:
  - Short scan outputs tropospheric column + surface concentration
  - Long scan outputs same products + partial columns

Key advantages of method:

- Circumvents time consuming online radiative transfer simulations
- Uses real atmospheric measurements for parameterizations in lieu of AMF look-up tables

Surface intercomparisons

NO_2 measurement statistics across all co-located sites:

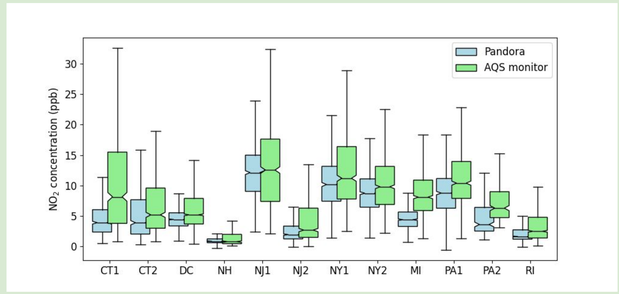


Figure 4. Boxplot showing NO_2 measurement statistics for co-located Pandora/AQS monitors across Eastern US from 2021-2022

- Pandora shows a median bias of -22% across all sites used in the analysis
- Direction of bias in line with expectation between 'true' surface measurement (AQS) and extrapolated near-surface measurement (Pandora)
- Best agreement observed at NJ1 (Bayonne, NJ) site with a median bias of -6%
- Largest differences observed at MI, CT1 and PA2 sites:
  - Differences at CT1 and MI could be driven by local vs regional NOx sources
  - PA2 discrepancy likely due to calibration offset in AQS monitor

Possible drivers of measurement discrepancies:

1. Maximum scan elevation angles

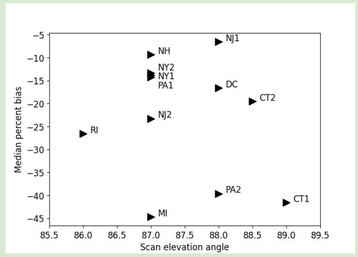
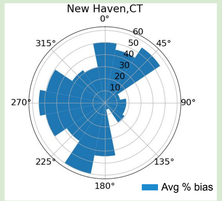


Figure 5. Median percent NO_2 biases for each site plotted against pandora maximum elevation angle

- Extrapolation of aerosol scattering from maximum elevation angle less than 89 degrees can lead to more uncertainty in retrieval
- Surface comparisons showed no observed relationship between measurement biases and max elevation angle, indicating NO_2 differences more sensitive to other factors

2. Local vs regional NO_2 influences

a)



b)

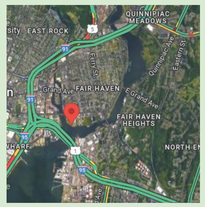


Figure 6. a) Pandora/AQS absolute median NO_2 biases (blue slices) plotted vs. wind direction for the New Haven, CT site. b) Location of New Haven site situated between major highways

- Biases heavily reduced when wind comes from the SE where plumes are least impacted by highway emissions
- Largest biases between Pandora and AQS occurs from W and SW where site is closest to highways

Vertical profile comparisons

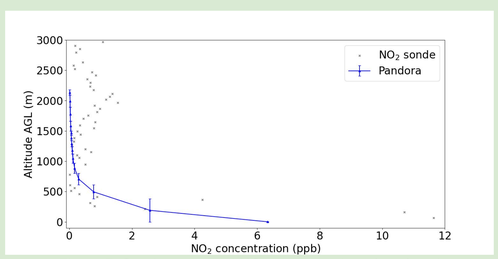


Figure 7. Sonde measured NO_2 concentrations (gray) and Pandora partial column concentrations (blue) measured nearest to time of flight vs. altitude AGL.

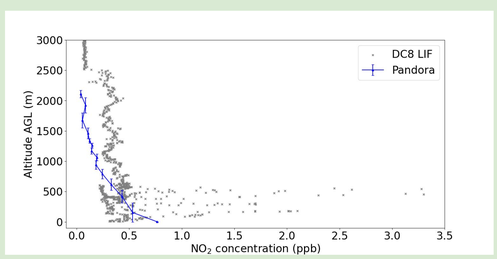


Figure 8. LIF measurements of NO_2 onboard the DC8 (gray) and Pandora partial column concentrations (blue) measured nearest to time of flight vs. altitude AGL.

- Good agreement between Sonde and Pandora from near-surface up to 1.5km
- Elevated NO_2 above 1.5km 'missed' by Pandora 2, possibly due to techniques reduced sensitivity to higher layers

- Pandora captures general NO_2 profile observed by aircraft during Northern section of flight from surface up to 500m
- Pandora 74 measurements of NO_2 mixing ratios also approach 0 ppb above 1.5km implying a more shallow boundary layer than measured by the DC8

Many more profile comparisons to come from ALEGROS and SARP summer 2024 field campaigns!

Methods

Pandora comparisons with surface observations

- Measurements taken from 12 US EPA AQS sites with a co-located pandora instrument across Eastern US (Figure 9) from a 2021-2022 measurement period.
- Pandora surface NO_2 measurements hourly averaged to match reported AQS values and filtered using $\pm$ 1 median rms and measurement uncertainty < 20%

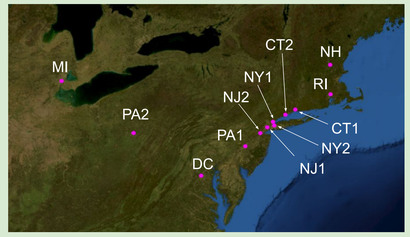


Figure 9. Map of co-located pandora/AQS sites used in the present study. Sites used in alphabetical order are: CT1 (New Haven, CT), CT2 (Westport, CT), DC (Washington, DC), NH (Londonderry, NH), NJ1 (Bayonne, NJ), NJ2 (New Brunswick, NJ), NY1 (Bronx, NY), NY2 (Queens, NY), MI (Detroit, MI), PA1 (Pittsburgh, PA), PA2 (Philadelphia, PA), and RI (East Providence, RI)

Pandora comparisons with airborne observations

A) Comparison of pandora vertical columns with NO_2 sonde

a)

b)

Figure 10. a) Map showing locations of Greenbelt, MD and Beltsville, MD with the pandora (triangle) and MAX-DOAS scanning direction are marked in red. b) Photo of the NO_2 sonde launch in Beltsville.

- NO_2 sonde launched in Beltsville, MD 5km away from nearest pandora instrument
- Sonde NO_2 measurements made using cavity-enhanced absorption with precision of $\pm$ 94 pptv (1s)
- Comparison done using closest pandora scan to time of launch

B) Comparison of pandora vertical columns with airborne measurements

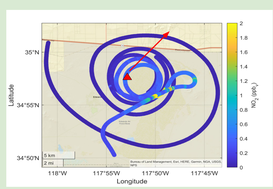


Figure 11. Flight track of DC8 spiral over Edwards Air Force Base, CA on June 23 with flight tracks colored by NO_2 concentration. The pandora (triangle) and MAX-DOAS scanning direction are marked in red

- DC8 aircraft spiraled over Edwards Air Force Base in California on June 23,2023 during the AEROMMA field campaign
- DC8 NO_2 measurements made using laser-induced fluorescence with precision of $\pm$ 50 ppt (1s)
- Comparison done using closest pandora scan to flight spiral

Data access and availability

All pandora instrument data available at:

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

US EPA AQS network data available at:

https://aqs.epa.gov/aqsweb/