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Assessment of the TROPOMI tropospheric NO₂ product based on recurrent airborne campaigns

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D. Schuettemeyer, M. Van Roozendael

S5PVT meeting, Taormina, 11-10-2022



- **Broader context: S5P campaigns**
 - S5P campaigns: SVANTE project and QA4EO project
- **SVANTE airborne data format + central processor v1.1**
- **Recurrent airborne campaigns over Berlin and Bucharest**
- **S5P NO₂ validation - Preliminary results**
- **Conclusion and perspectives**

ESA SVANTE and QA4EO campaigns – S5P validation

Talk K. Lange

Talk S. Iancu

Talk M. K. Sha

- S5PVAL-DE-RUHR
 - S5PVAL-DE-BERLIN
 - S5PVAL-RO
 - S5PVAL-BE
 - S5PVAL-TRANS
 - NITROX
 - MAGIC
 - ACCLIP
 - S5PVAL-KOLKATA
 - COCCON
- NO₂
SO₂
HCHO
- CO
CH₄

Legend

-  Airborne UV-VIS
-  Airborne IR
-  Airborne UV-VIS & IR
-  Ground-based IR

S5pcampaigns.aeronomie.be



SVANTE airborne data format

- **NetCDF format (python script to convert from own format and fill attributes)**
- **Following largely Climate and Forecast (CF) metadata conventions and TROPOMI L2 product definitions**
- **Global attributes**
 - Campaign description: ROI, date, aircraft, instrument, operator, etc.
 - Algorithm parameters – DOAS fit + reference spectrum
 - Algorithm parameters – RTM
 - ERA-5 wind, PBL, surface temperature (average and st. dev.)
 - Fully traceable for user how data was processed
 - Allows for different versions to exist next to each other
- **Data**
 - VCD + intermediate products such as AMF, (D)SCD
 - RTM input: albedo, RAA, VZA, SZA, etc.
 - Uncertainties on VCD, DSCD, SCDref and AMF
 - Lat, Lon, time for each pixel
 - Similar to TROPOMI L2 NO₂ product
- **Data format can be used for all projects involving airborne imaging data, e.g. future S4/S5 cal/val**

```
SVANTE_SWING2_FUBCESSNA_20210614.nc
├── METADATA
│   ├── ALGORITHM_SETTINGS
│   │   ├── DOASFIT
│   │   ├── RTM
│   │   └── CAMPAIGN_DESCRIPTION
│   ├── air_mass_factor_troposphere
│   ├── air_mass_factor_troposphere_uncertainty
│   ├── id
│   ├── latitude
│   ├── longitude
│   ├── nitrogendioxide_differential_slant_column_density
│   ├── nitrogendioxide_residual_slant_column_density_uncertainty
│   ├── nitrogendioxide_slant_column_density
│   ├── nitrogendioxide_slant_column_density_uncertainty
│   ├── nitrogendioxide_tropospheric_column
│   ├── nitrogendioxide_tropospheric_column_uncertainty
│   ├── qa_value
│   ├── root_mean_square_error_of_fit
│   ├── solar_azimuth_angle
│   ├── solar_zenith_angle
│   ├── surface_albedo_nitrogendioxide_window
│   ├── time.UTC
│   ├── viewing_azimuth_angle
│   └── viewing_zenith_angle
```

■ Central airborne data processor v1.1

- Key objectives
 - Collect and process data from different campaigns and different imaging instruments
 - **Consistent** a priori assumptions (albedo, NO_2 profile, aerosol scenario, SCD_{ref}) in processing of data from different campaigns/instruments
 - **Process in a harmonized way** in order to obtain **independent reference data sets** to compare with TROPOMI L2 products
- 1) **Step 1: DOAS spectral fitting, georeferencing and pre-processing**
- 2) **Step 2: DSCD to VCD processing**
 - SCD stratospheric and temperature correction
 - $\text{AMF}_{\text{tropo}}$ - LIDORT 2.6 RTM based on MODIS MCD43A3 albedo, TM5 a priori NO_2 profile, sun/viewing geometry, etc.
- 3) **Step 3: harmonized gridding tools and spatiotemporal comparison tools with satellite**
- Airborne format and code is well-documented (can be used in other projects and for S-4/S-5 cal/val)
- Improvements/changes regarding format will be implemented in v1.2 (similar to satellite data processors)

S5PVAL-DE-BERLIN and S5PVAL-RO

- **Recurrent** airborne mapping of tropo NO₂ over **Berlin + Bucharest** with **SWING imager**
- 12 flights during one year **covering different conditions**: pollution levels, meteorology and geo-physical parameters, S-5p overpass angular dependence, etc.
- SWING+ (UV-VIS – 0,7 nm – 170 x 170 m) operated from **INCAS BN-2 (RAMOS)**, **FUB Cessna 207T**, **FUB motorglider ASK16** (integrated April 2022)
- Spatiotemporal coincidence with TROPOMI overpass

SWING+ specifications (at 3 km a.g.l.)

	SWING+
Wavelength range	280-550 nm
Spectral resolution (FWHM)	0.7 nm
FOV across-track	100°
Ifov across track	3°
Swath width	2900 m
Ground speed	60 m/s
Exposure time	0.5 s
Spatial resolution	170 m
Weight	3 kg
Size (LxWxH)	20 x 20 x 30 cm ³
Scanning	Whiskbroom
Target platform	UAV/aircraft

SWING+ on INCAS BN-2



SWING+ on FUB Cessna 207T



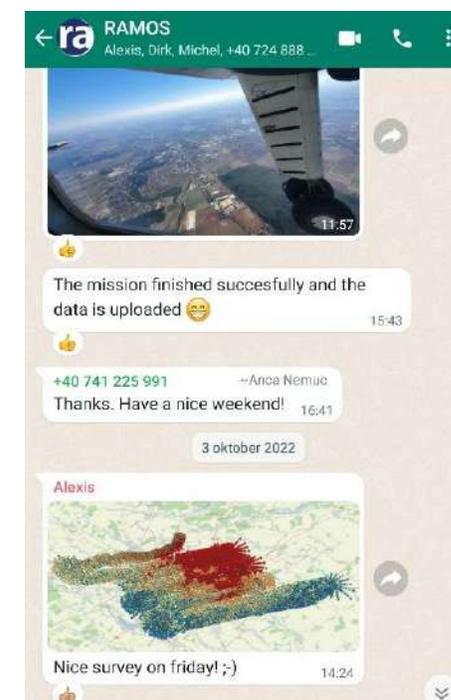
SWINGPOD on FUB ASK16 glider
(integrated since April 2022)



Intercomparison with TROPOMI

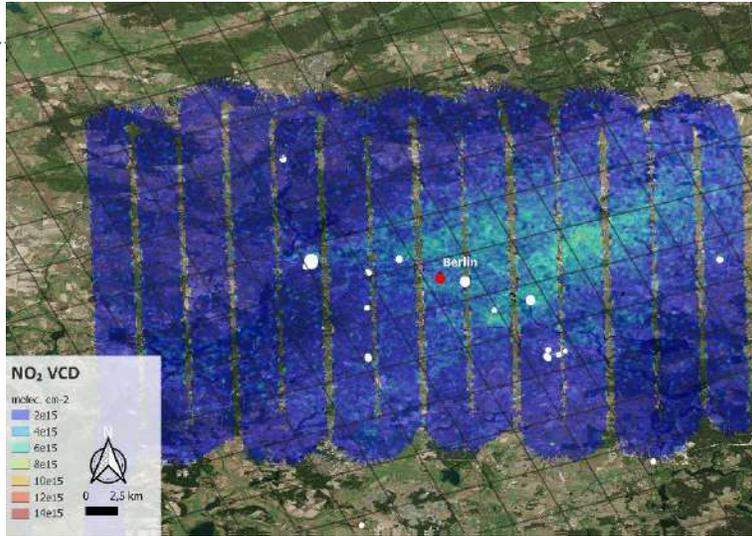
- Averaging airborne pixels ($\sim 0.17 \times 0.17 \text{ km}^2$) within each TROPOMI pixel ($\sim 3.5 \times 5.5 \text{ km}^2$)

	SWING-TROPOMI intercomparison
Constraints	
-Data quality	-TROPOMI QA value ≥ 0.75 -SWING slant error $\leq 3 \times$ detection limit ($\sim 7 \times 10^{15} \text{ molec. cm}^{-2}$)
-Spatial	TROPOMI pixel covered at least 50% by airborne data
-Temporal	$\Delta T < 1$ hour (difference between airborne vs spaceborne overpass)
-Weather	Clear-sky conditions
Flights	
-Bucharest	~ 20 flights since 01/07/2021
-Berlin (Cessna 207 T)	6 flights since 14/06/2021
-Berlin (Glider ASK 16)	7 (test) flights since 06/04/2022
-Next slides	4 flights over Berlin + 4 flights over Bucharest are analysed, mostly in autumn conditions
TROPOMI products	Comparisons with OFFL , PAL , OFFL-CAMS and PAL-CAMS
TROPOMI versions	-01/01/2021 \rightarrow 01/07/2021: TROPOMI NO₂ v1.4 -01/07/2021 \rightarrow 15/11/2021: TROPOMI NO₂ v2.2 -15/11/2021 \rightarrow 17/07/2022: TROPOMI NO₂ v2.3

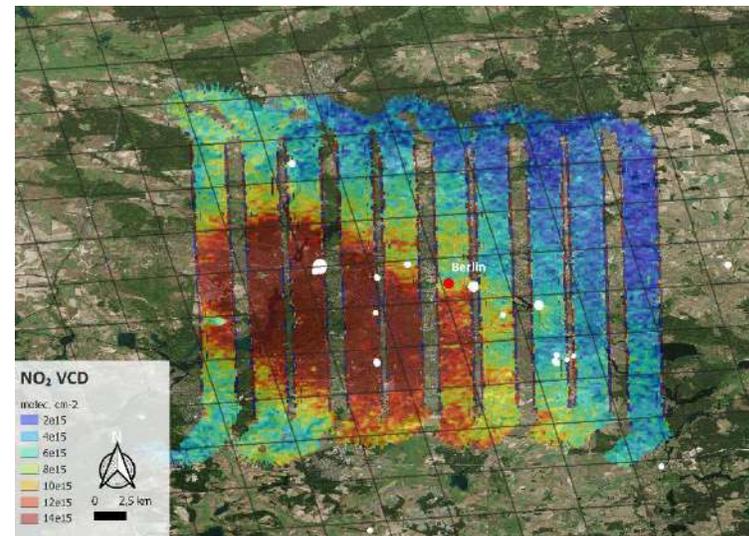


Preliminary results (NO₂ VCD maps) – Berlin, DE

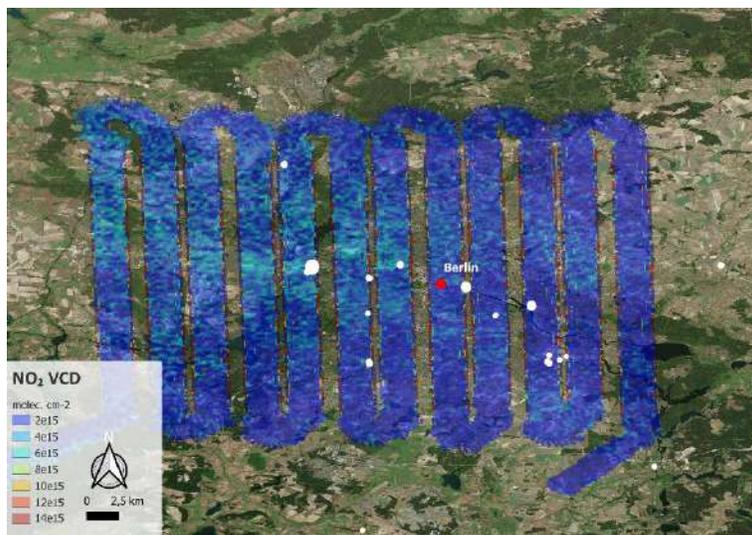
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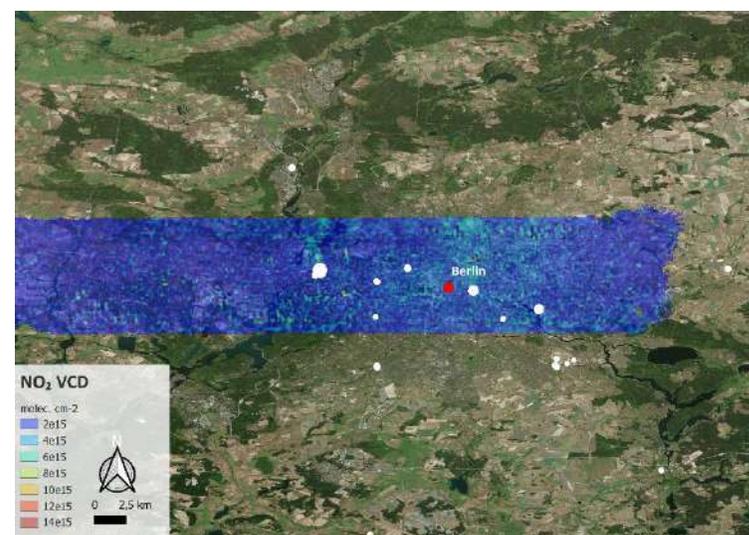
07-10-2021 (Thursday)



09-10-2021 (Saturday)

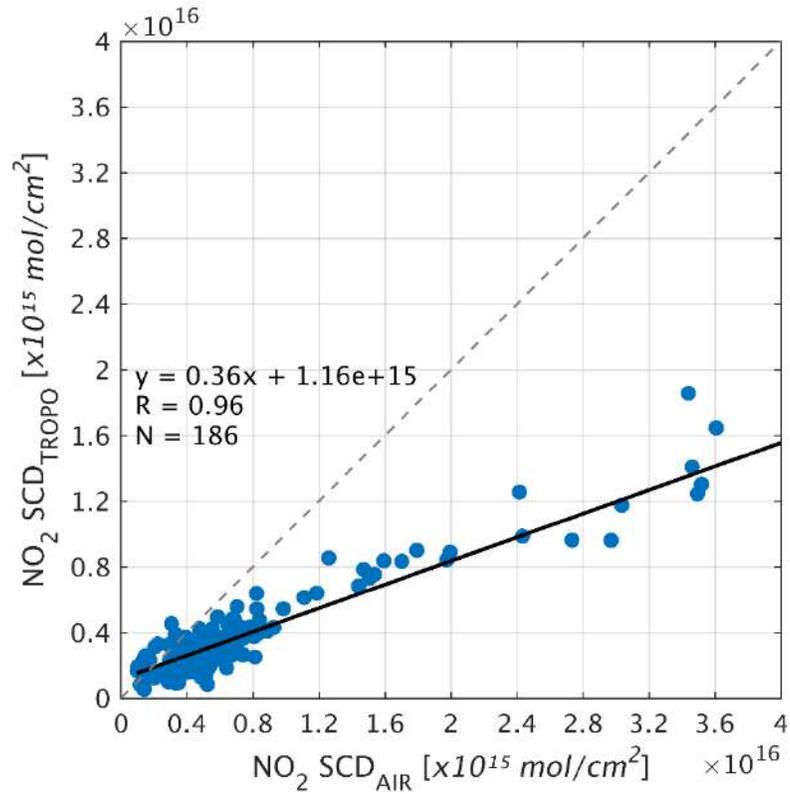


24-10-2021 (Sunday)

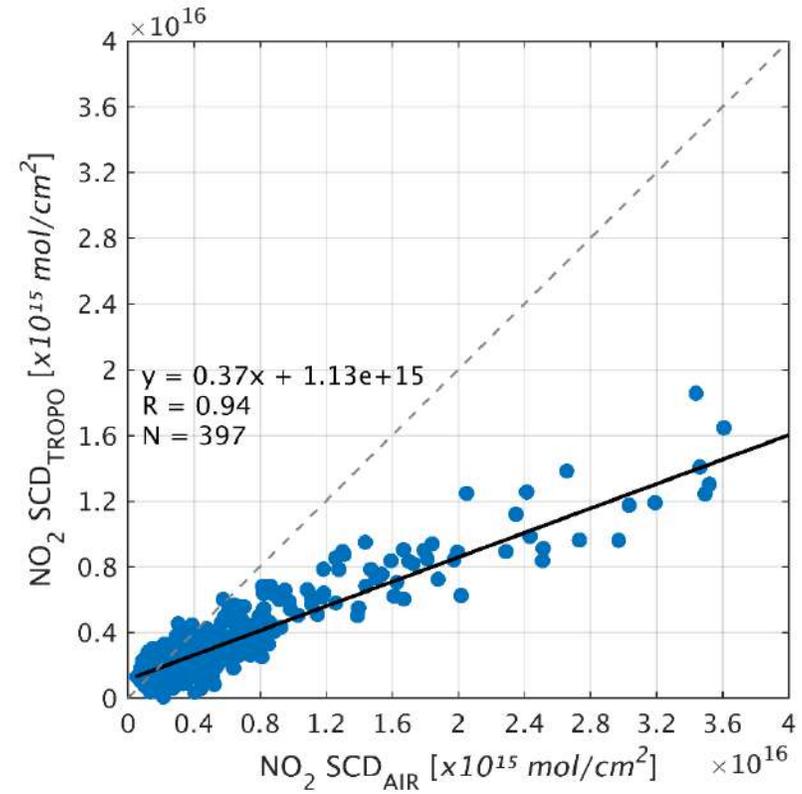


Preliminary results (SCD) – Berlin, DE

Ensemble 4 flights (OFFL v2.2 - 50% overlap - <=1 hour)

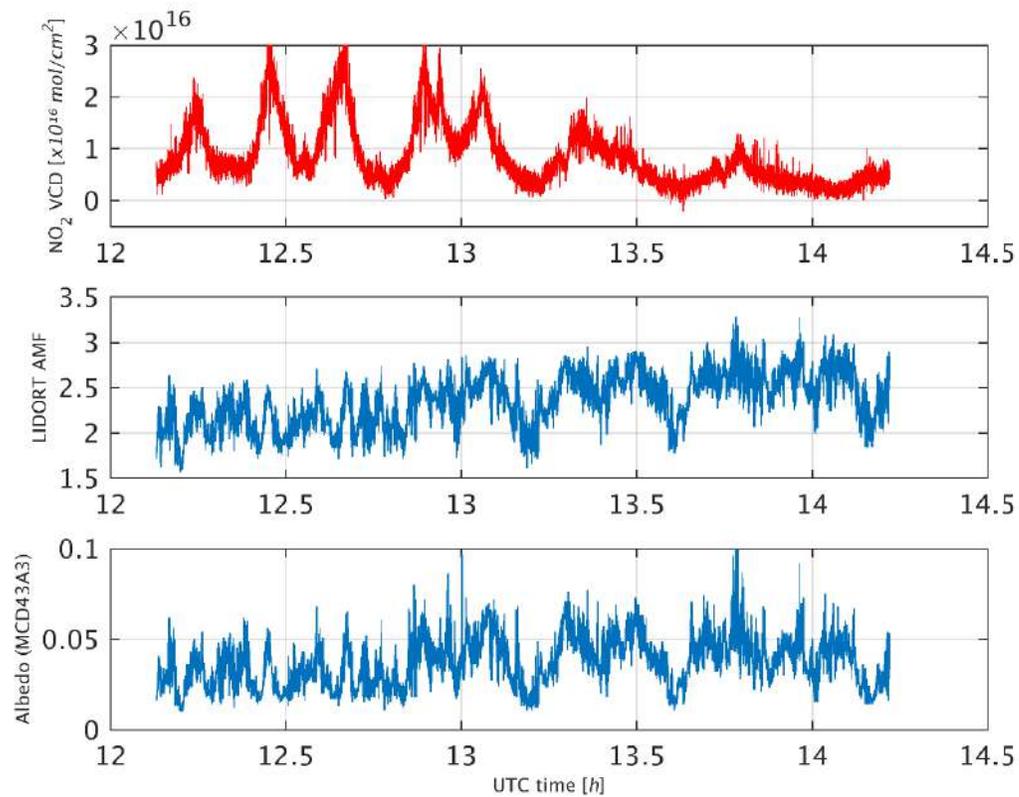


Ensemble 4 flights (OFFL v2.2 – no spatiotemp. constraints)

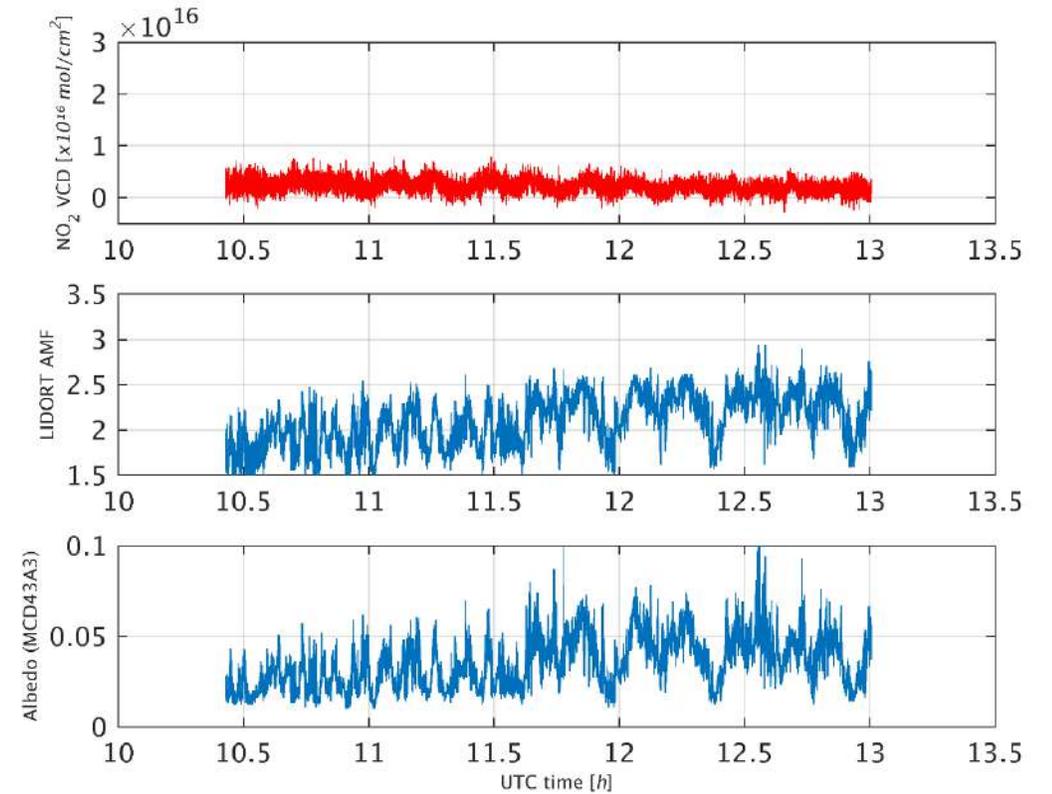


Preliminary results (VCD) – Berlin, DE

07-10-2021

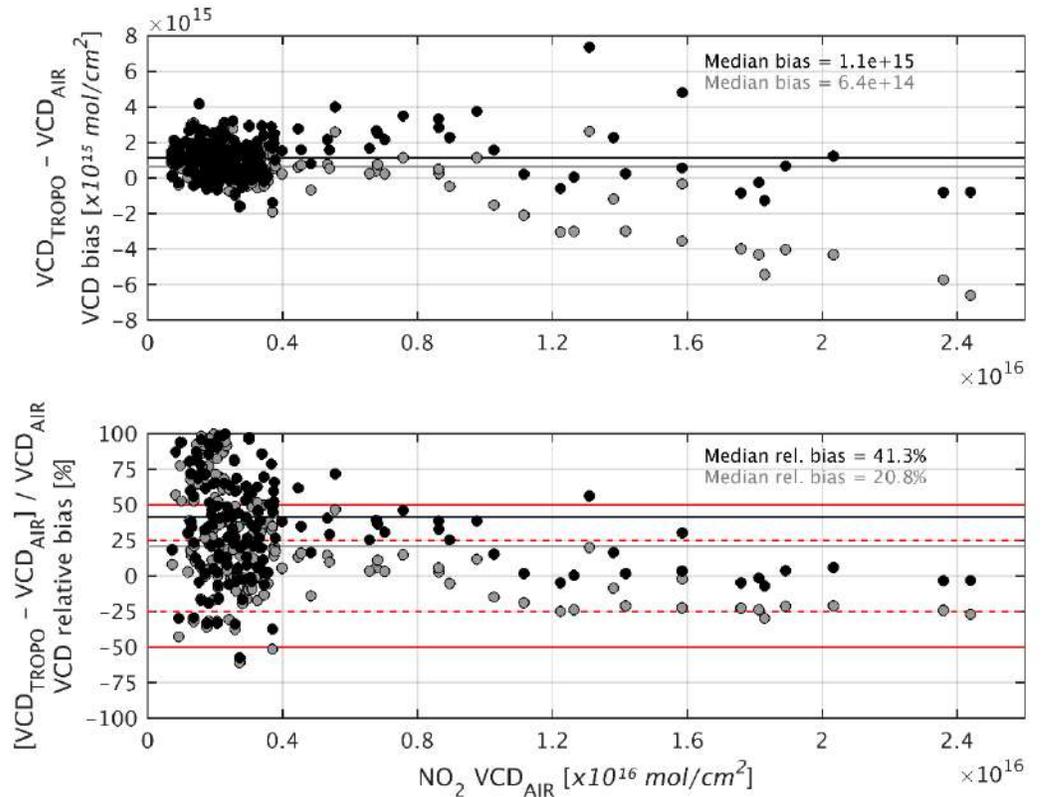
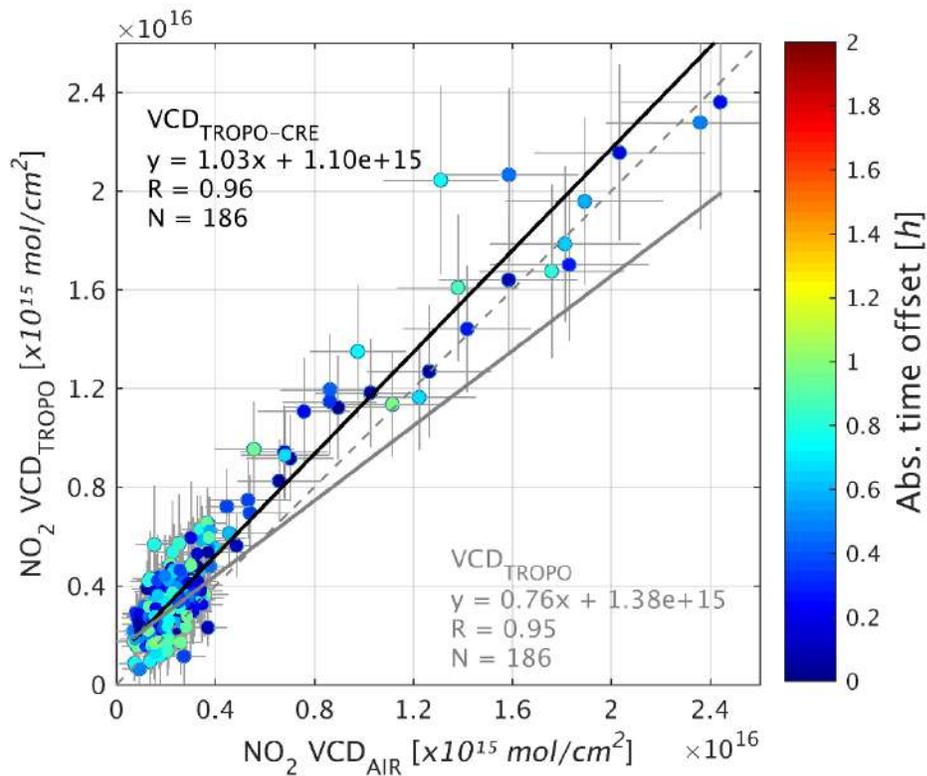


09-10-2021



Preliminary results (S5P NO₂ validation) – Berlin

Ensemble 4 flights (OFFL(-CAM5) v2.2 - 50% overlap - <=1 hour)



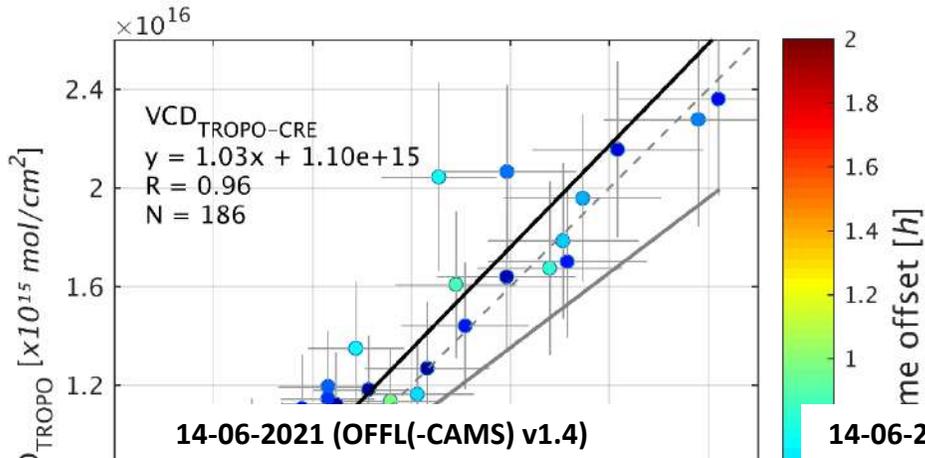
Error bars

$$\sigma_{\text{VCD}_{\text{TROPO}}} = \sqrt{
 \begin{aligned}
 & \left(\frac{\sigma_{\text{SCD}_{\text{TROPO}}}}{\text{AMF}_{\text{TROPO}}} \right)^2 \\
 & + \left(\frac{\sigma_{\text{SCD}_{\text{TROPO}}^{\text{strato}}}}{\text{AMF}_{\text{TROPO}}^{\text{strato}}} \right)^2 \\
 & + \left(\frac{\text{SCD}_{\text{TROPO}} - \text{SCD}_{\text{TROPO}}^{\text{strato}}}{\text{AMF}_{\text{TROPO}}^2} \right)^2 \\
 & + \left(\sigma_{\text{AMF}_{\text{TROPO}}} \right)^2
 \end{aligned}
 }$$

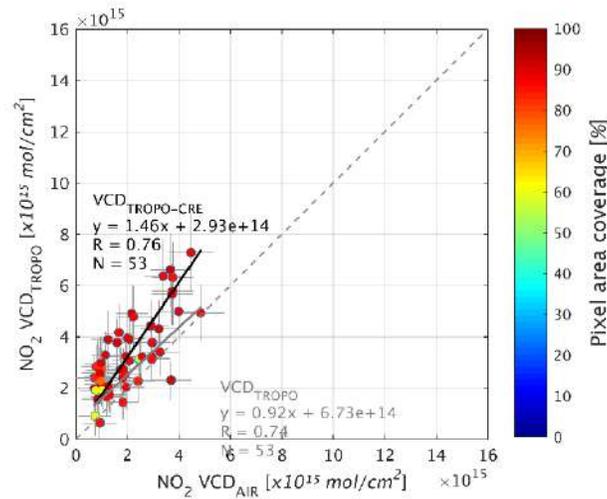
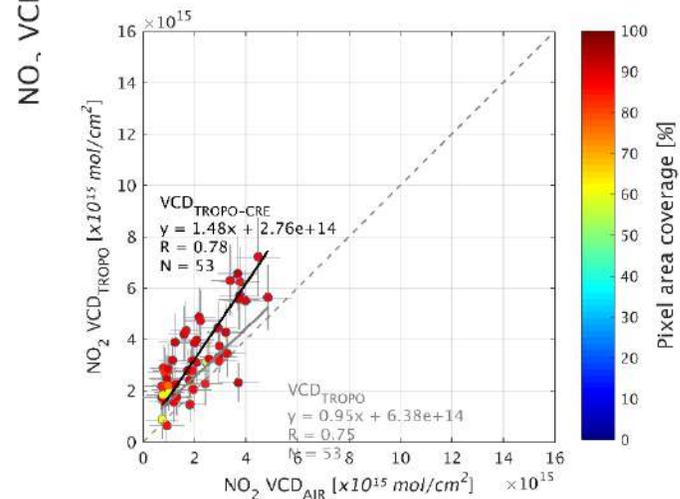
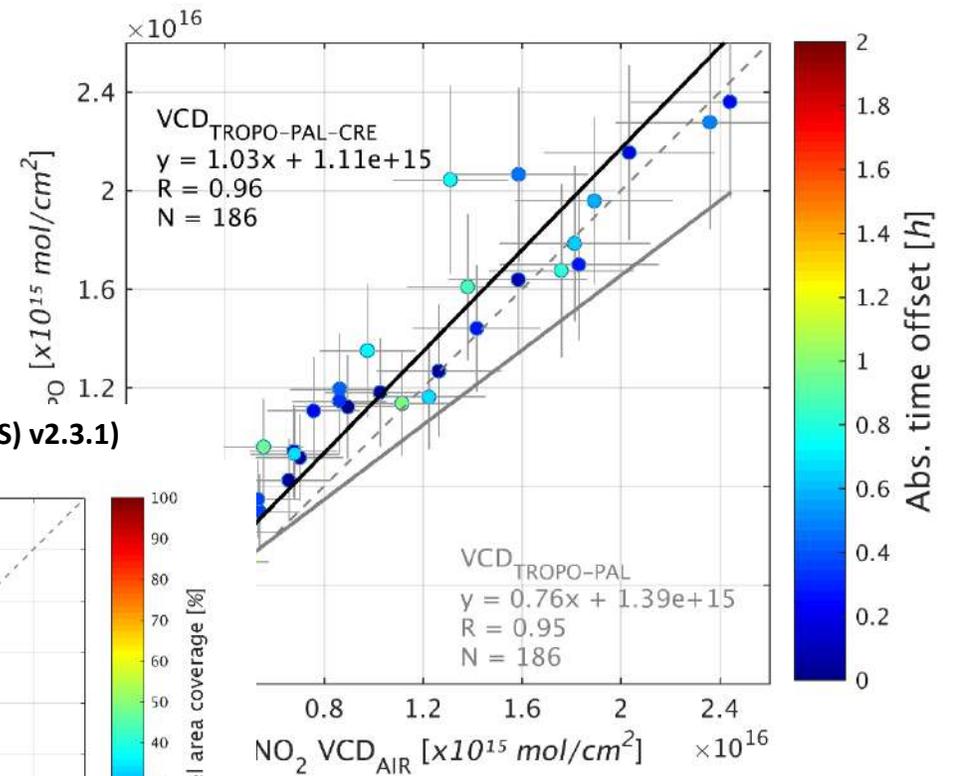
$$\sigma_{\text{VCD}_{\text{APEXI}}} = \sqrt{
 \begin{aligned}
 & \left(\frac{\sigma_{\text{SCD}_{\text{APEXI}}}}{\text{AMF}_{\text{APEXI}}} \right)^2 \\
 & + \left(\frac{\sigma_{\text{SCD}_{\text{ref}}}}{\text{AMF}_{\text{APEXI}}} \right)^2 \\
 & + \left(\frac{\text{SCD}_{\text{APEXI}}}{\text{AMF}_{\text{APEXI}}} \cdot \sigma_{\text{AMF}_{\text{APEXI}}} \right)^2
 \end{aligned}
 }$$

Preliminary results (S5P NO₂ validation) – Berlin

Ensemble 4 flights (OFFL(-CAMS) v2.2 - 50% overlap - <=1 hour)

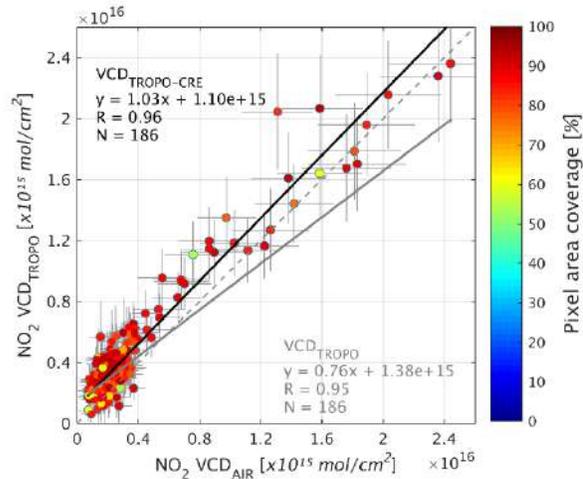


Ensemble 4 flights (PAL(-CAMS) v2.3.1 - 50% overlap - <=1 hour)

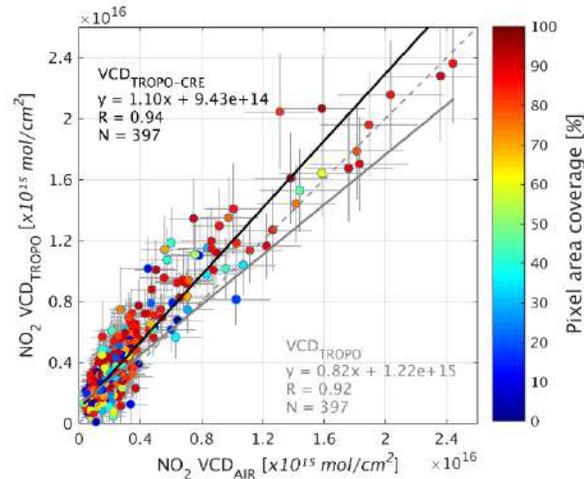


Preliminary results (S5P NO₂ validation) – Berlin

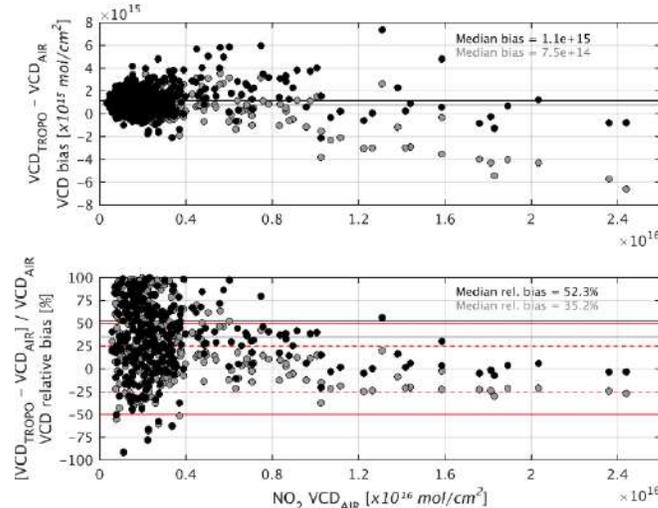
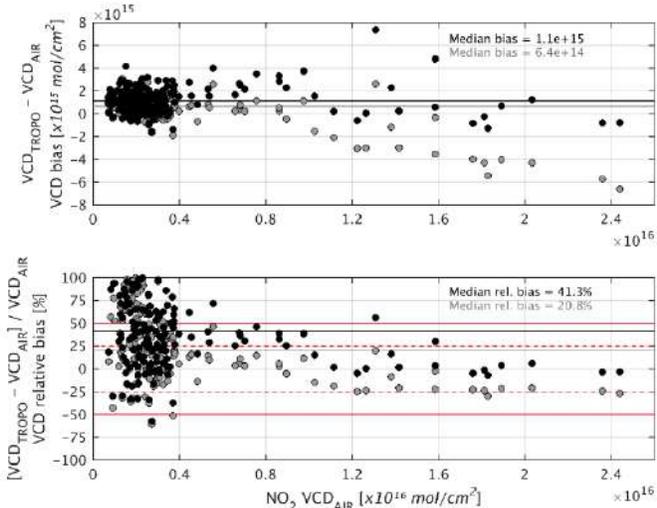
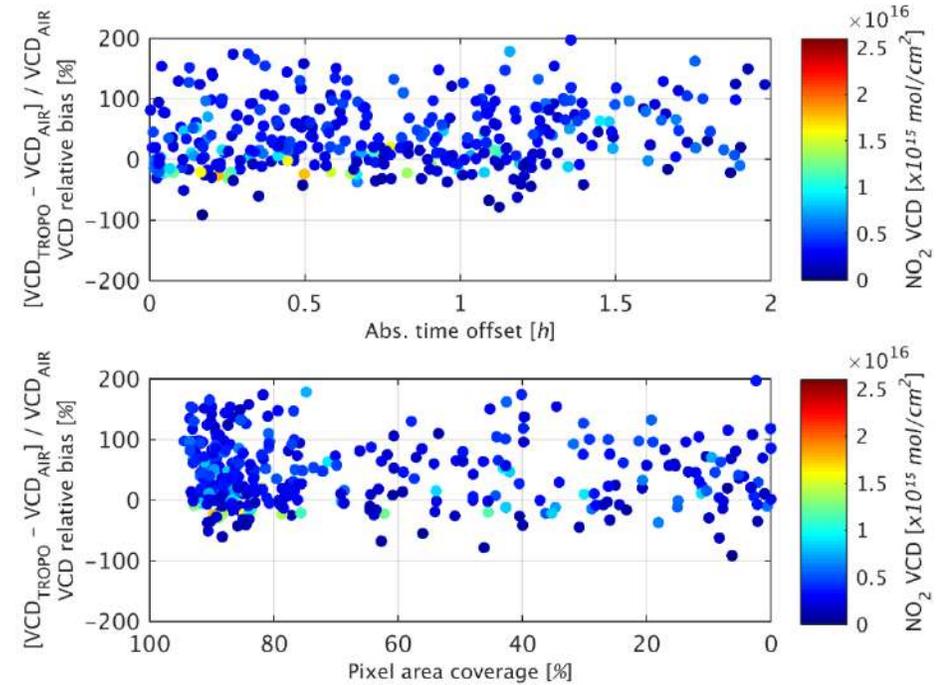
Ensemble 4 flights
(OFFL(-CAMS) v2.2 - 50% overlap - <=1 hour)



Ensemble 4 flights
(OFFL(-CAMS) v2.2 - No spatiotemp. constraints)

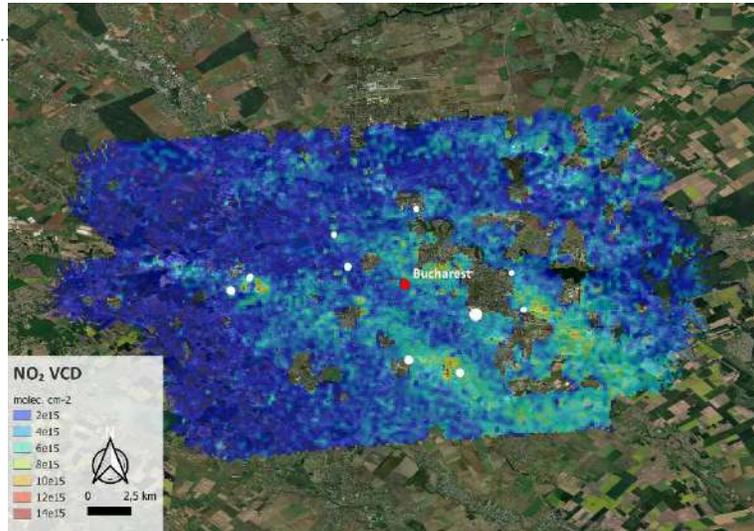


Ensemble 4 flights – Impact spatiotemporal variability

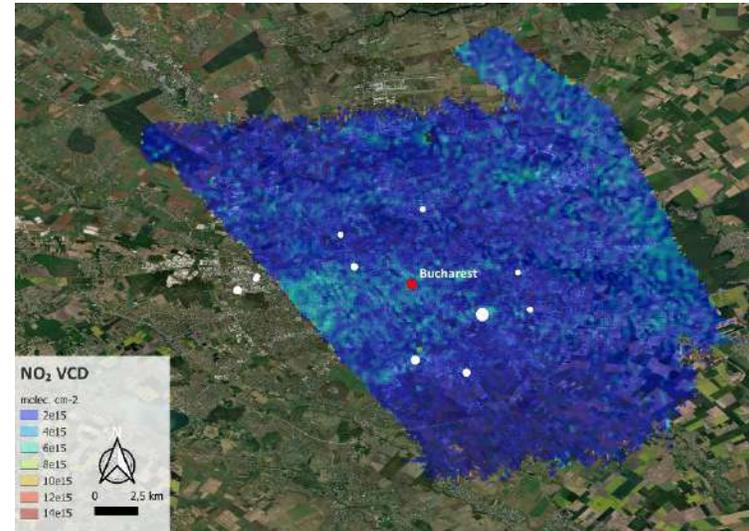


Preliminary results (NO₂ VCD maps) – Bucharest, RO

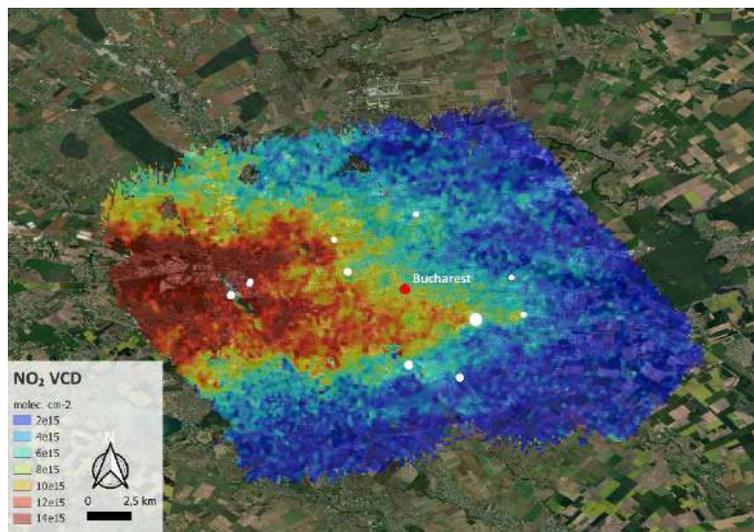
05-07-2021 (Monday)



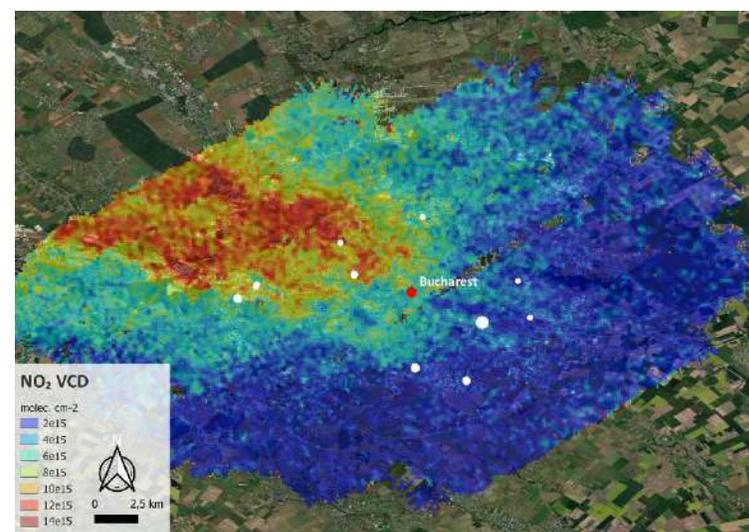
10-07-2021 (Saturday)



29-10-2021 (Friday)

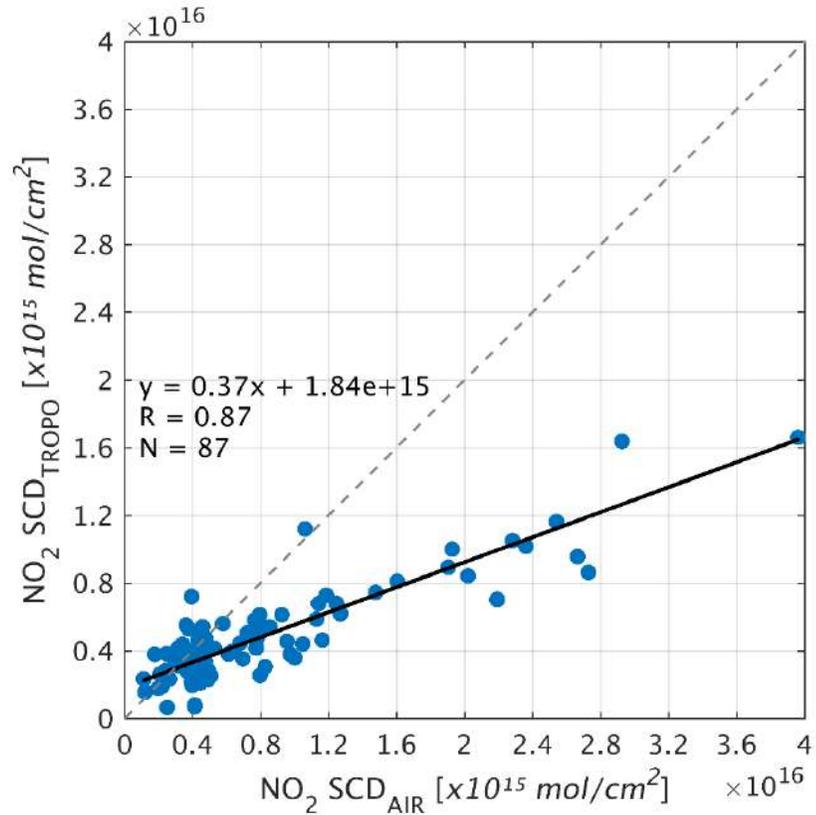


23-12-2021 (Thursday)

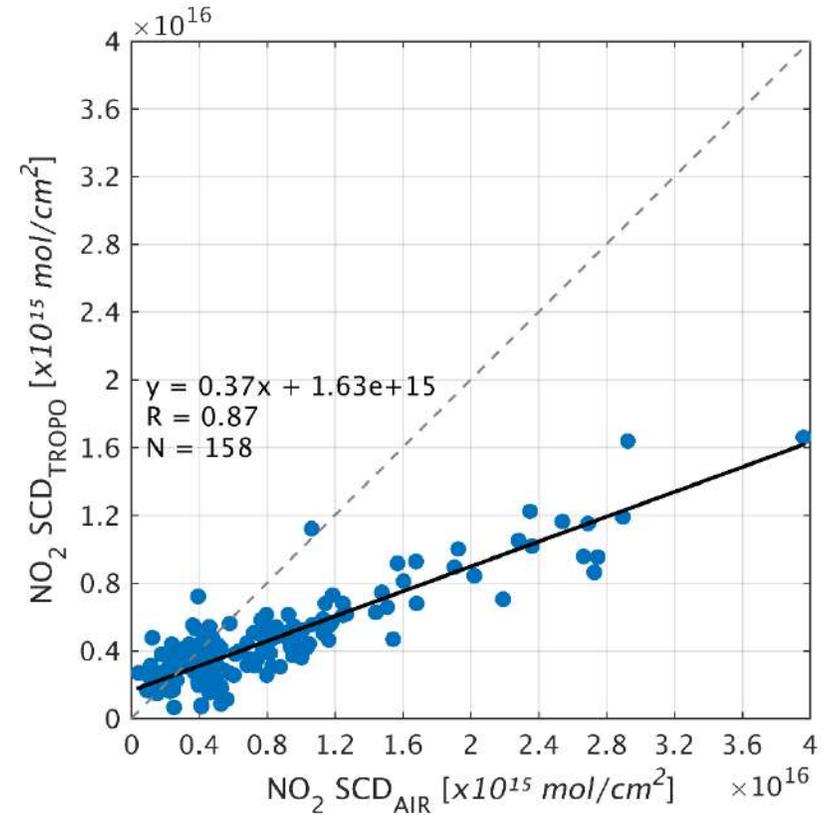


Preliminary results (SCD) – Bucharest, RO

Ensemble 4 flights (OFFL v2.2 - 50% overlap - ≤ 1 hour)

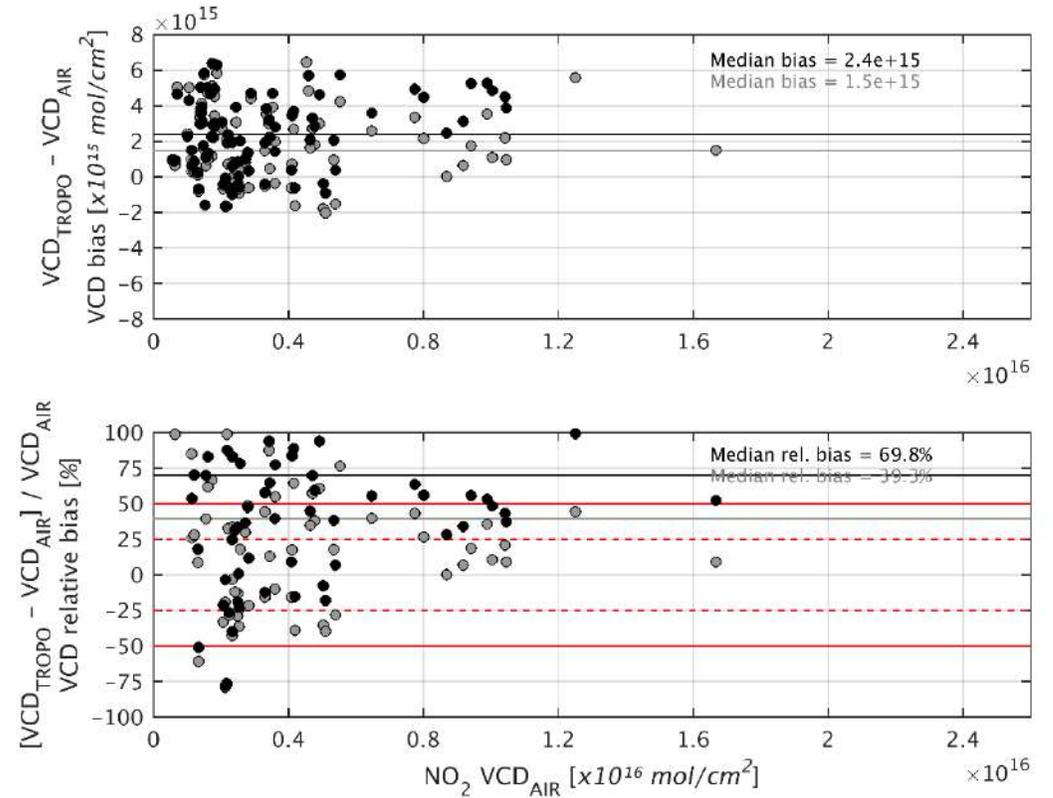
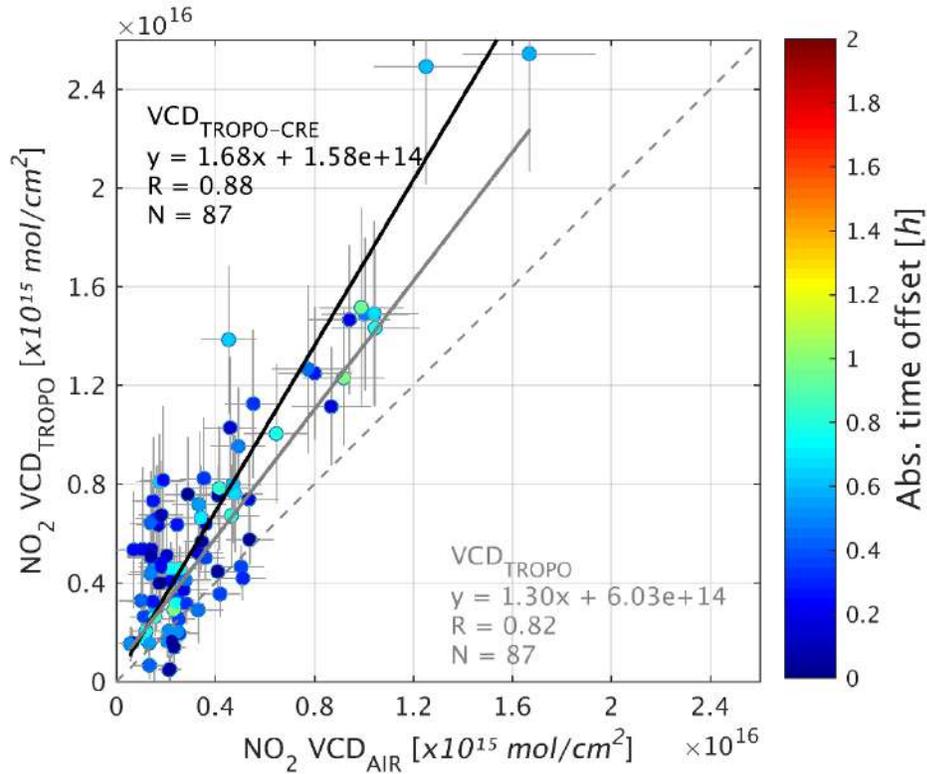


Ensemble 4 flights (OFFL v2.2 – no spatiotemp. constraints)



Preliminary results (S5P NO₂ validation) – Bucharest

Ensemble 4 flights (OFFL(-CAM5) v2.2 - 50% overlap - <=1 hour)





Conclusions – next steps

- **Central processor v1.1 (developed in context of ESA SVANTE/QA4EO projects)**
 - NetCDF CF data format for airborne imaging
 - Central processing code: DOAS spectral fitting + AMF computation
 - Airborne–satellite automatic independent validation tools
 - Important step to **harmonize/standardize data acquisition and processing** of airborne imaging data
- **Assessment of TROPOMI tropospheric NO₂ product**
 - Clear NO₂ patterns can be retrieved over urban/industrialised areas based on airborne imaging data
 - L2 TROPOMI NO₂ VCDs are well correlated ($R = 0.95$ (Berlin); $R = 0.82$ (Bucharest)) but biased (21% (Berlin); 40% (Bucharest)) with respect to airborne SWING retrievals.
 - CAMS product can have 20-30% impact on slope; small differences between OFFL and PAL for analysed period
 - Typically retrieved VCDs were relatively low for urban areas; mostly autumn conditions
- **Next steps**
 - Apply central processing and TROPOMI comparison tools on AirMAP data from Ruhr campaign
 - Process all available SWING data sets from recurrent flights → improve statistics
 - Further harmonize/standardize by best practice documents, joint standards, protocols, etc.



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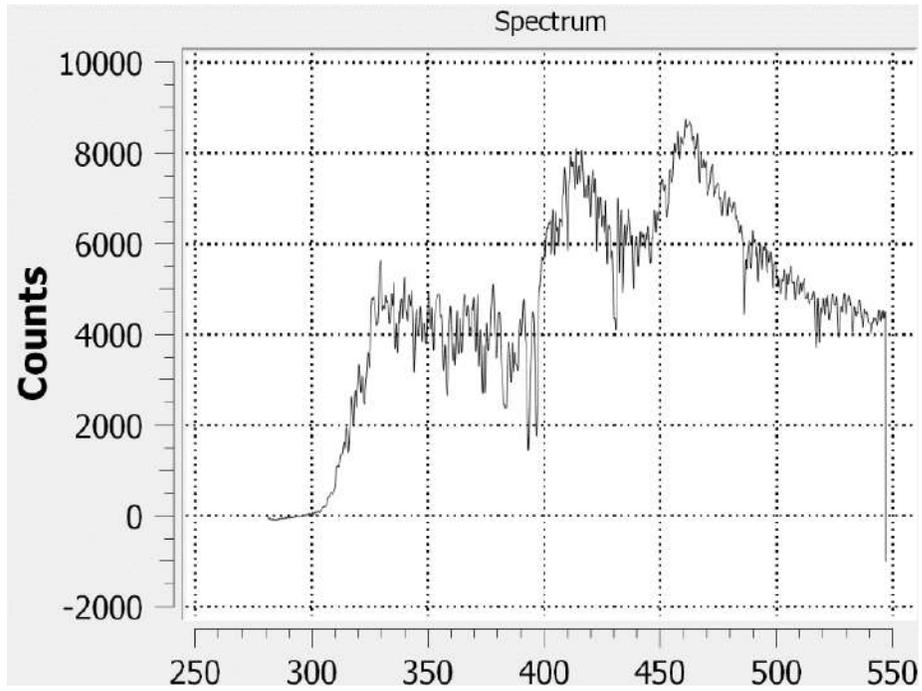
...Thank you! Questions?

[S5pcampaigns.aeronomie.be](https://s5pcampaigns.aeronomie.be)

Contact: frederik.tack@aeronomie.be

■ Post flight quicklooks – Raw data check

- Download of the SWING spectra and GPS-IMU data
- Check of the spectra, fixing corrupted file if needed

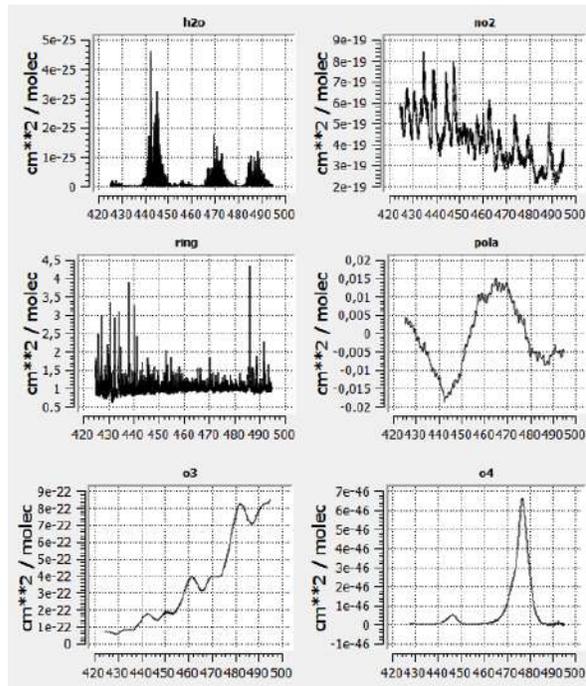


S5PVAL-RO/RAMOS Flight on 23-12-2021

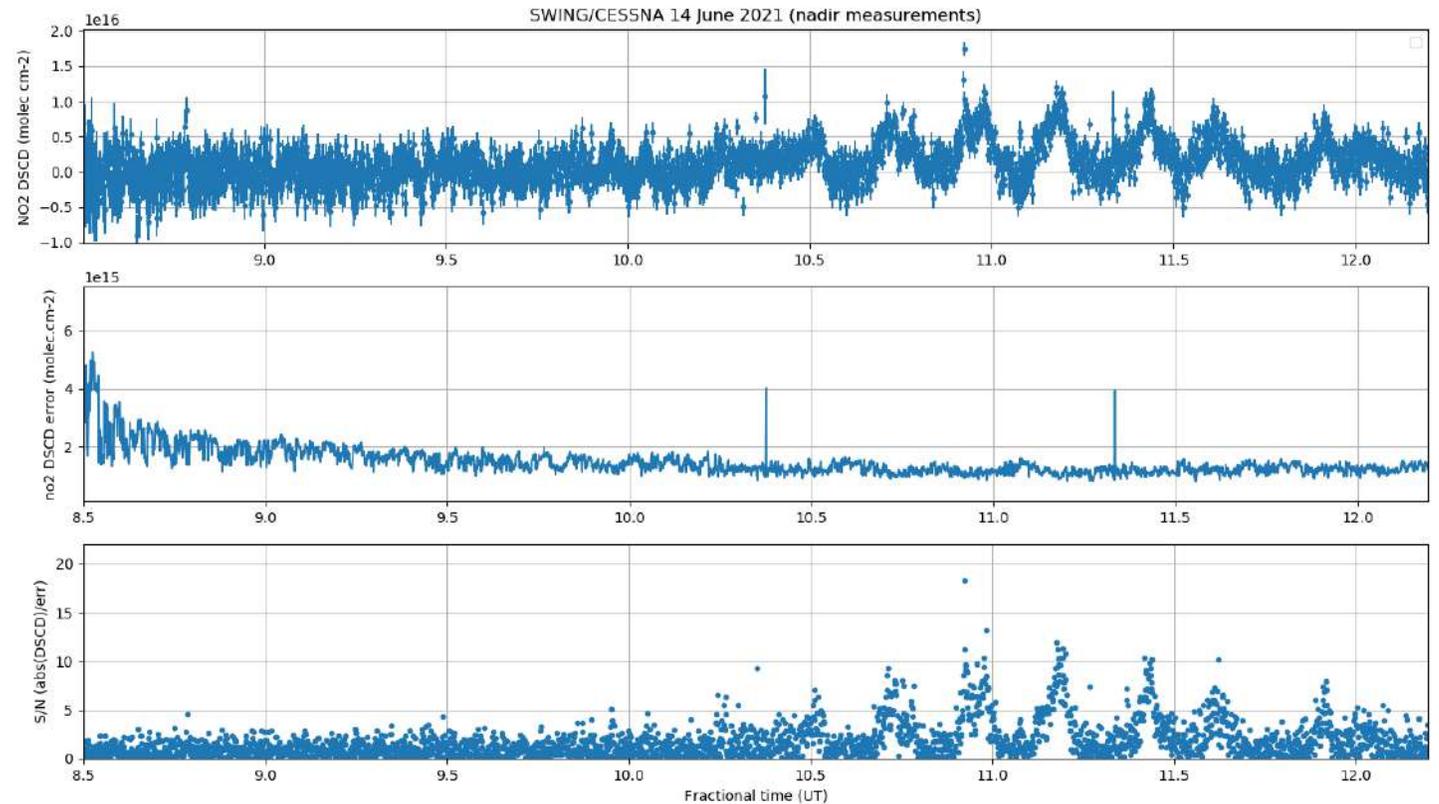
DOAS analysis and pre-processing

Post flight quicklooks – DOAS analysis

- DOAS analysis with a fixed reference spectrum (average of 25 SWING spectra)

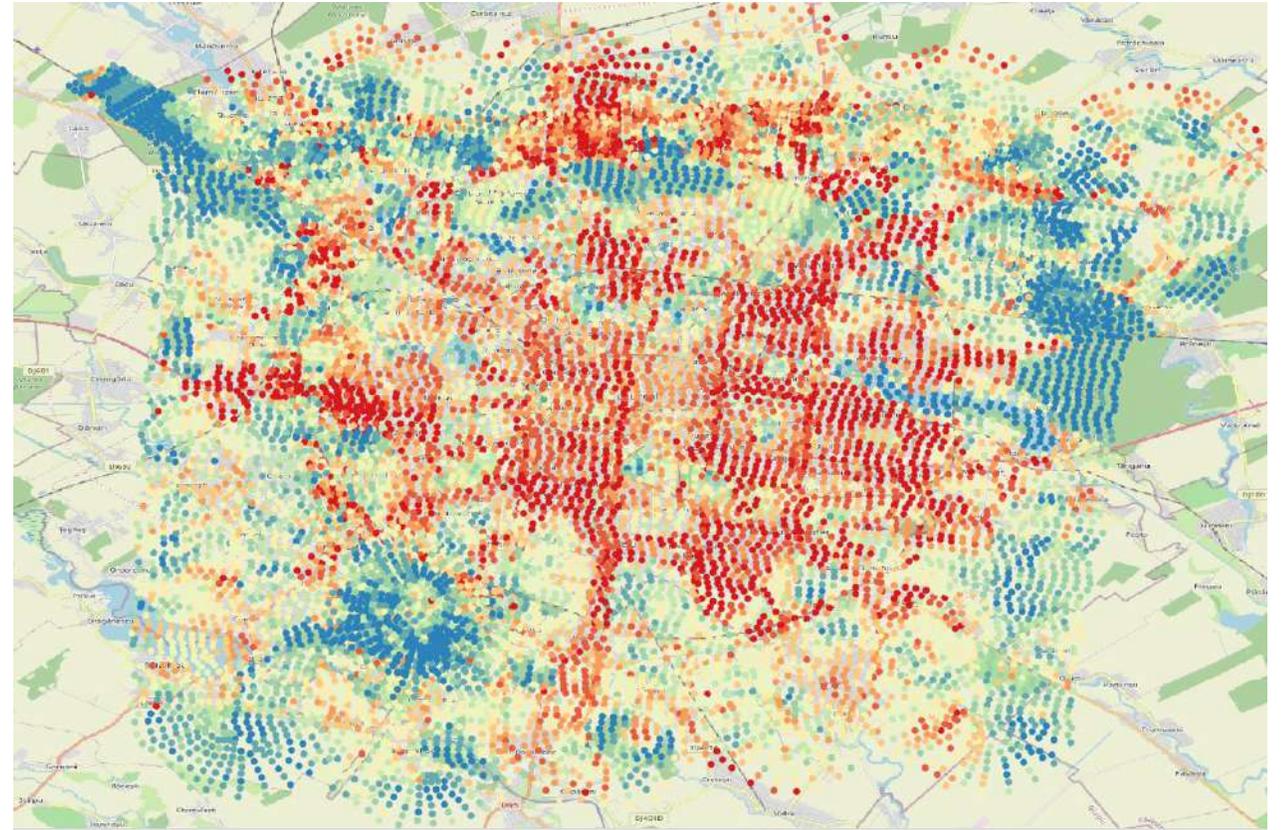


Fitted cross-sections



S5PVAL-DE flight on 14-06-2021

- **Post flight quicklooks – Georeferencing**
 - Georeference the DSCD with the GPS-IMU data
 - Check of the flux map vs ground albedo

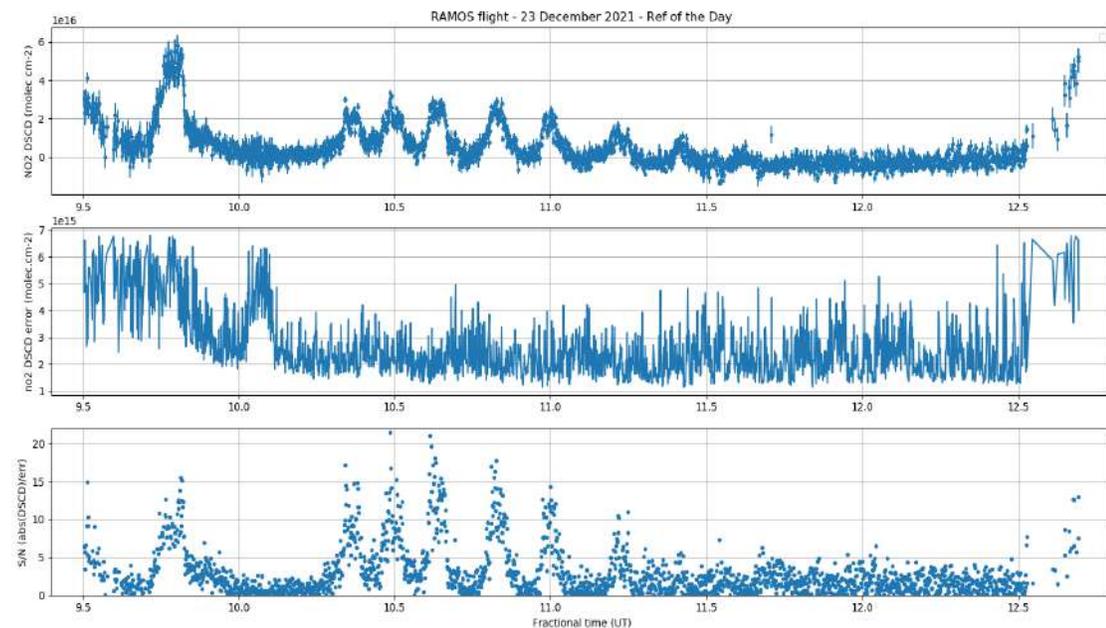
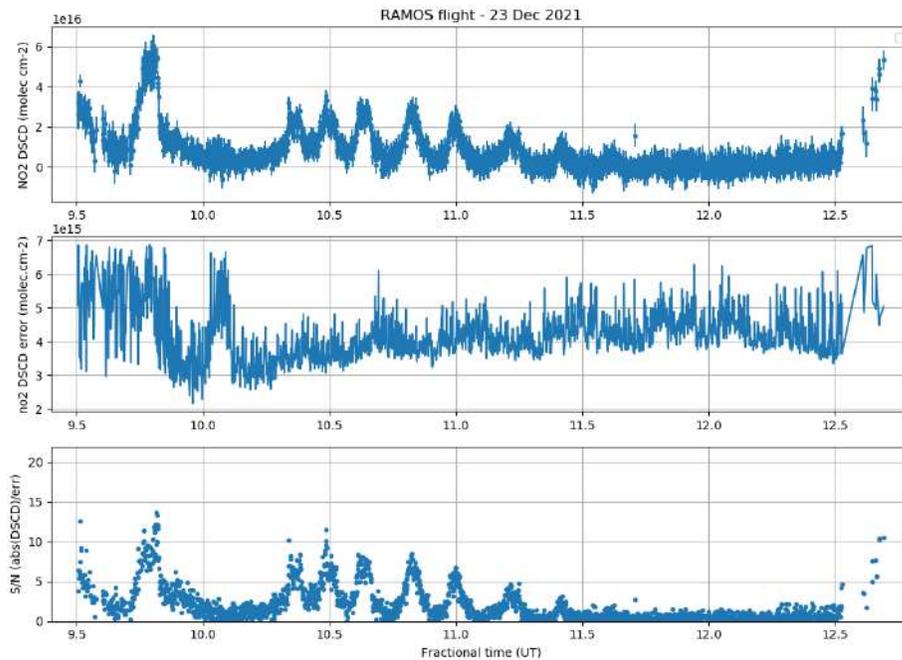


S5PVAL-RO/RAMOS Flight on 11-11-2021

DOAS analysis and pre-processing

Input for central processing

- Finetuned DOAS analysis and georeferencing with a reference spectrum (average of 25 spectra) of the day
- Fill metadata info for the day (operator, possible comment on weather, place and time of the reference, etc.)
- Create input .nc file for central processing, discarding spectra with altitude < 3000 m, NO₂ fit RMS > 1, and flagging NO₂ fit RMS > 0.005

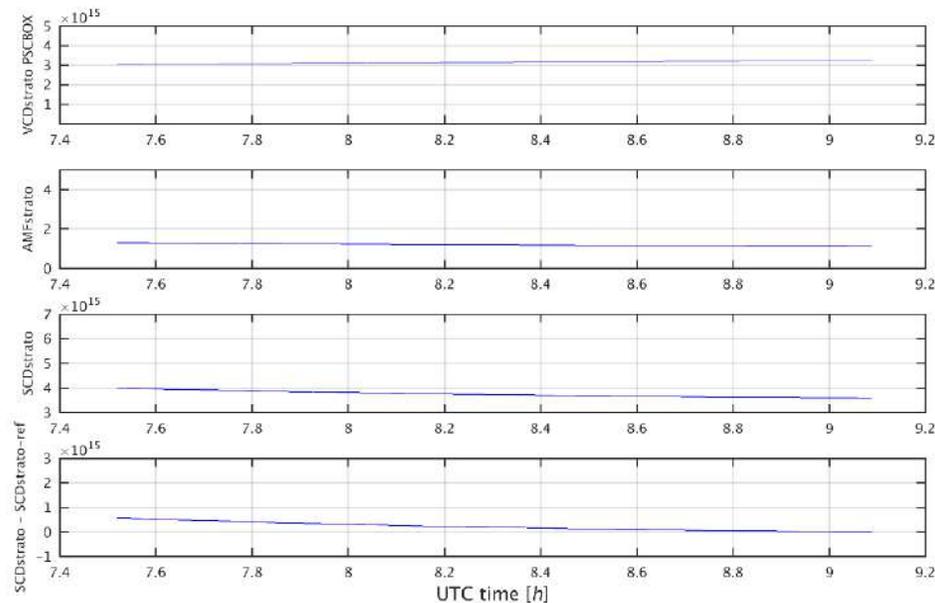


DSCD → VCD processing

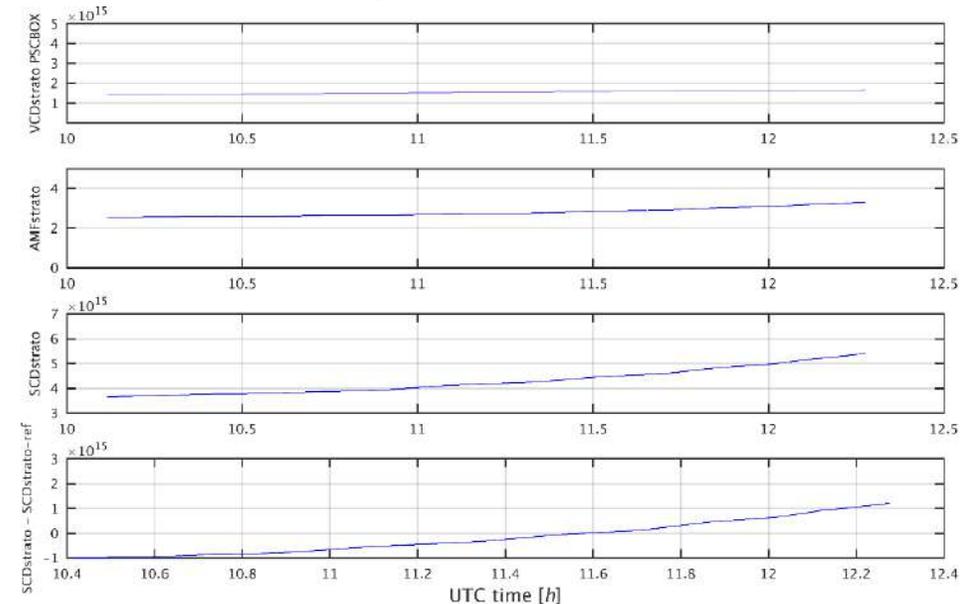
■ SCD stratospheric correction

- Compensates for **changes in the stratospheric field** between reference area and actual measurements
- Based on 1) modeled SCDstrato from stacked box photochemical model PSCBOX, 2) averaged SCDstrato from coincident TROPOMI overpass for scaling, and 3) geometric AMF
- Effect generally quite small ($< 1e15$ for 2h flight), but can become significant at larger SZA (autumn-winter flight) or long flight time with reference at start or end of flight

Flight on 01-07-2021



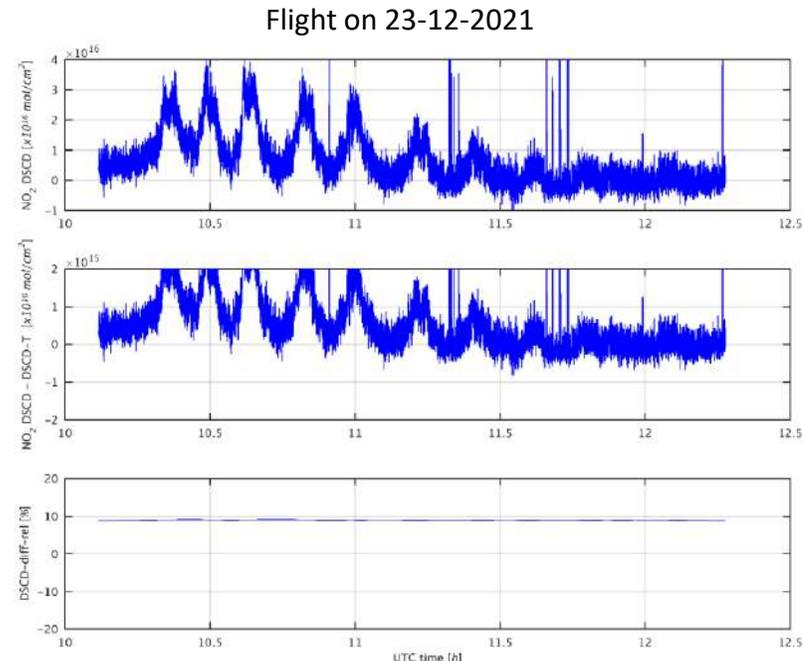
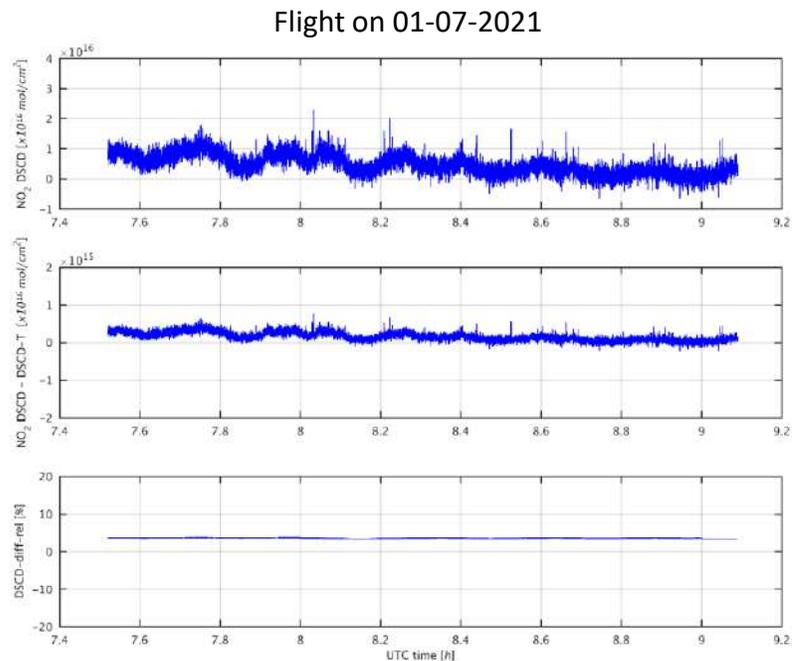
Flight on 23-12-2021



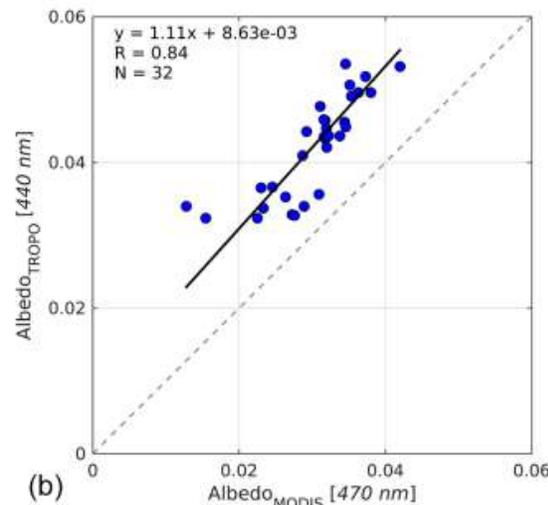
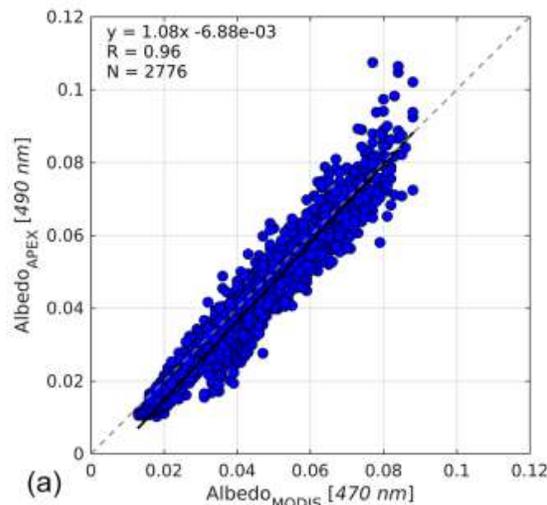
DSCD → VCD processing

■ DSCD temperature correction

- Correct for **temperature dependence of NO₂ cross-section**
 - $T_{\text{eff}} = T_{\text{surf}} - 6.5 \cdot \text{PBL} / 2 \rightarrow$ Laps rate of 6.5° per km
 - $\text{SCD}_T = \text{SCD} \cdot (1 + 0.0035 \cdot (T_{\text{eff}} - T_{\text{ref}}))$
- Surface temperature obtained from ERA-5 (global, hourly product at 0.25° spatial resolution)
- Overestimation of about <5% (summer) to <10% (winter) on SCD when not corrected



- AMF_{tropo} -- LIDORT 2.6 RTM (Spurr, 2008)
- **Surface albedo in the fit window**
 - **User specified**, e.g. based on at-sensor radiance when absolutely calibrated
 - Or **interpolated on MODIS MCD43A3** Black-sky albedo / MCD43A1 BRDF L3 v006 product
 - Global products at **500 m resolution** produced daily using 16 days of Terra and Aqua MODIS data
 - Band 3 (470 nm) used for NO_2
 - MODIS MCD43A3 (BRDF) vs MCD43A1 (BSA) → impact of less than 2% on NO_2 VCD
 - Product compared to OMI LER, used for TROPOMI albedo, in Tack et al. (2021). OMI LER tends to overestimate



- **AMF_{tropo} -- LIDORT 2.6 RTM (Spurr, 2008)**
- **A priori NO₂ profile**
 - Box profile (based on ERA-5 PBL height) or interpolated TM-5 profile (1° spatial resolution)
 - Box profile (500 m) VS TM-5 model profile → VCDs 6-9% lower when model profile is used
 - Box profile (1000 m) VS TM-5 model profile → VCDs within 1%
- **Aerosol scenario (AOD, SSA, etc)**
 - based on CIMEL observations (if available)
 - Pure Rayleigh atmosphere
- VZA, SZA, RAA, analysis wavelength, platform altitude, etc. available in NetCDF file
- **Online computation for each airborne pixel → output are intensities and/or 1D Box-AMFs**