IDEAS-QA4EO Cal/Val

Synergies between Pandora and MAX-DOAS systems for the retrieval of tropospheric aerosol and trace gas vertical profiles, as well as total NO$_2$ columns

Dimitris Karagkiozidis, Dimitris Nikolis, Alkis Bais and Dimitris Balis

Laboratory of Atmospheric Physics, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece
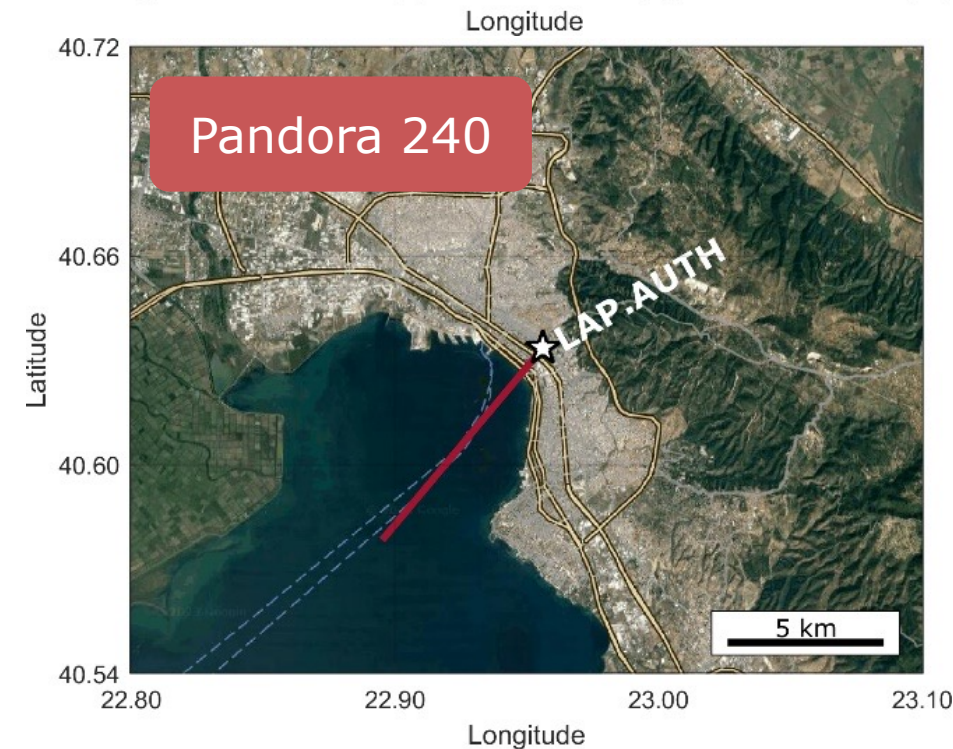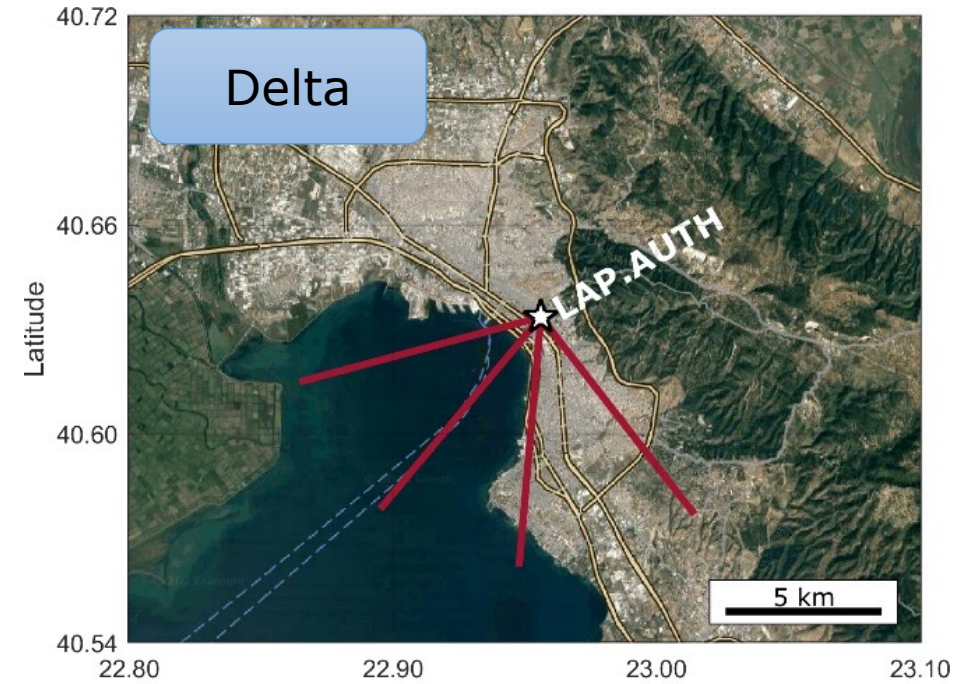
MAX-DOAS measurements at Thessaloniki

Delta

- Research-grade system
- Increased accuracy in trace gas measurements
- Direct sun and MAX-DOAS observations
- NO_2, HCHO, Aerosols

Pandora 2S 240

- Part of PGN
- Two spectrograph units (UV and VIS)
- Direct sun and MAX-DOAS observations
- NO_2, HCHO, O_3, SO_2

Delta

Pandora 240

Aim

❑ Retrieval of tropospheric aerosol NO_2 and HCHO vertical profiles in Thessaloniki using as input Pandora's spectra and dSCDs

❑ Comparison with the operational MAX-DOAS products

❑ Comparison with the operational Pandora L2 products

Operational schedule of Pandora sky-radiance observations

Elevation angles: 1, 2, 15, 30 and 89°

Adjusted schedule

Elevation angles: 1, 2, 3, 4, 5, 6, 8, 10, 12, 15, 30 and 89°

Aerosol and trace gas profiling
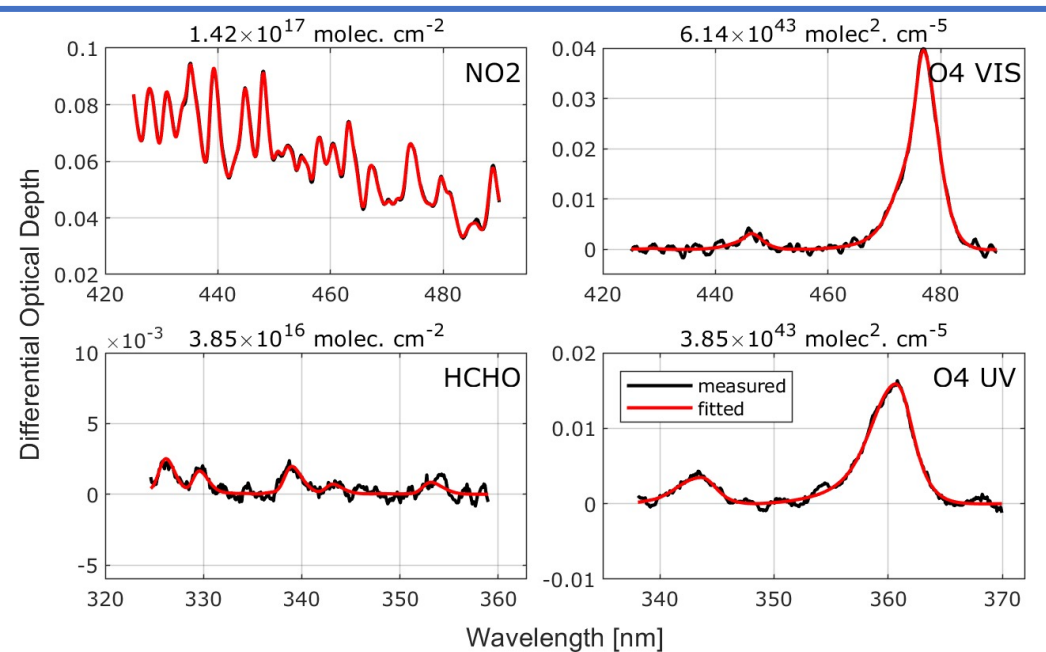
Mexican MAXDOAS Fit v2020_04 (MMF)
Friedrich et al., 2019

Optimal Estimation Method

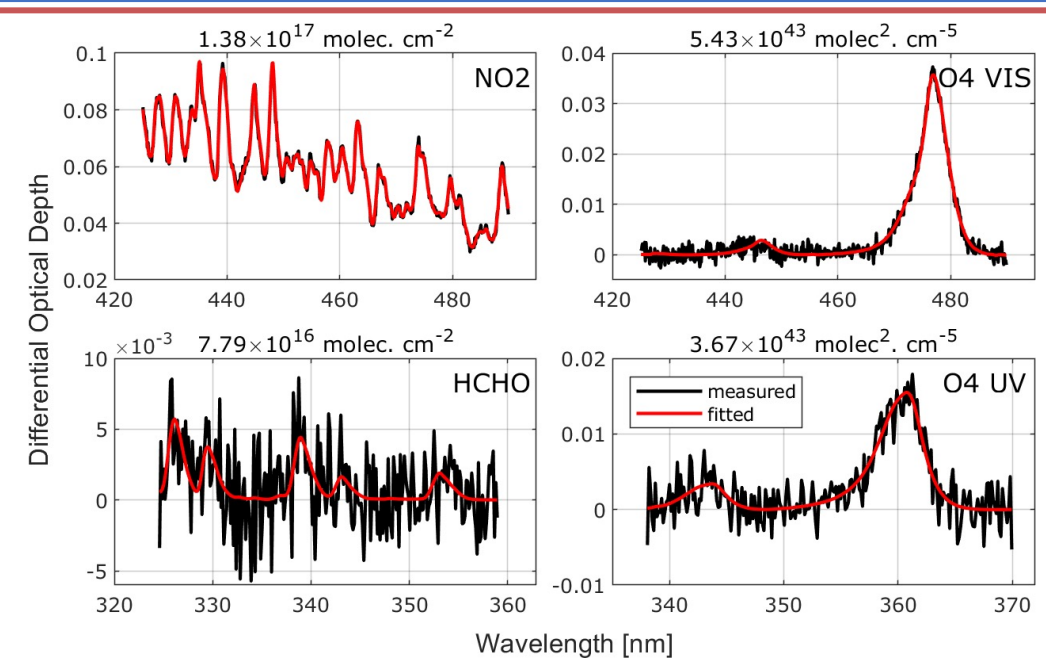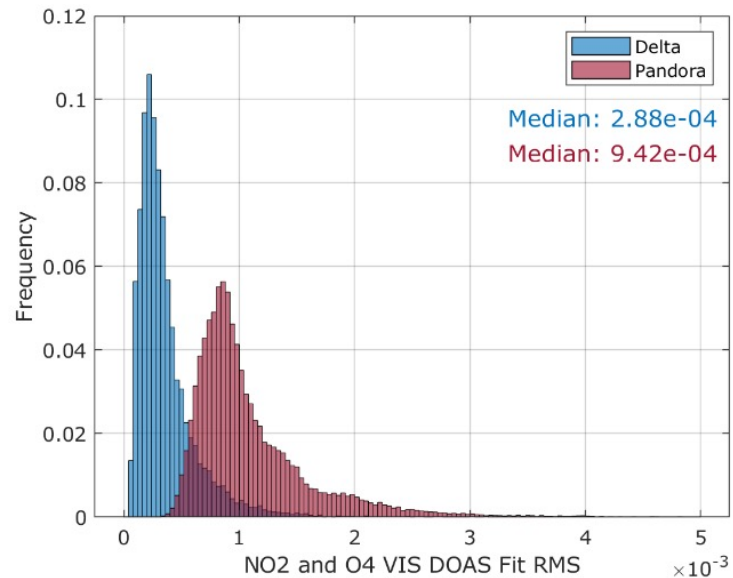Mainz Profile Algorithm v0.98 (MAPA)
Beirle et al., 2019

Parameterization Approach

❑ dSCDs have been recalculated with QDOAS using the sequential zenith-sky spectra as reference

❑ DOAS retrieval settings based on recommendations of CINDI-2 (Kreher et al., 2020)
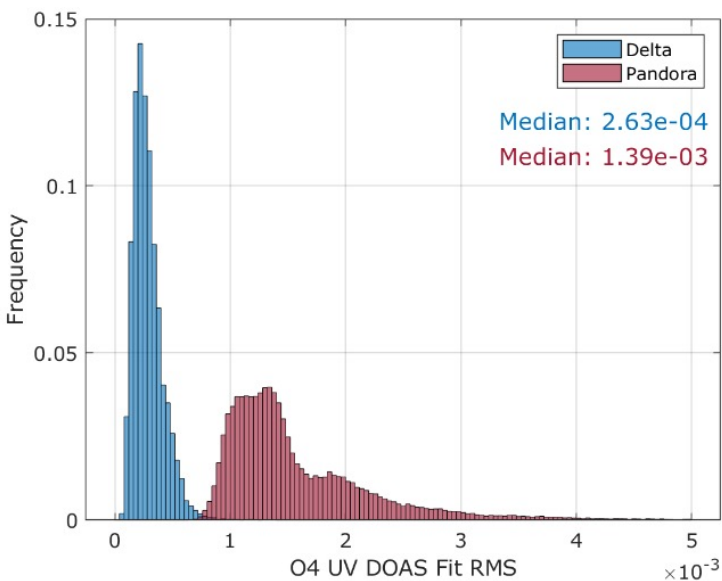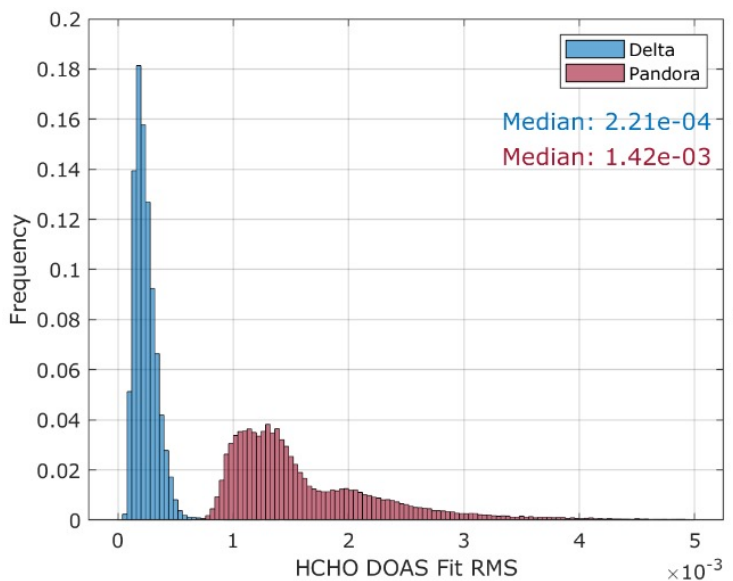
❑ Period of study: Nov 2023 – Apr 2024

Evaluation of retrieved dSCDs (Delta vs Pandora)

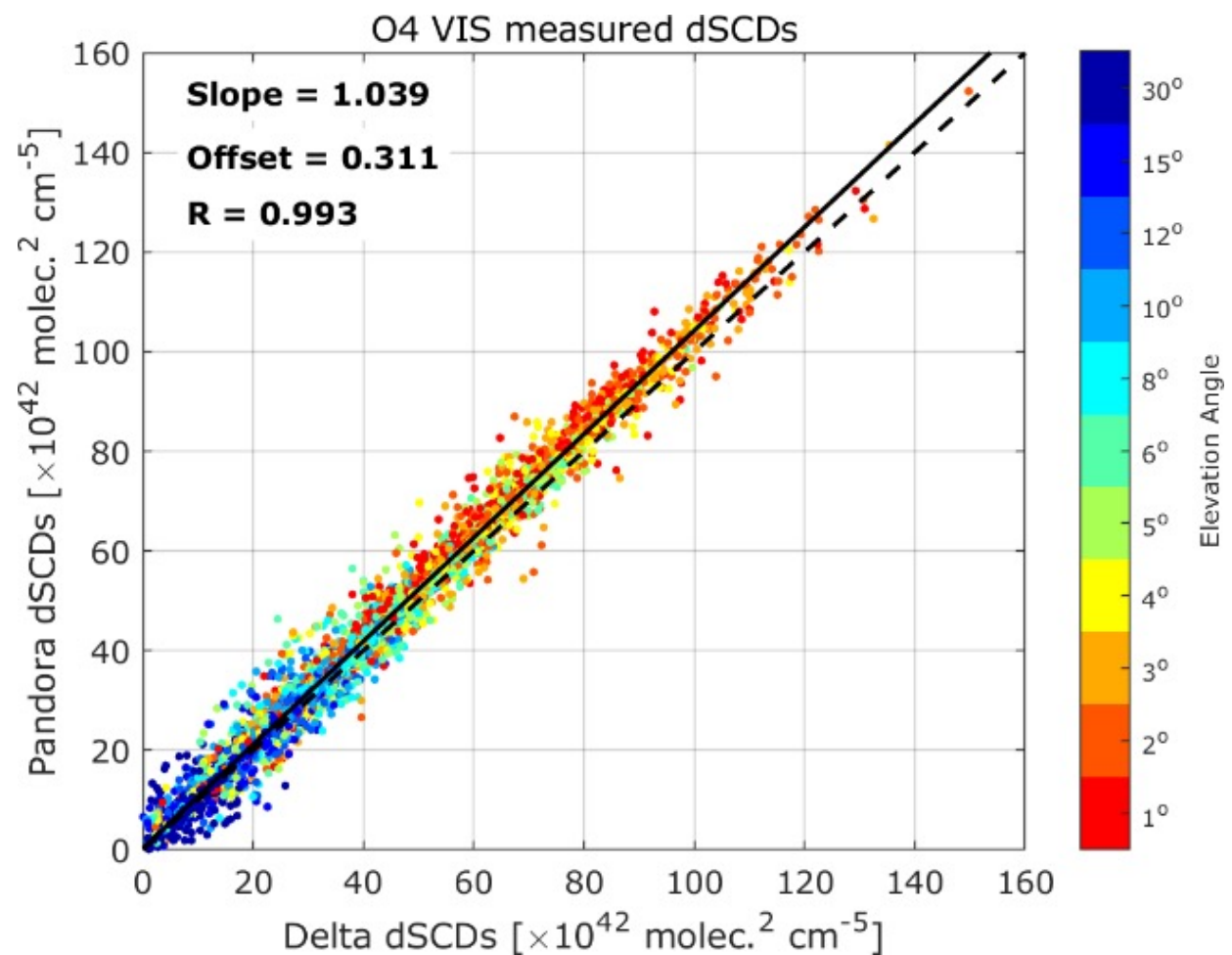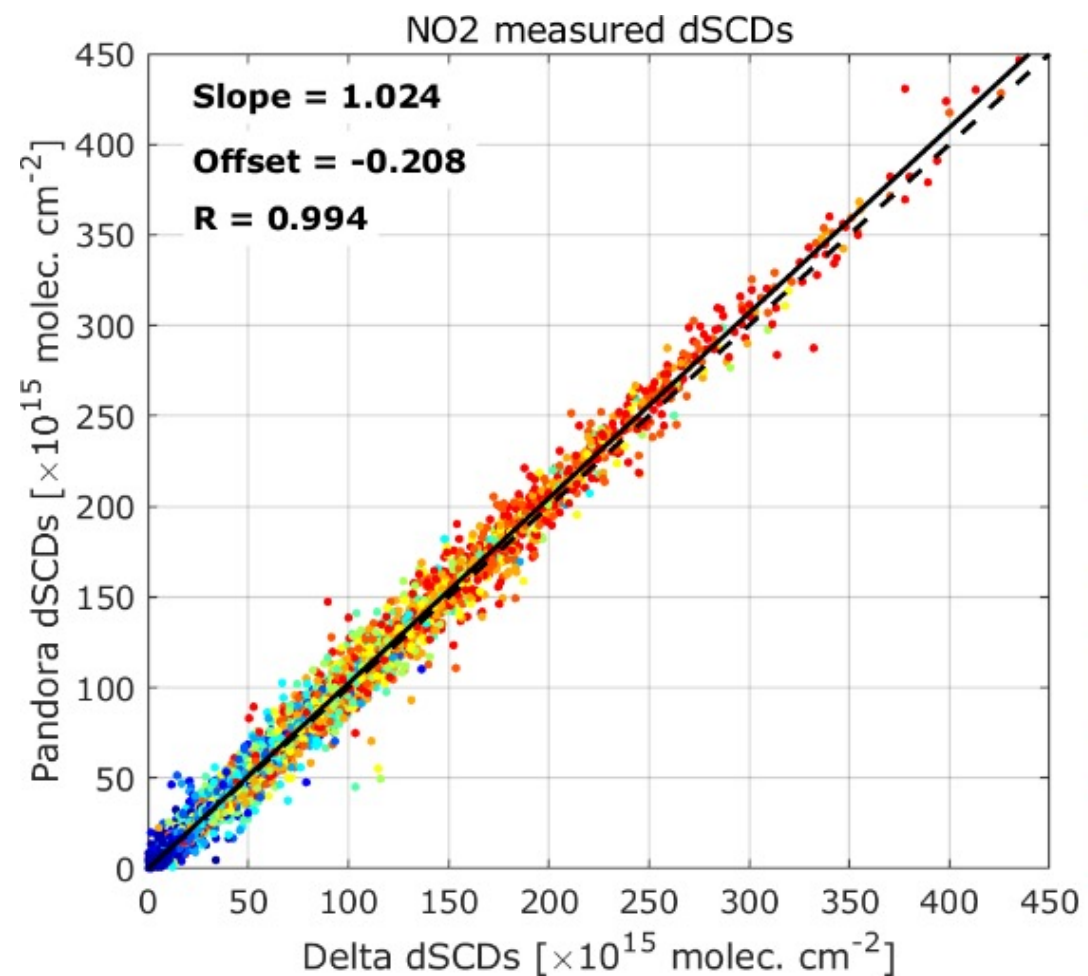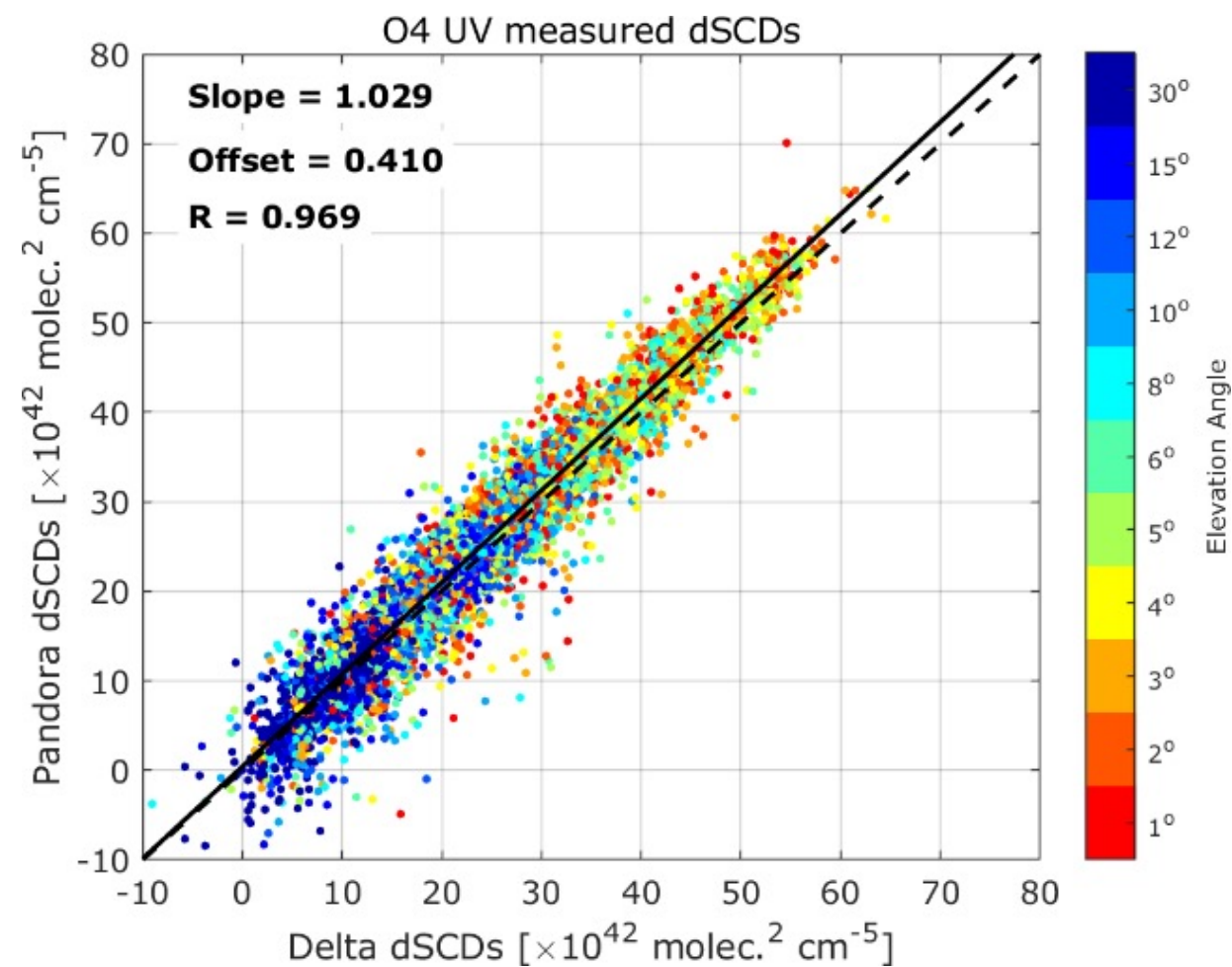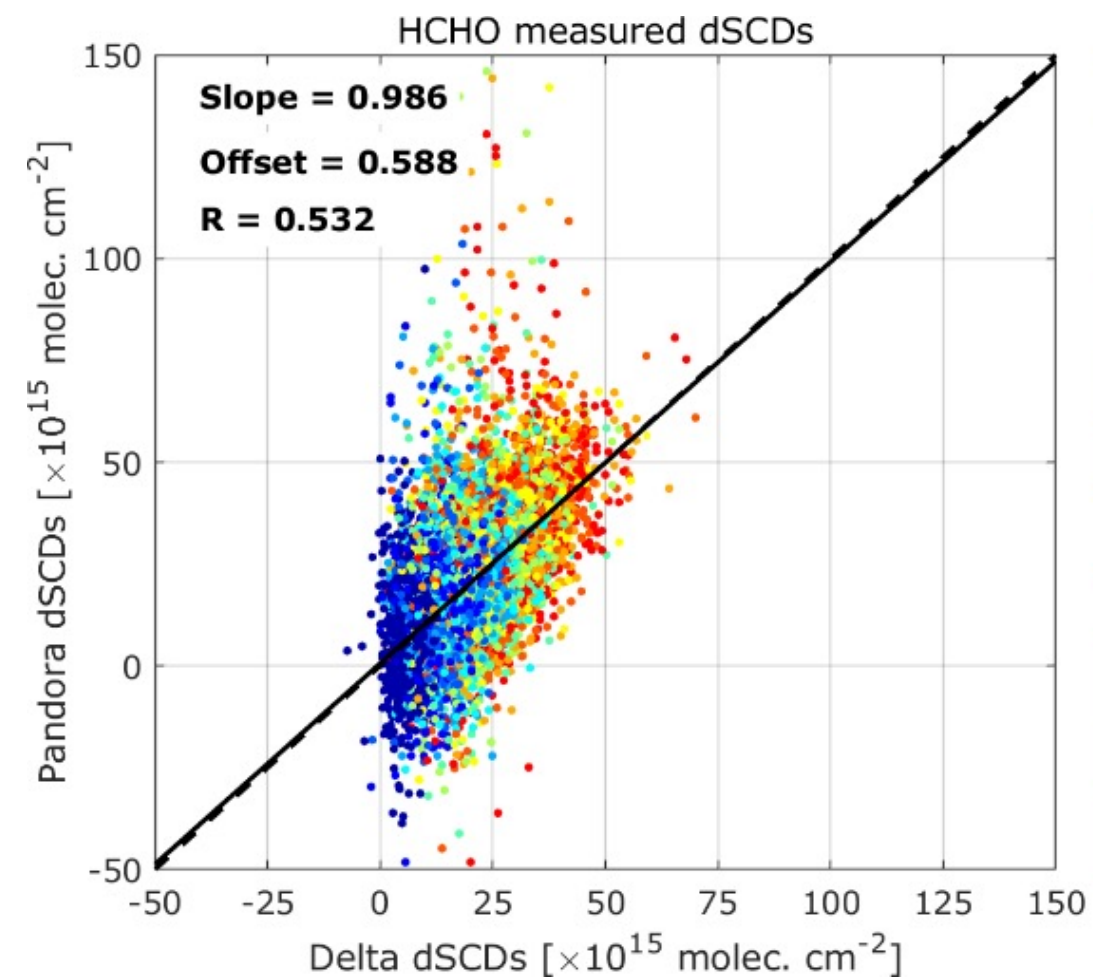# Comparison of measured dSCDs

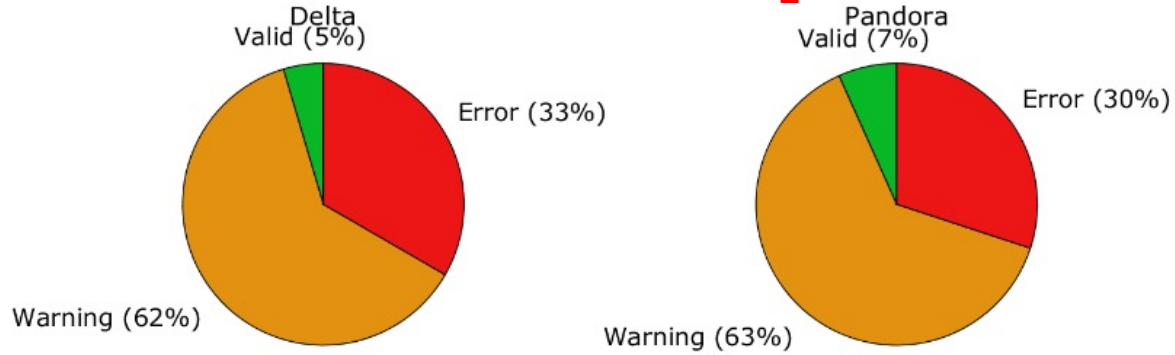Species in the visible range

Comparison of measured dSCDs

Species in the UV range

Flagging of data by the profiling algorithms
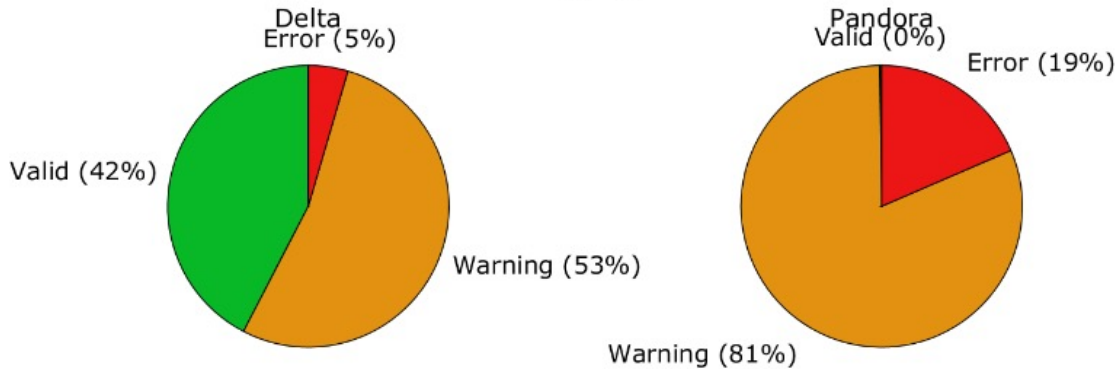
MMF flagging

MMF Flagging NO₂

Delta
Valid (5%)
Error (33%)
Warning (62%)

Pandora
Valid (7%)
Error (30%)
Warning (63%)

MMF Flagging O₄ VIS

Delta
Valid (0%)
Warning (45%)
Error (55%)

Pandora
Valid (0%)
Warning (48%)
Error (52%)

MMF Flagging HCHO

Delta
Error (5%)
Valid (42%)
Warning (53%)

Pandora
Valid (0%)
Error (19%)
Warning (81%)

MMF Flagging O₄ UV

Delta
Valid (0%)
Error (32%)
Warning (68%)

Pandora
Warning (5%)
Error (95%)
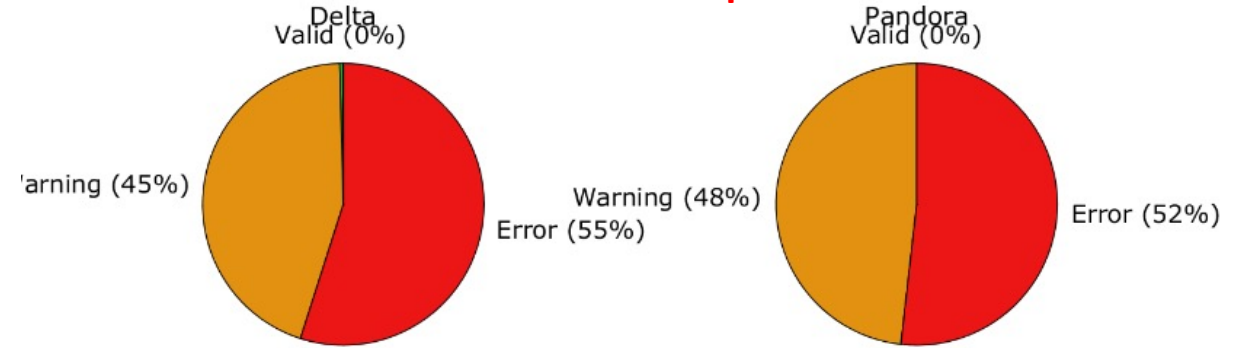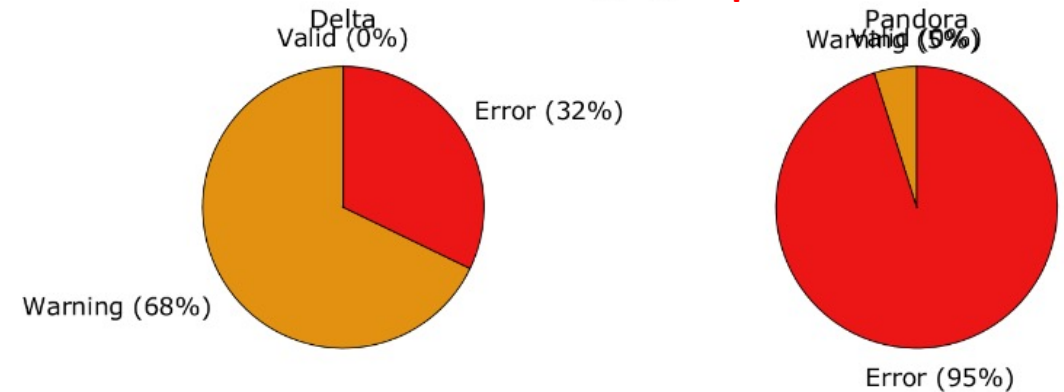
Flagging of data by the profiling algorithms

MAPA flagging

MAPA Flagging NO$_2$

Delta
Valid (30%)
Error (29%)
Warning (41%)

Pandora
Valid (26%)
Error (35%)
Warning (39%)

MAPA Flagging O$_4$ VIS

Delta
Error (28%)
Valid (36%)
Warning (36%)

Pandora
Valid (32%)
Error (33%)
Warning (35%)

MAPA Flagging HCHO

Delta
Valid (34%)
Error (38%)
Warning (28%)

Pandora
Valid (16%)
Error (50%)
Warning (34%)

MAPA Flagging O$_4$ UV

Delta
Error (37%)
Valid (40%)
Warning (23%)

Pandora
Valid (24%)
Error (48%)
Warning (28%)
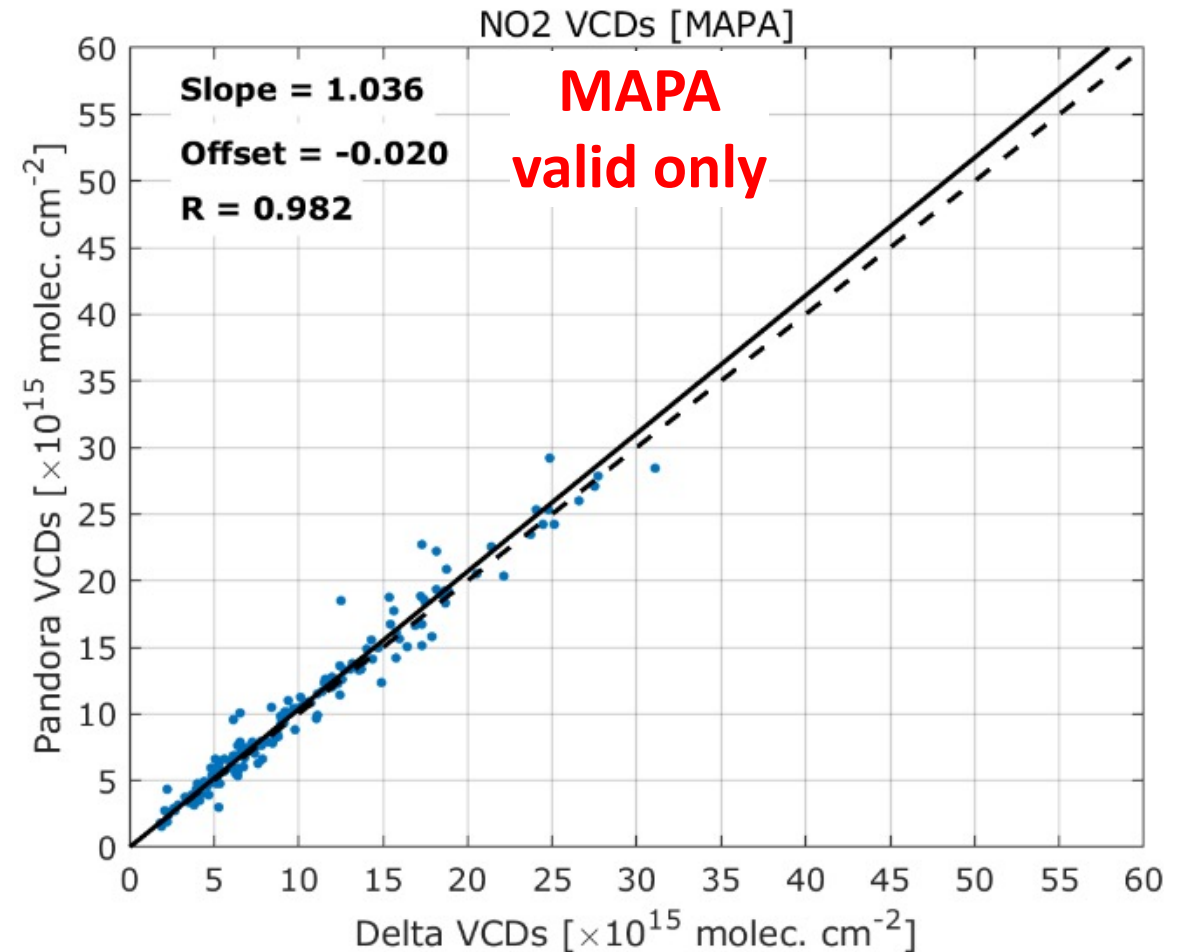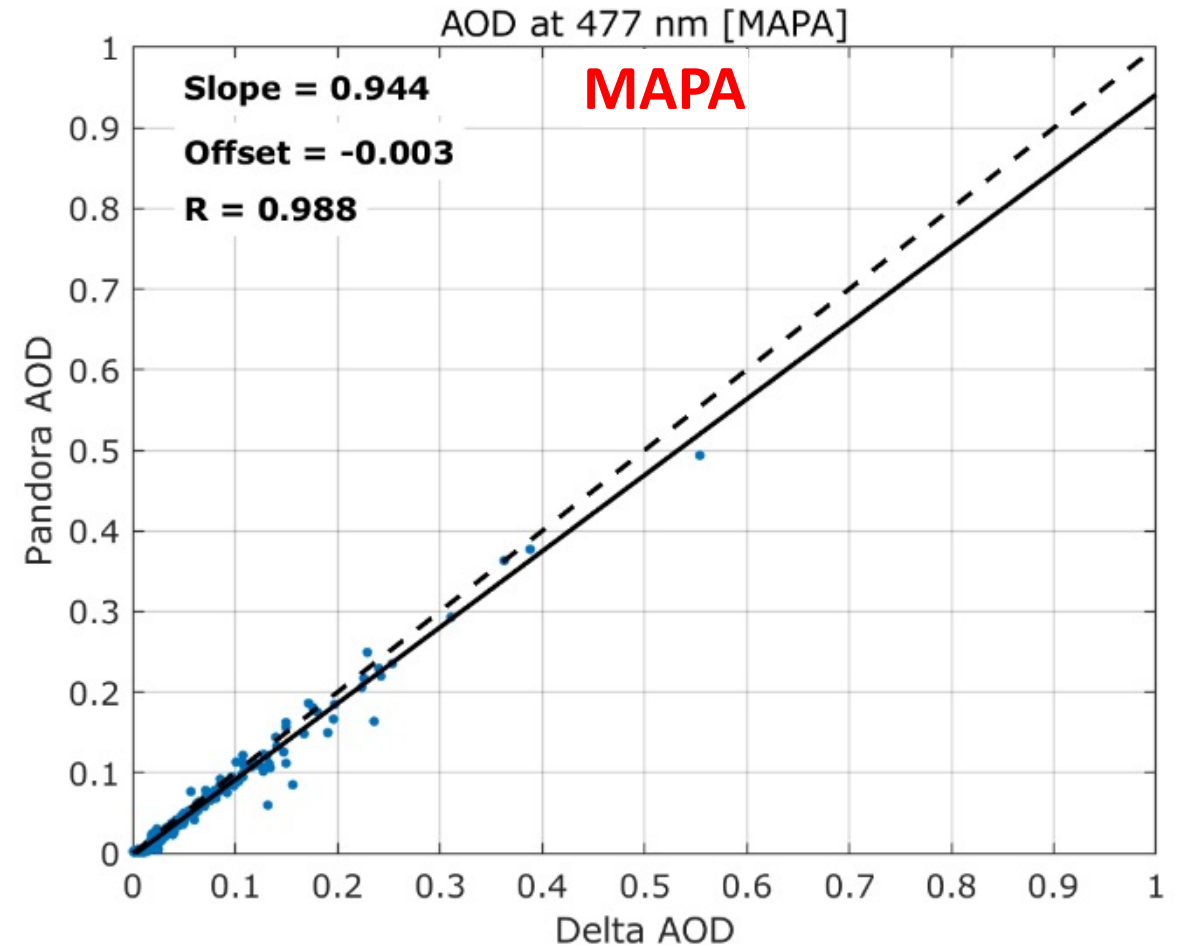
Comparison of profile-retrieved integrated columns

Species in the visible range — NO_2

NO2 VCDs [MMF]

Slope = 0.984

Offset = 0.247

R = 0.959

MMF
valid + warnings

Pandora VCDs [$\times 10^{15}$ molec. cm^{-2}]

Delta VCDs [$\times 10^{15}$ molec. cm^{-2}]

NO2 VCDs [MAPA]

Slope = 1.036

Offset = -0.020

R = 0.982

MAPA
valid only

Pandora VCDs [$\times 10^{15}$ molec. cm^{-2}]

Delta VCDs [$\times 10^{15}$ molec. cm^{-2}]

Comparison of profile-retrieved integrated columns
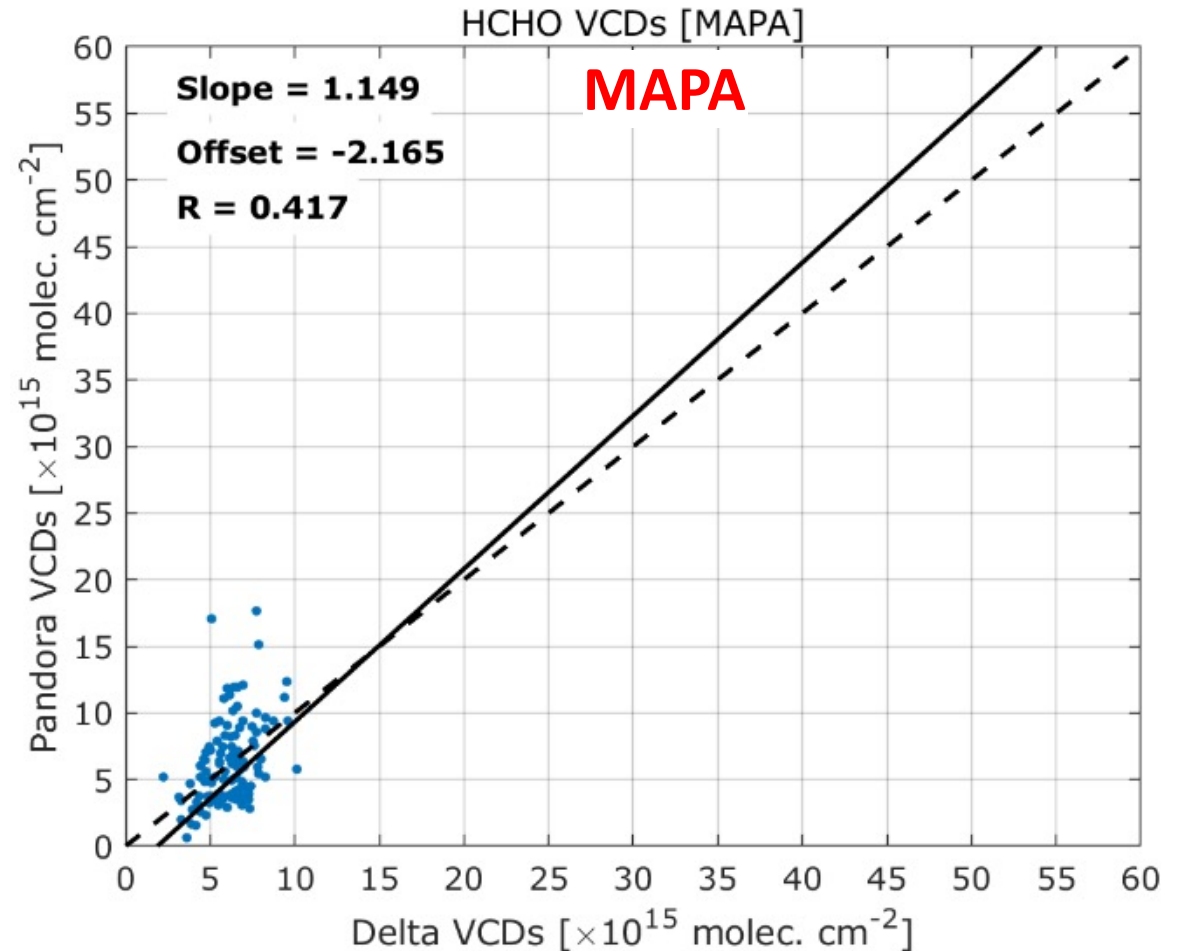
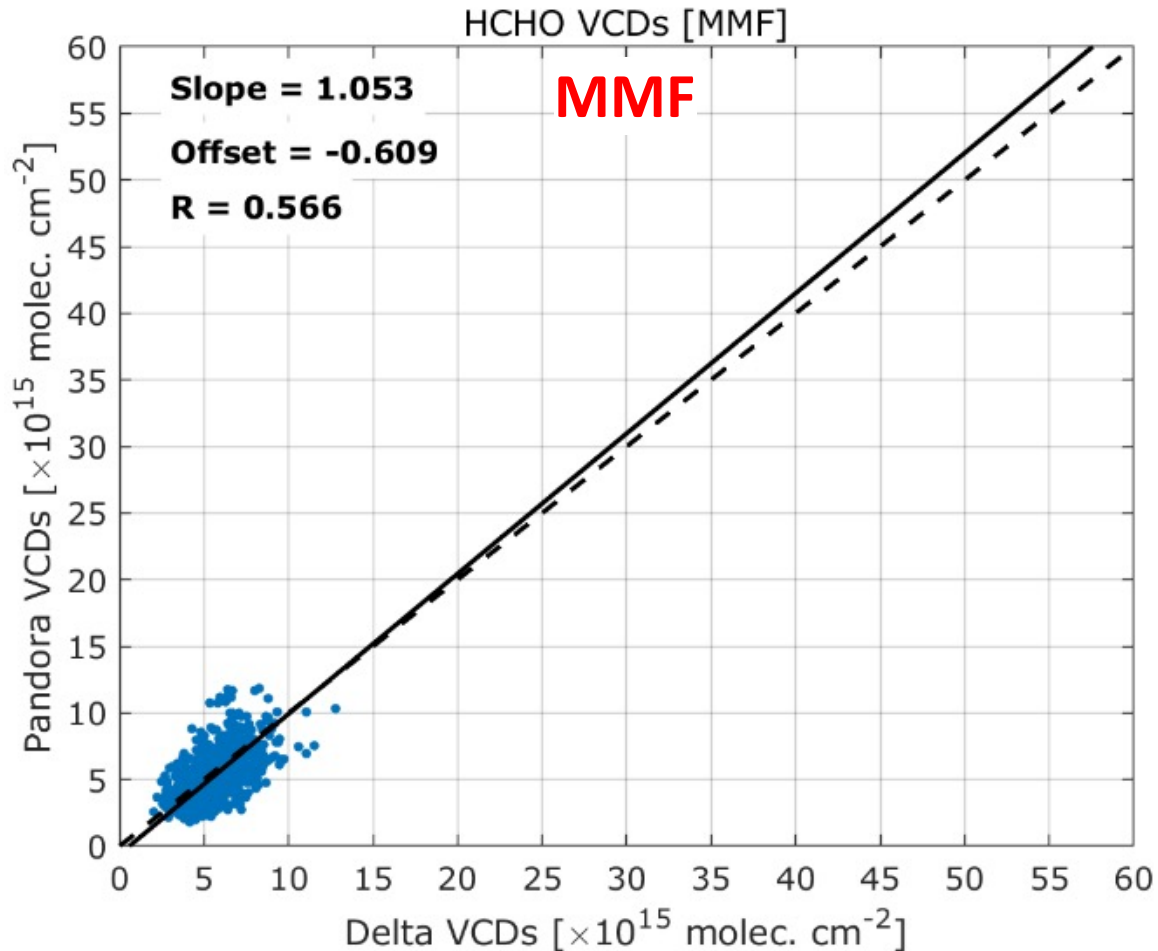Species in the visible range | AOD at 477 nm
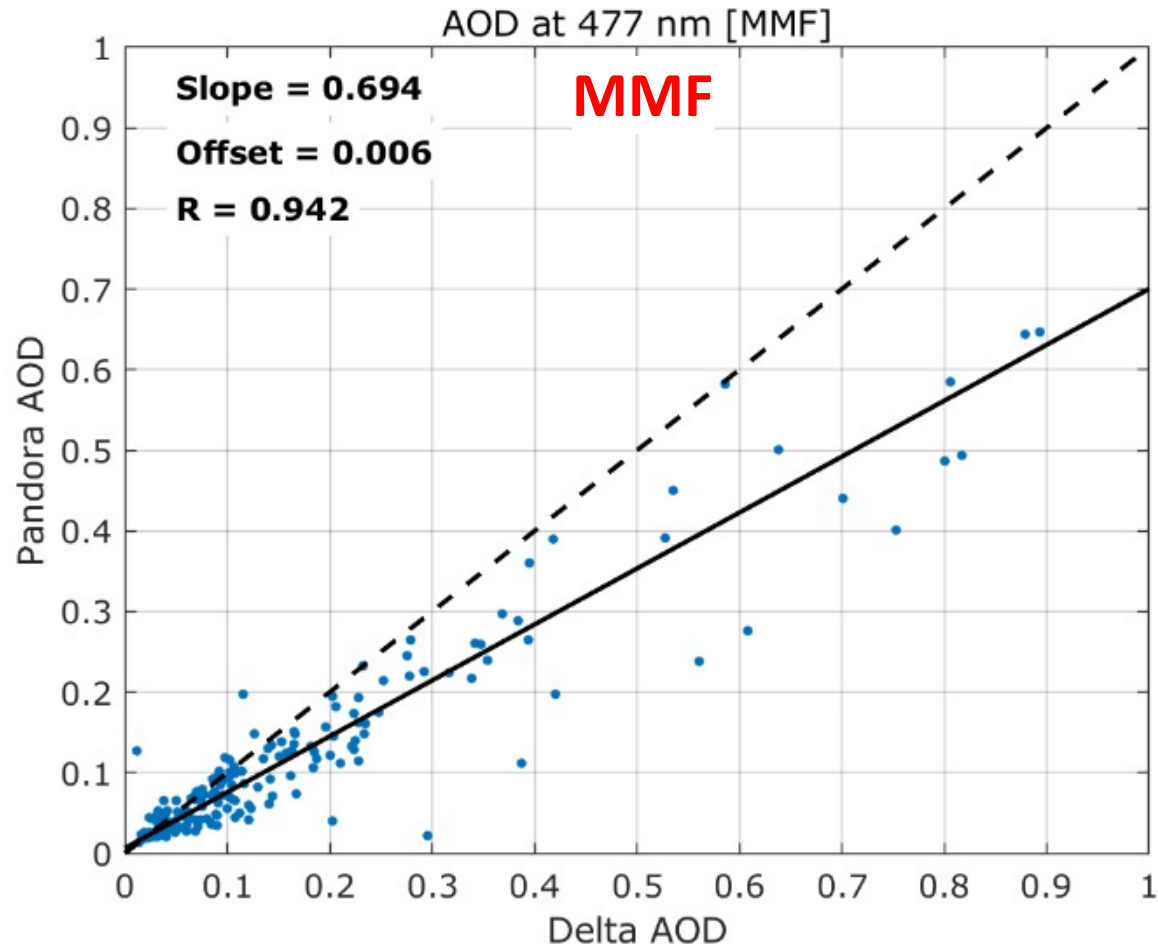
Comparison of profile-retrieved integrated columns
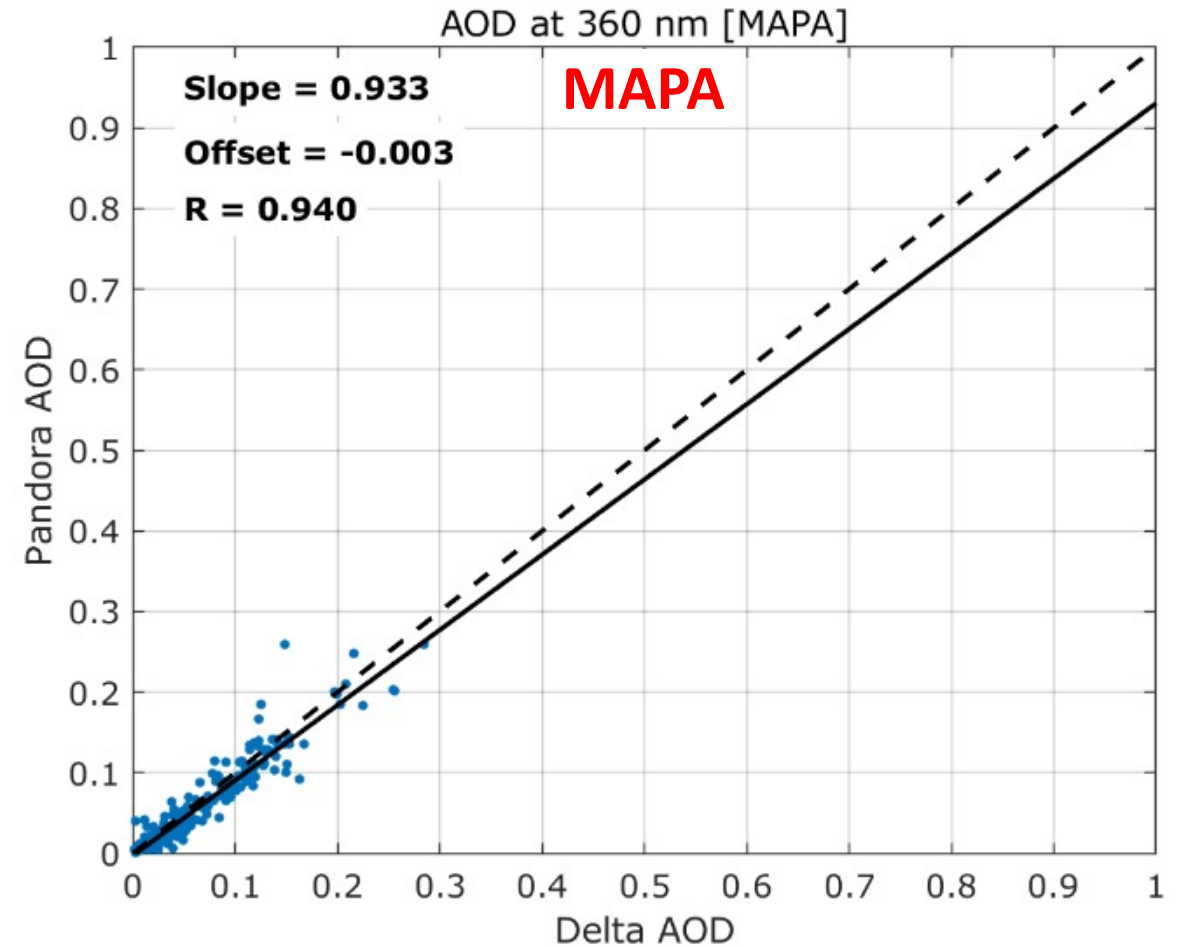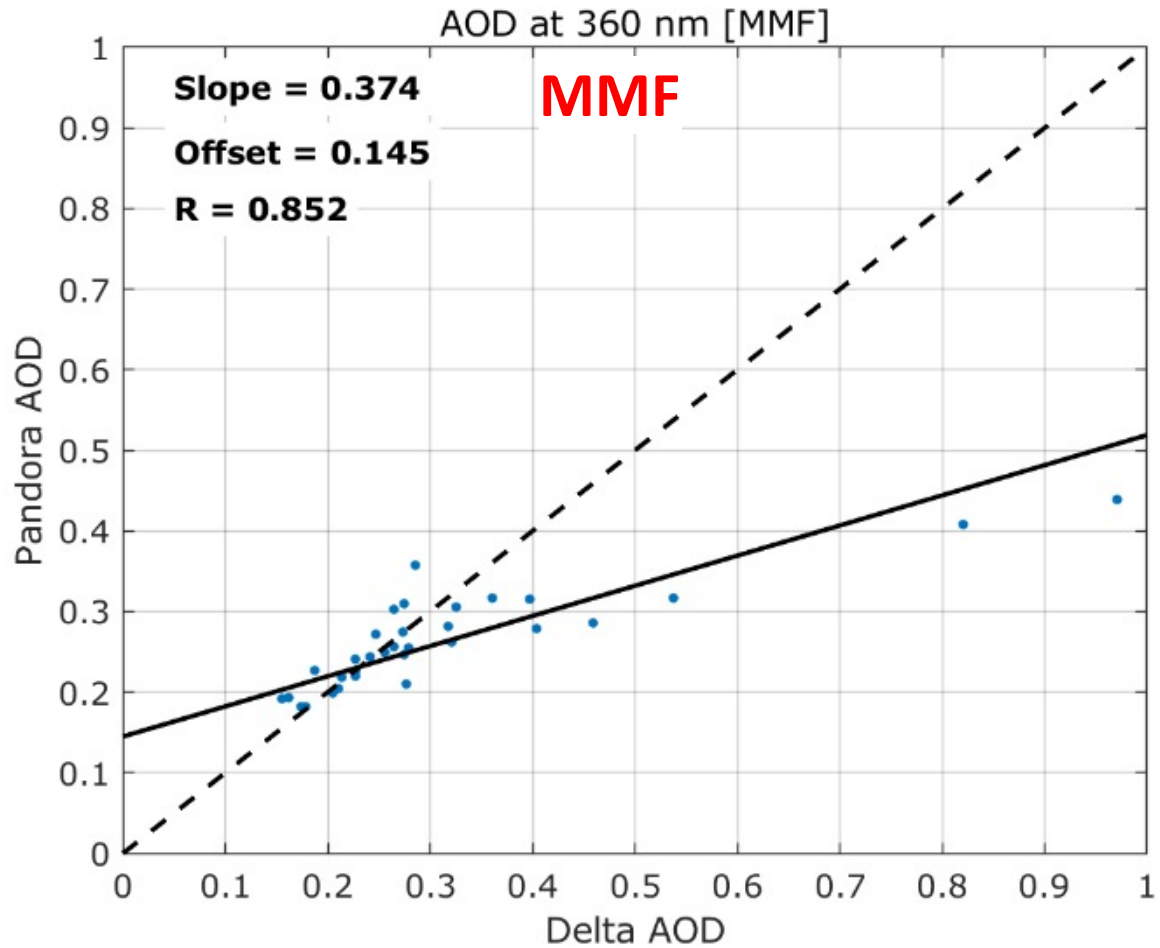
Species in the UV range   HCHO

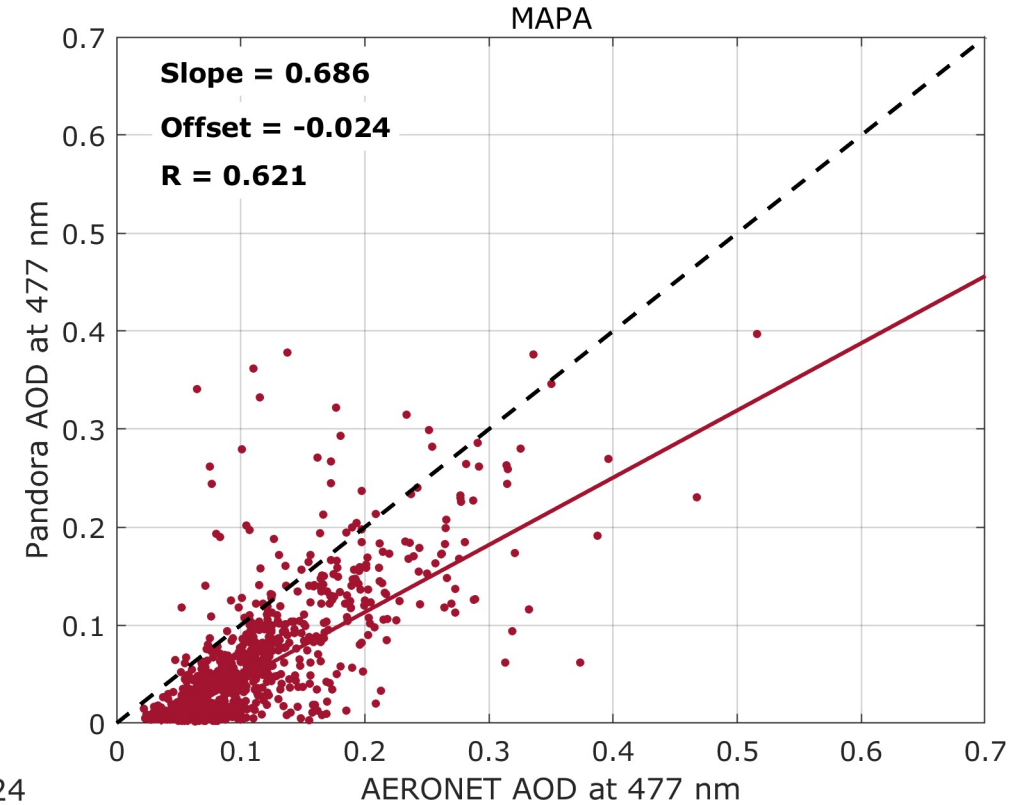# Comparison of profile-retrieved integrated columns
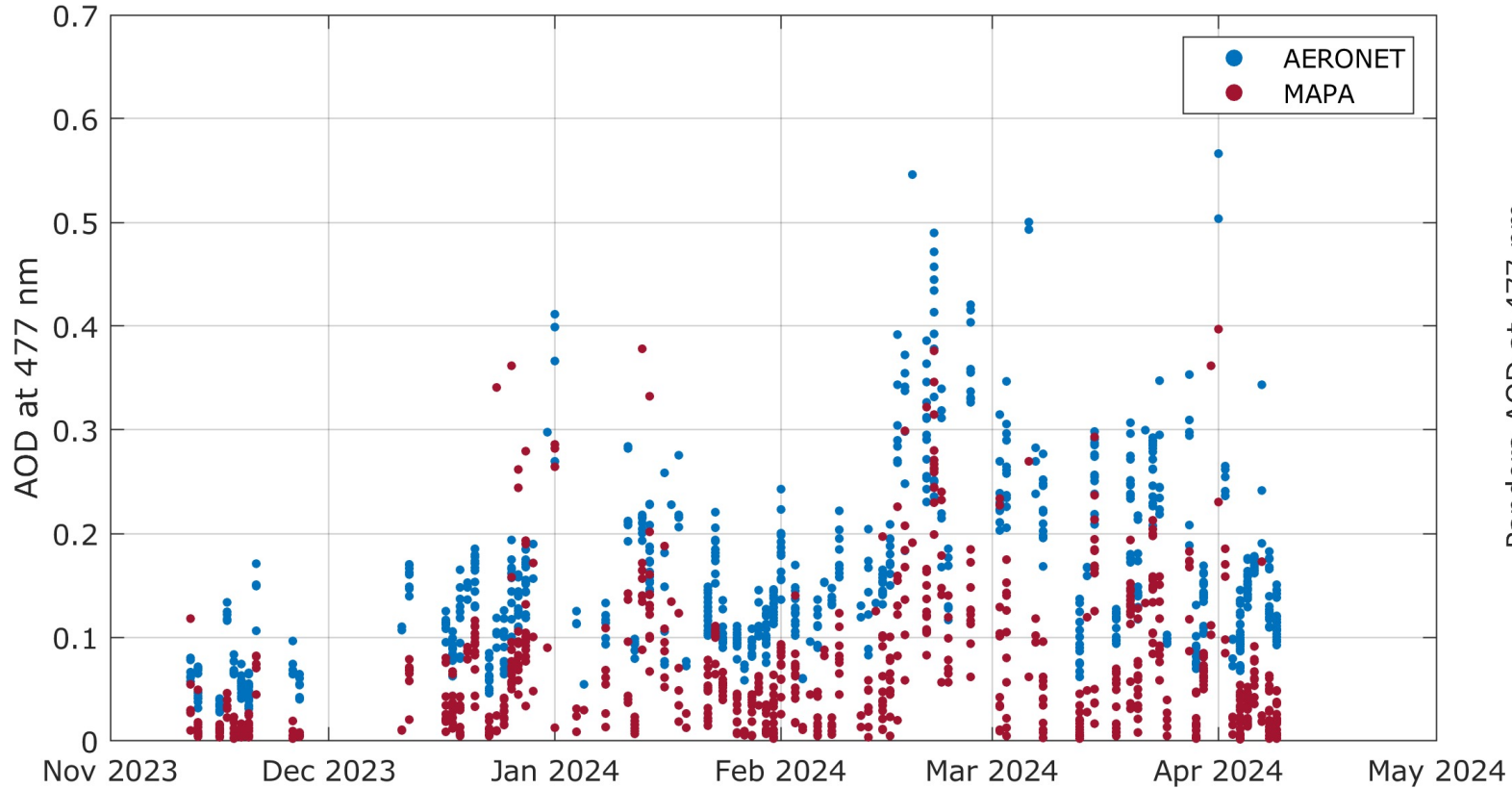
Species in the UV range   AOD at 360 nm

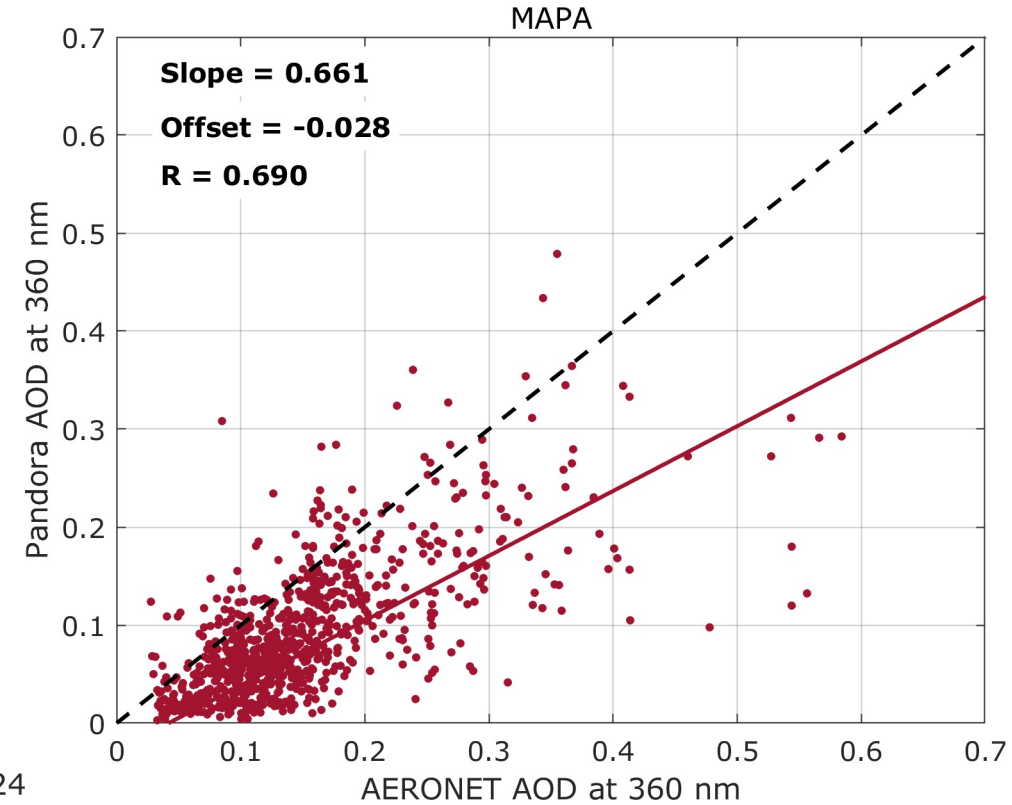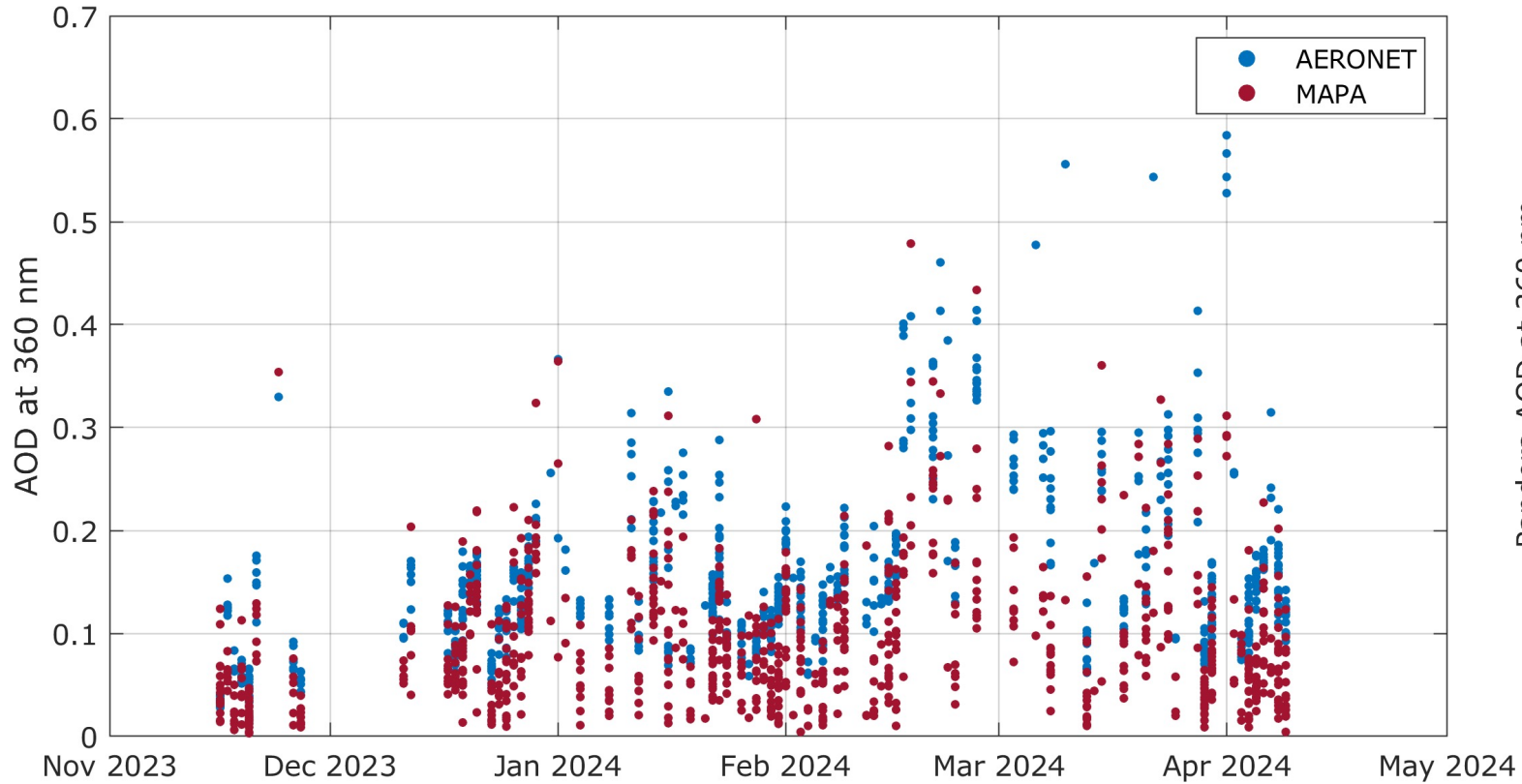# Comparison of Pandora AOD (MAPA) with AERONET data

Preliminary results

AOD at 477 nm

Comparison of Pandora AOD (MAPA) with AERONET data

Preliminary results

AOD at 360 nm

Retrieval of total NO₂ columns by Delta

Adaptation of a DOAS-based algorithm using direct-sun spectra by Delta
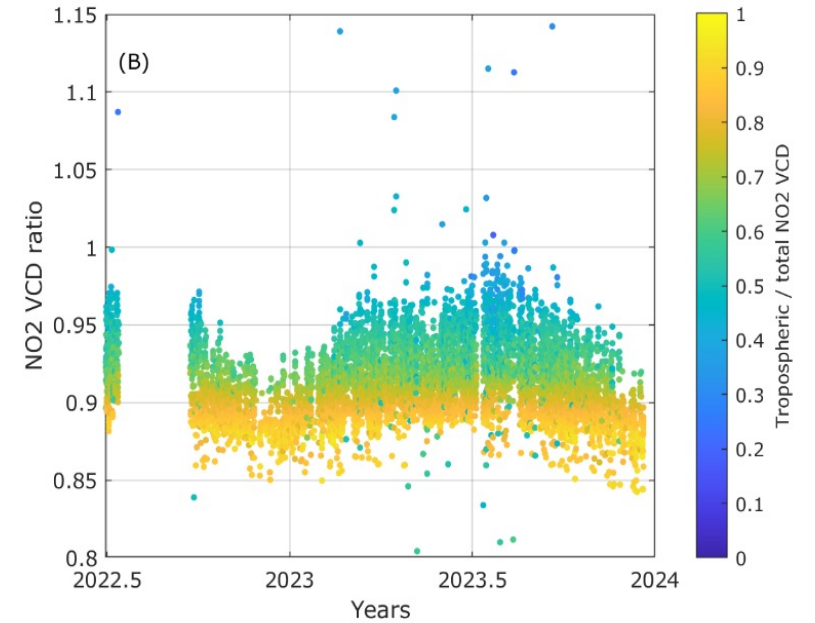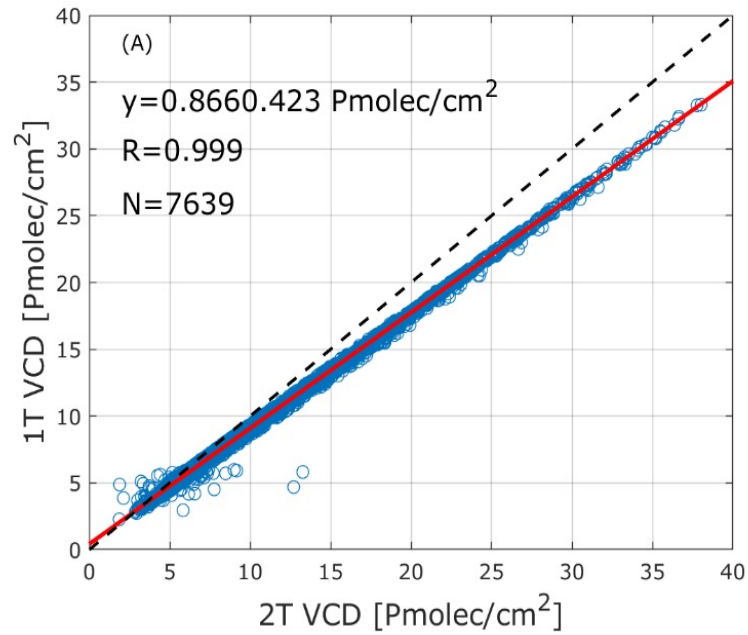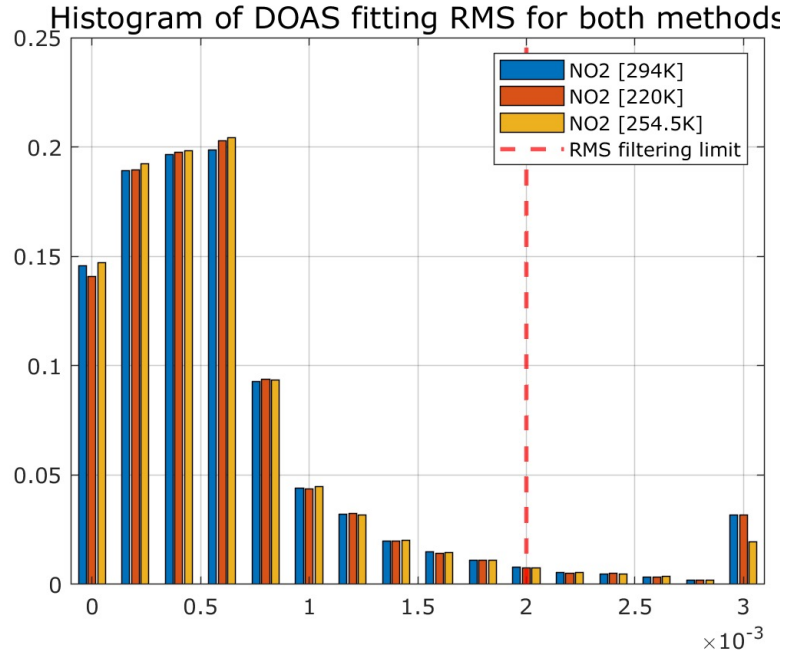
Two different methods:

- ❑ 2T method: NO_2 absorption cross sections at two temperatures for tropospheric (294K) and stratospheric absorption (220K) + climatology of stratospheric NO_2

- ❑ 1T method: NO_2 absorption cross section at one temperature (254.5K) (interpolated)

The SCD of the reference spectrum is estimated by applying the Bootstrap Estimation method (Herman et al., 2009)
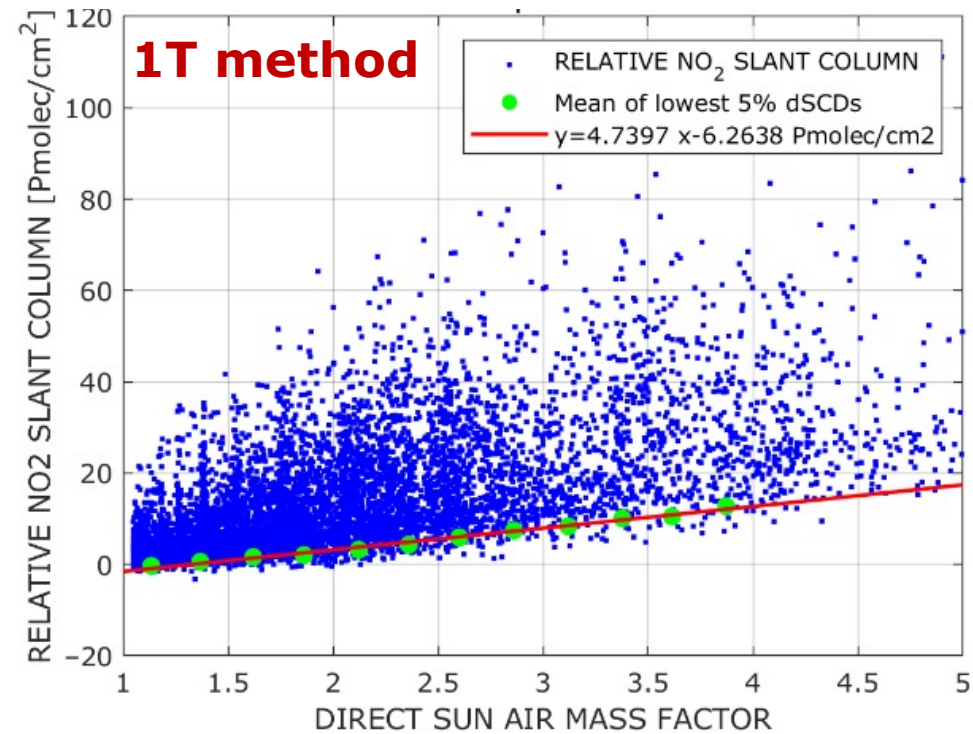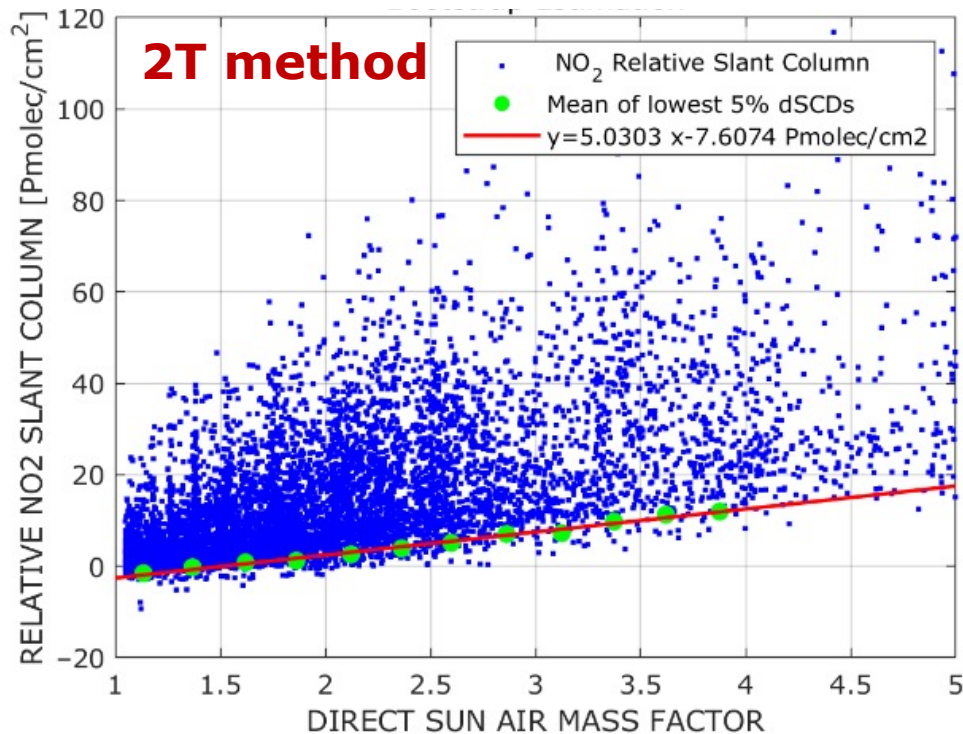
Evaluation of the total NO$_2$ columns by Delta

Frequency distribution of the DOAS Fit RMSE based on NO$_2$ cross sections at three temperatures

Comparison of the total NO$_2$ VCDs derived by the 1T and 2T methods

Time series of the ratio of NO$_2$ VCD derived by the 1T and the 2T methods

Differences between the two methods are minimal when the tropospheric NO2 VCD is low

The 2T method works better irrespective of tropospheric NO$_2$ VCDs

Evaluation of the retrieved total NO$_2$ columns
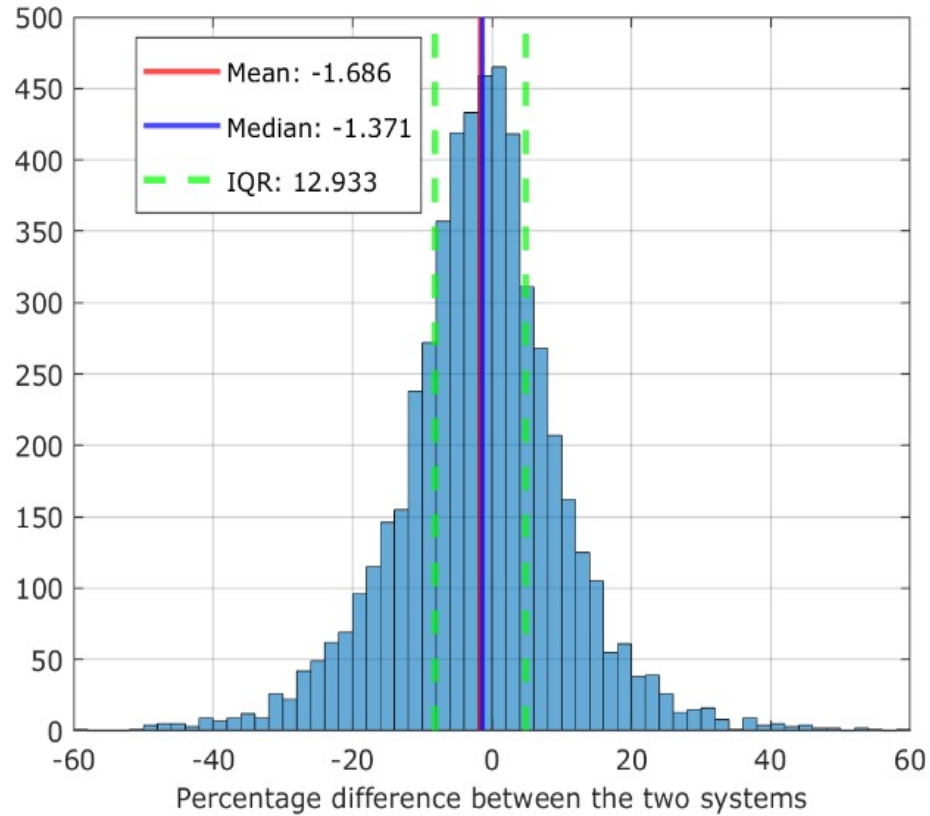
Histogram of differences in total NO$_2$ VCDs between Pandora and Delta
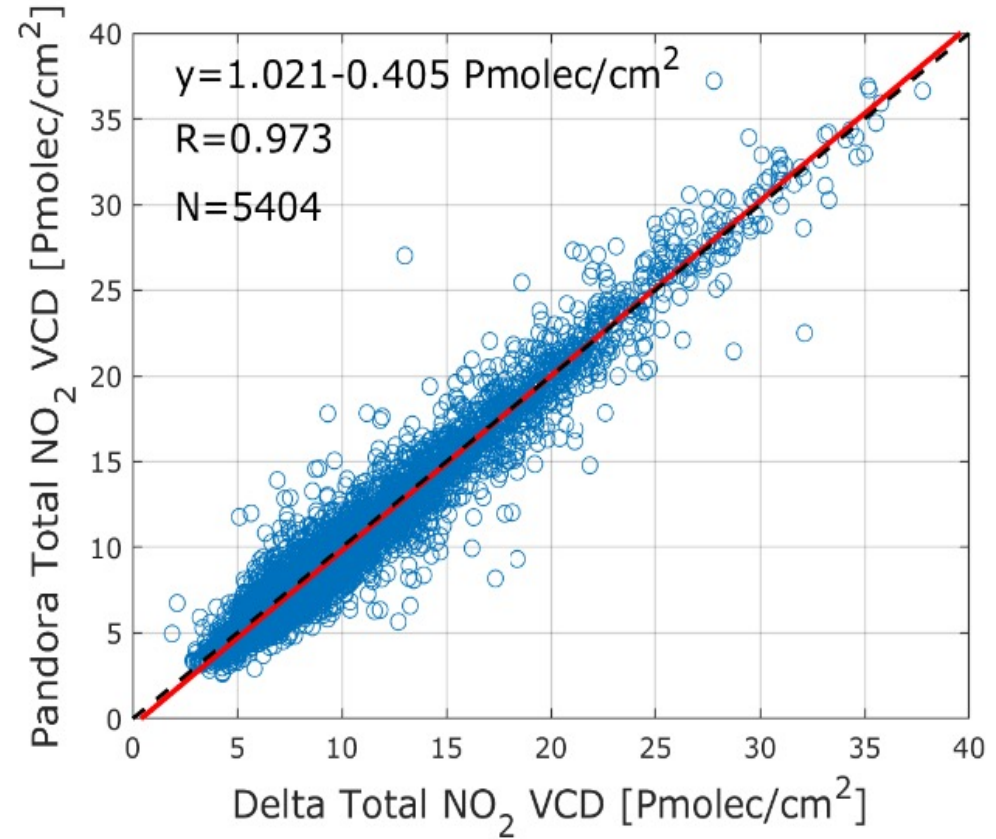
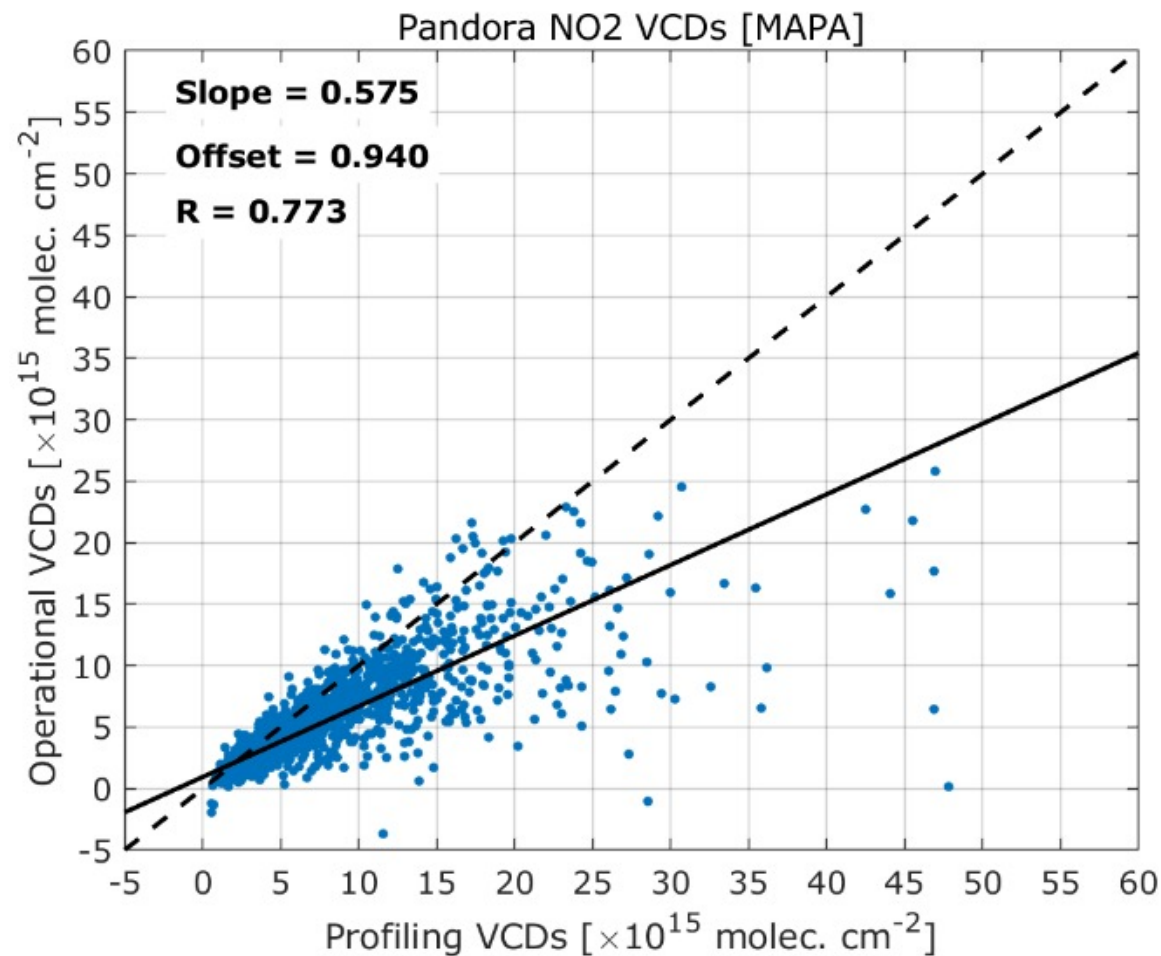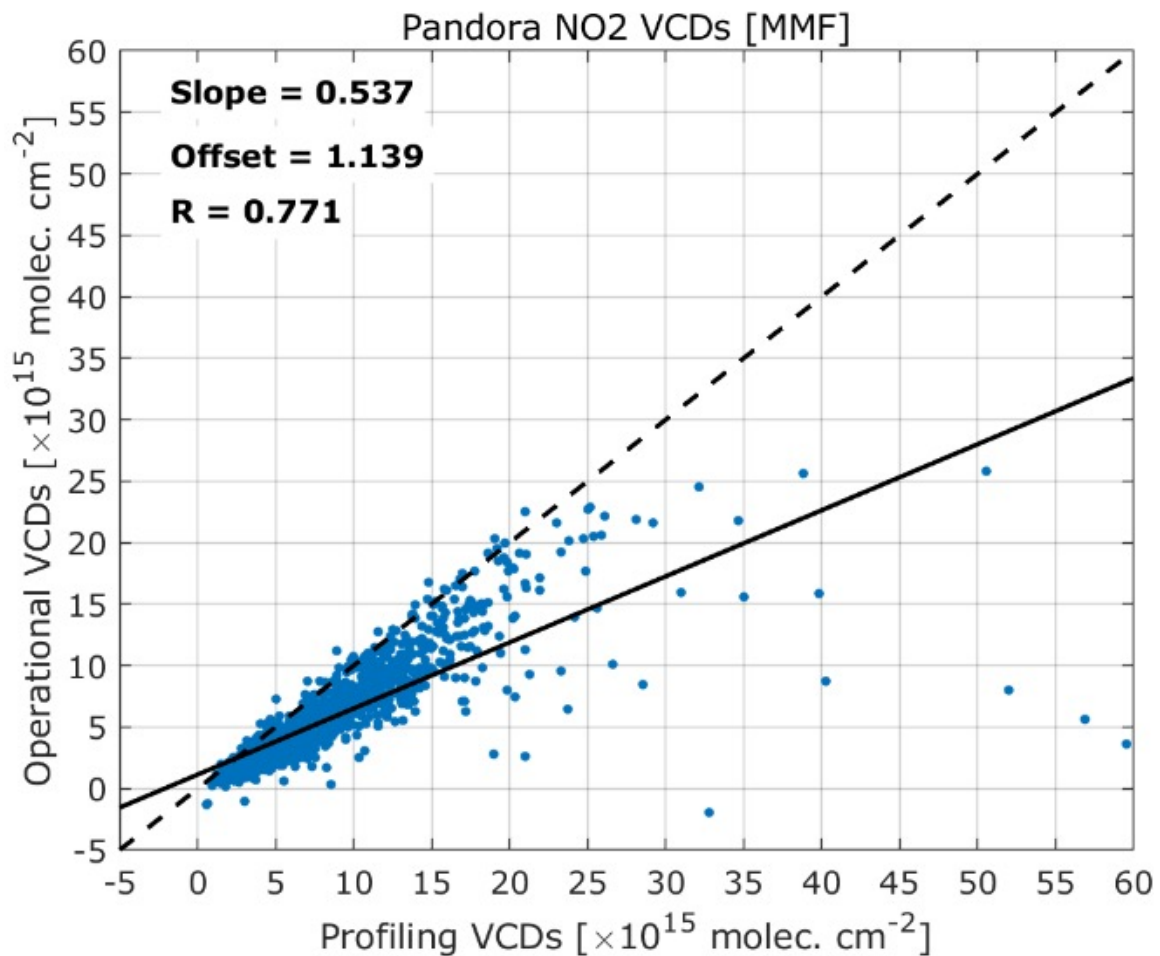The corresponding scatter plot using collocated data of the two systems

- Very good agreement with mean bias of 1.69% and correlation coefficient of 0.97.
- 50% of the data agree to within ±6.5%

Thanks for your attention!

Backup Slides

Comparison with the operational Pandora product

NO$_2$

Comparison with the operational Pandora product

HCHO