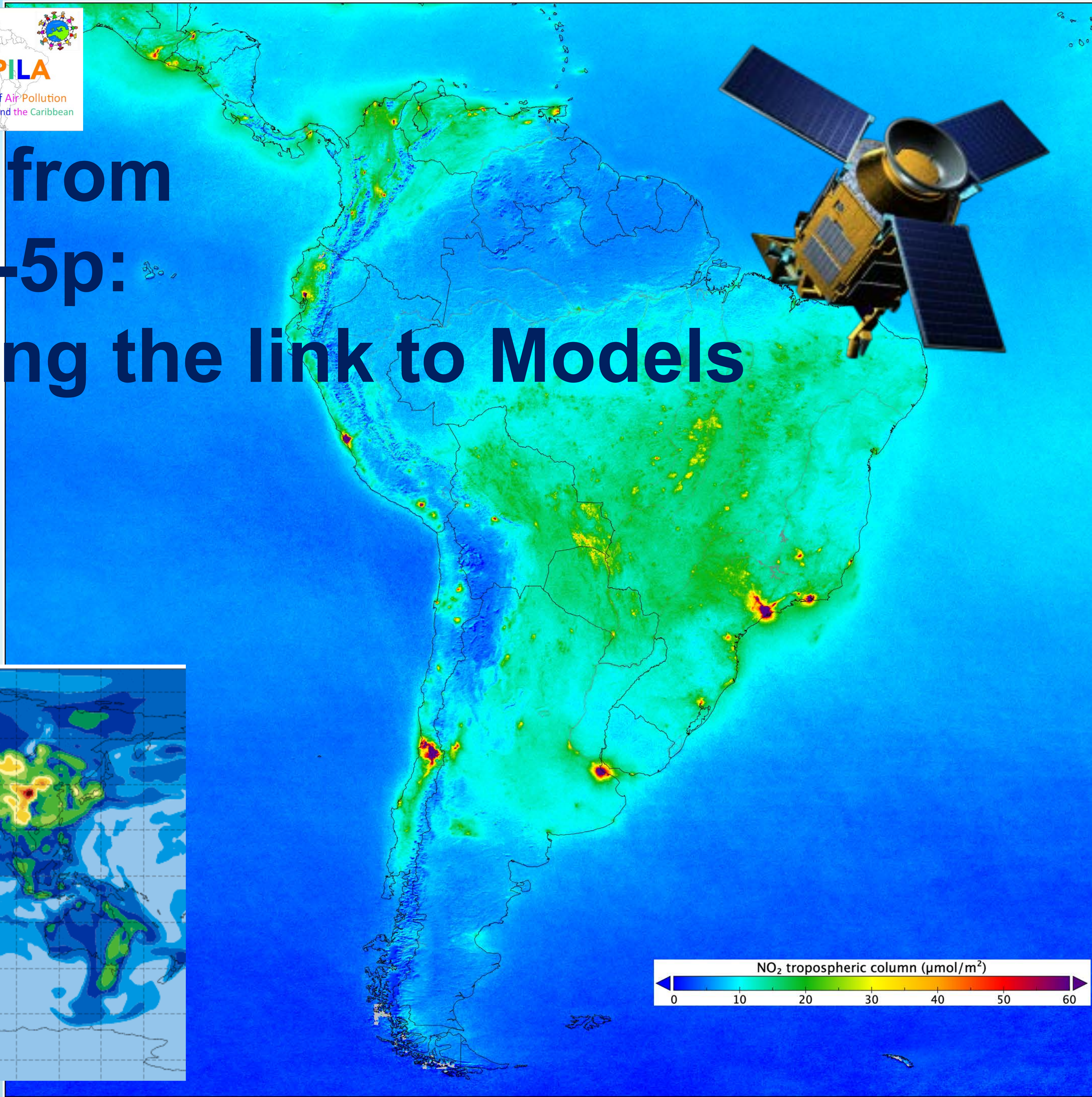
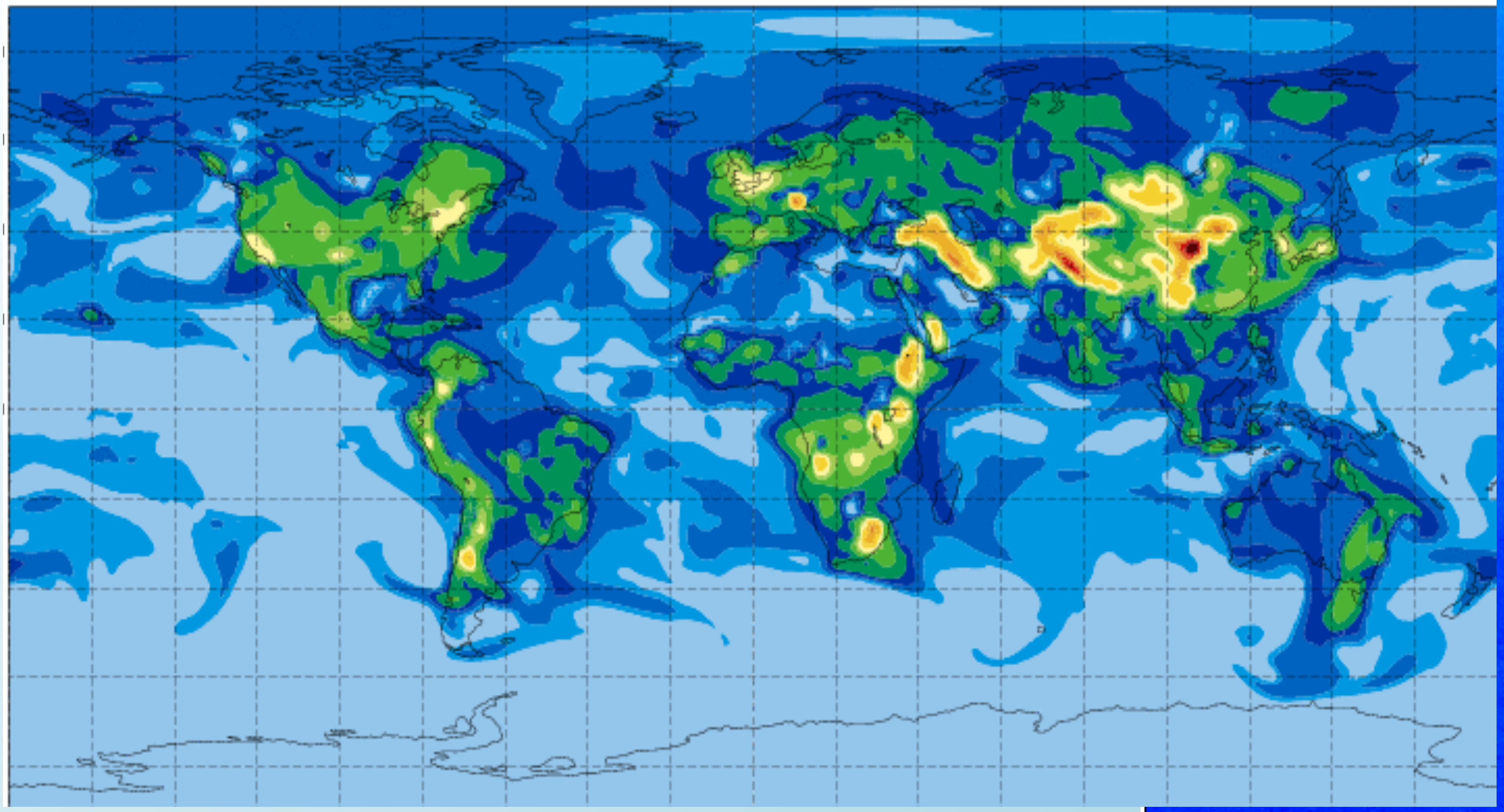
Satellite observations from TROPOMI on Sentinel-5p: Measurements & Making the link to Models

Henk Eskes, Deborah Stein Zweers
R&D Satellite Observation, KNMI

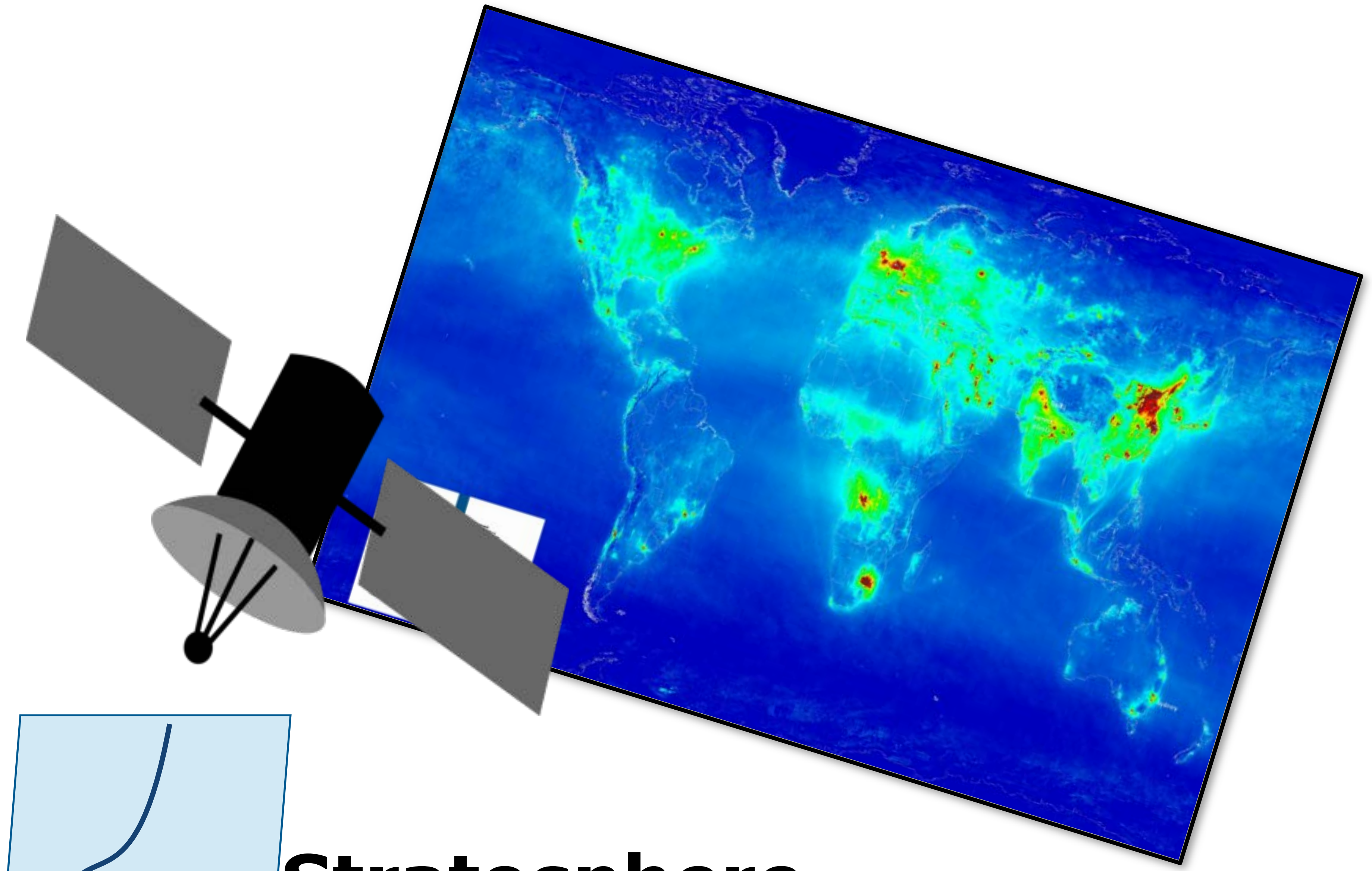
PAPILA summer school, 24 April 2020

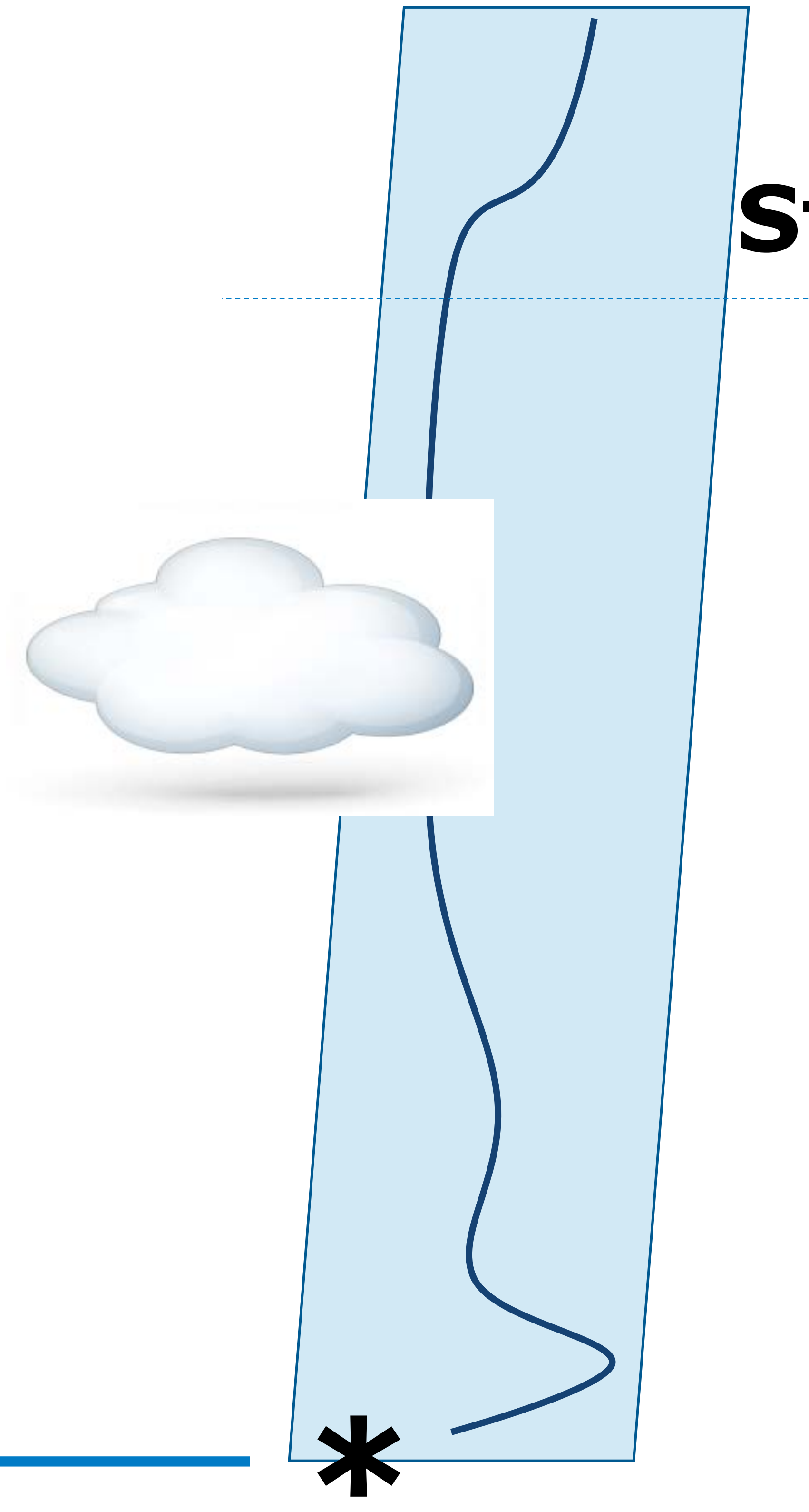




How does satellite data fit in global air quality monitoring?

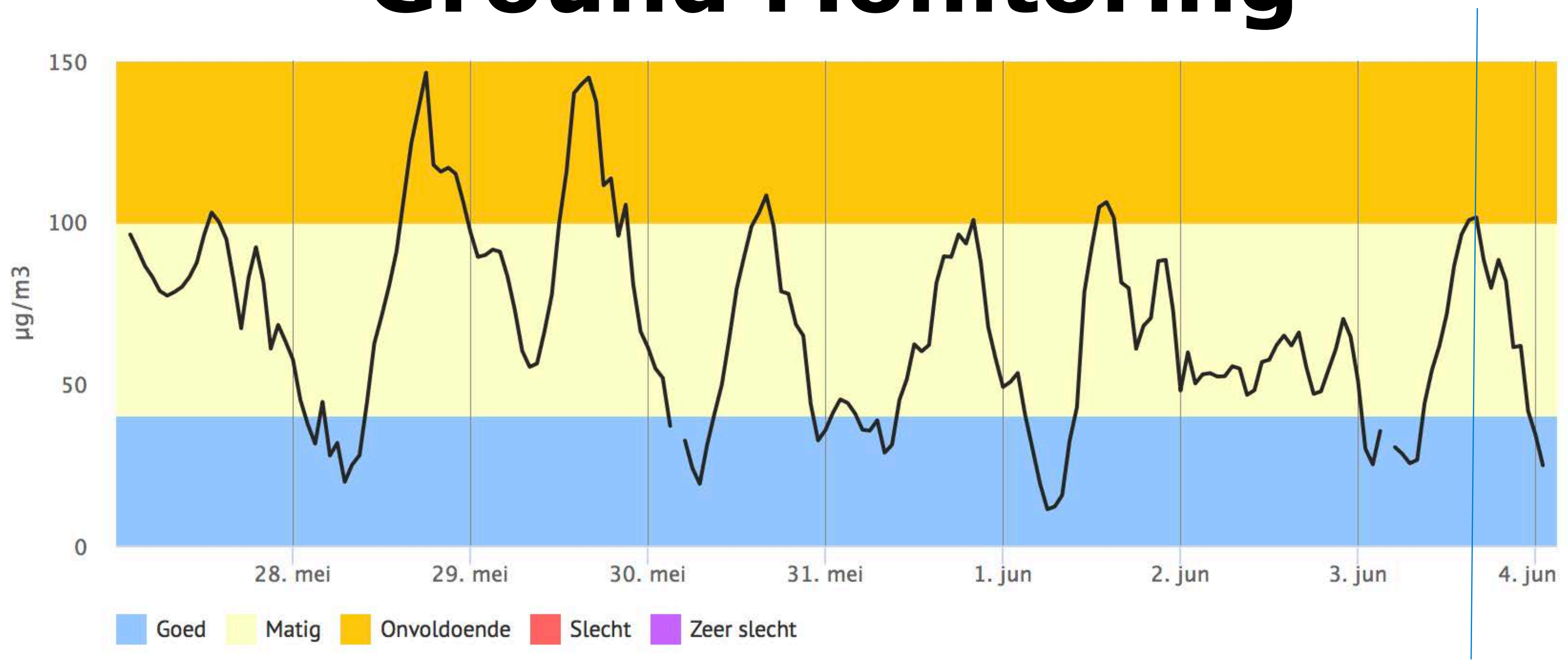
Vertical profile information



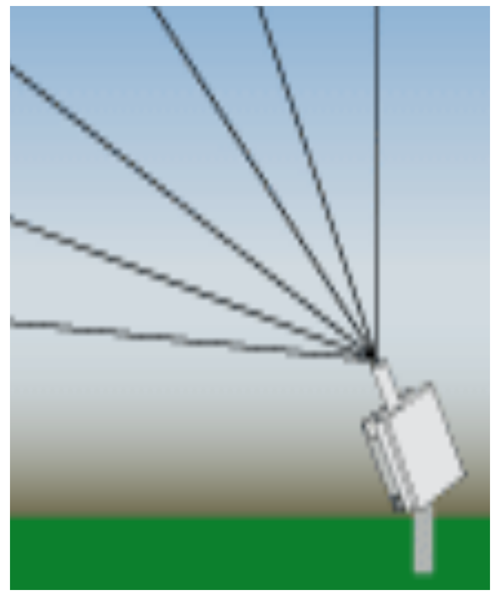


Stratosphere

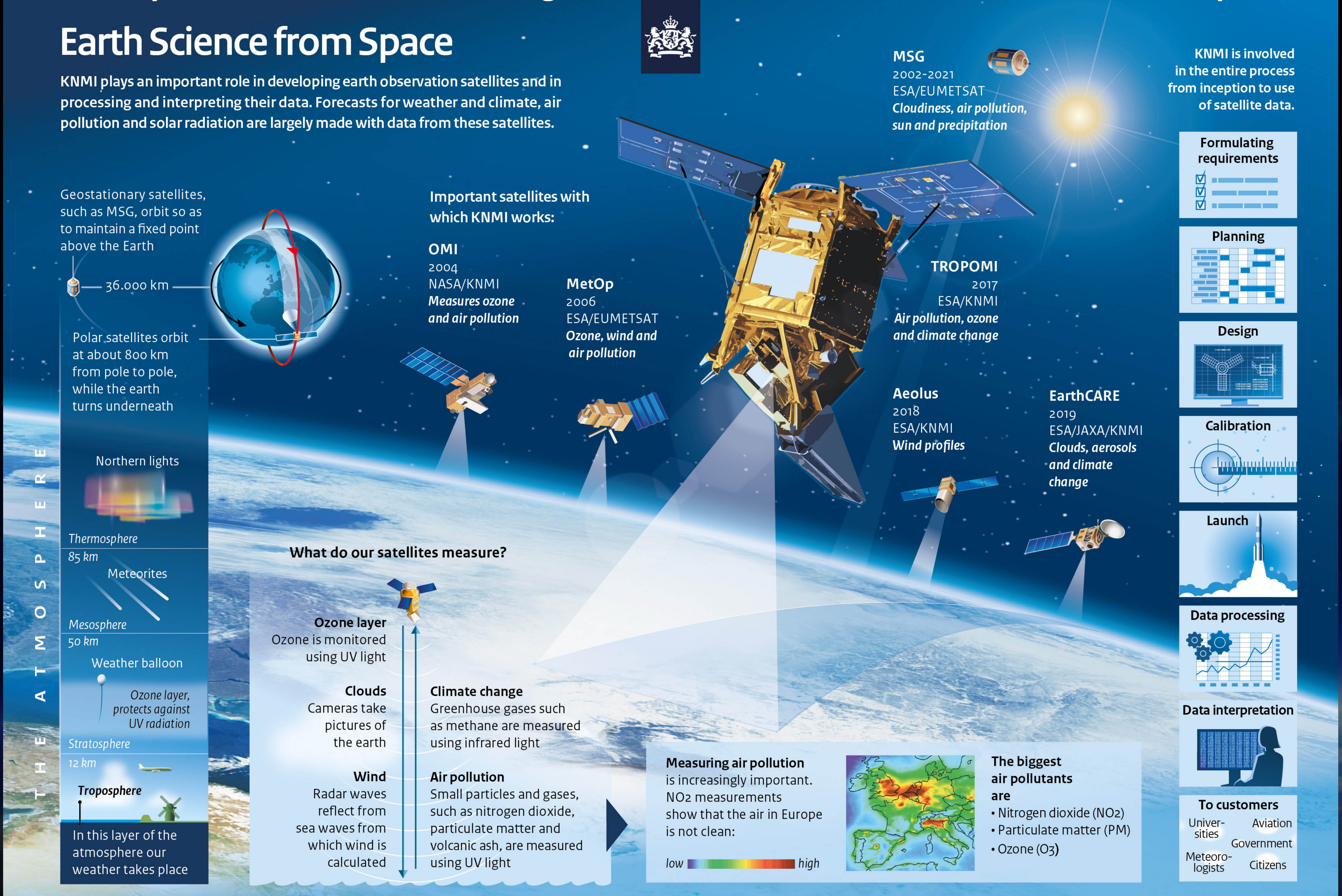
Ground Monitoring



MAX-DOAS, PANDORA



KNMI – Royal Netherlands Meteorological Institute -- R&D Satellite Observations Department

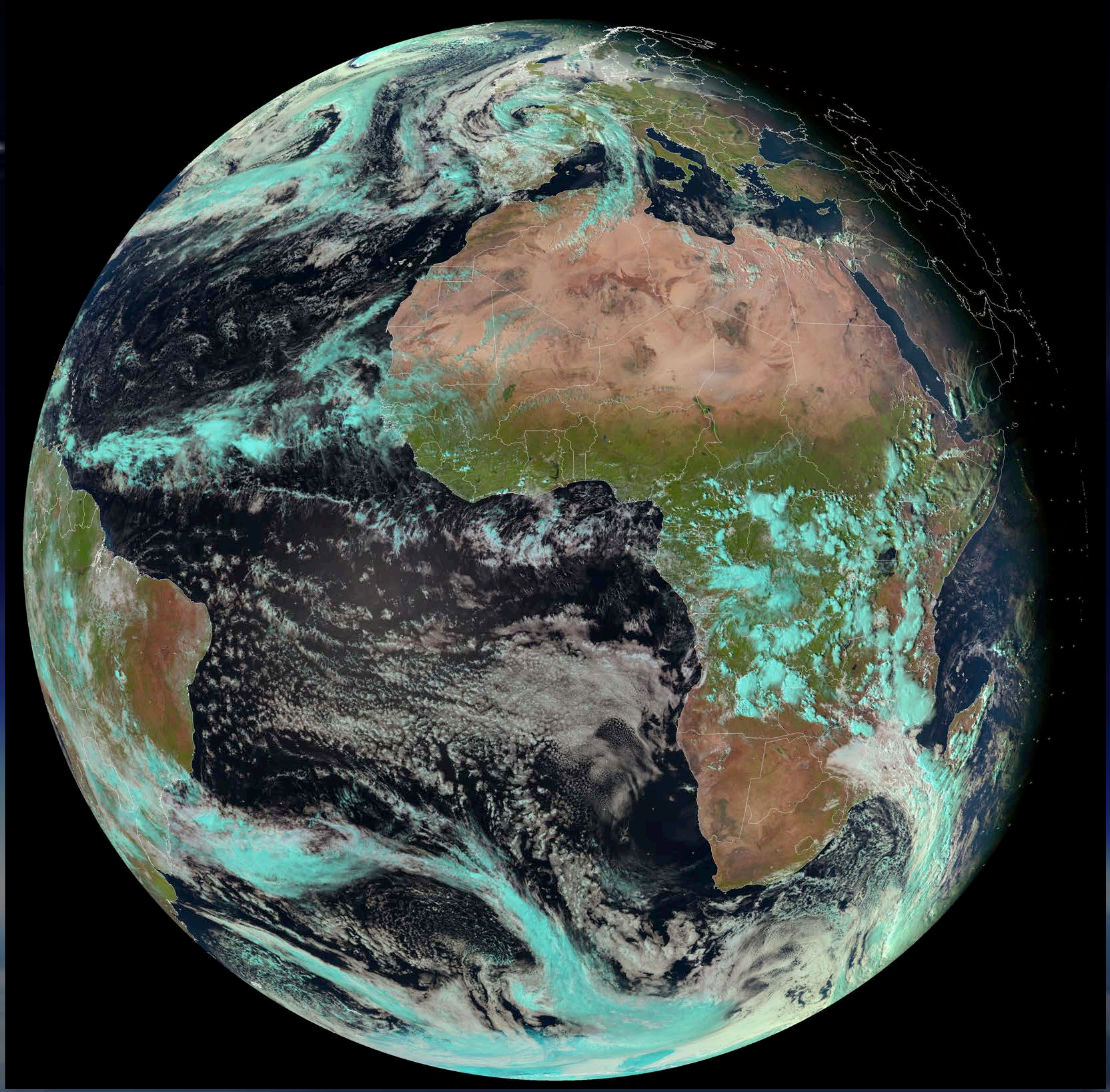


TROPOMI

Why Satellites?

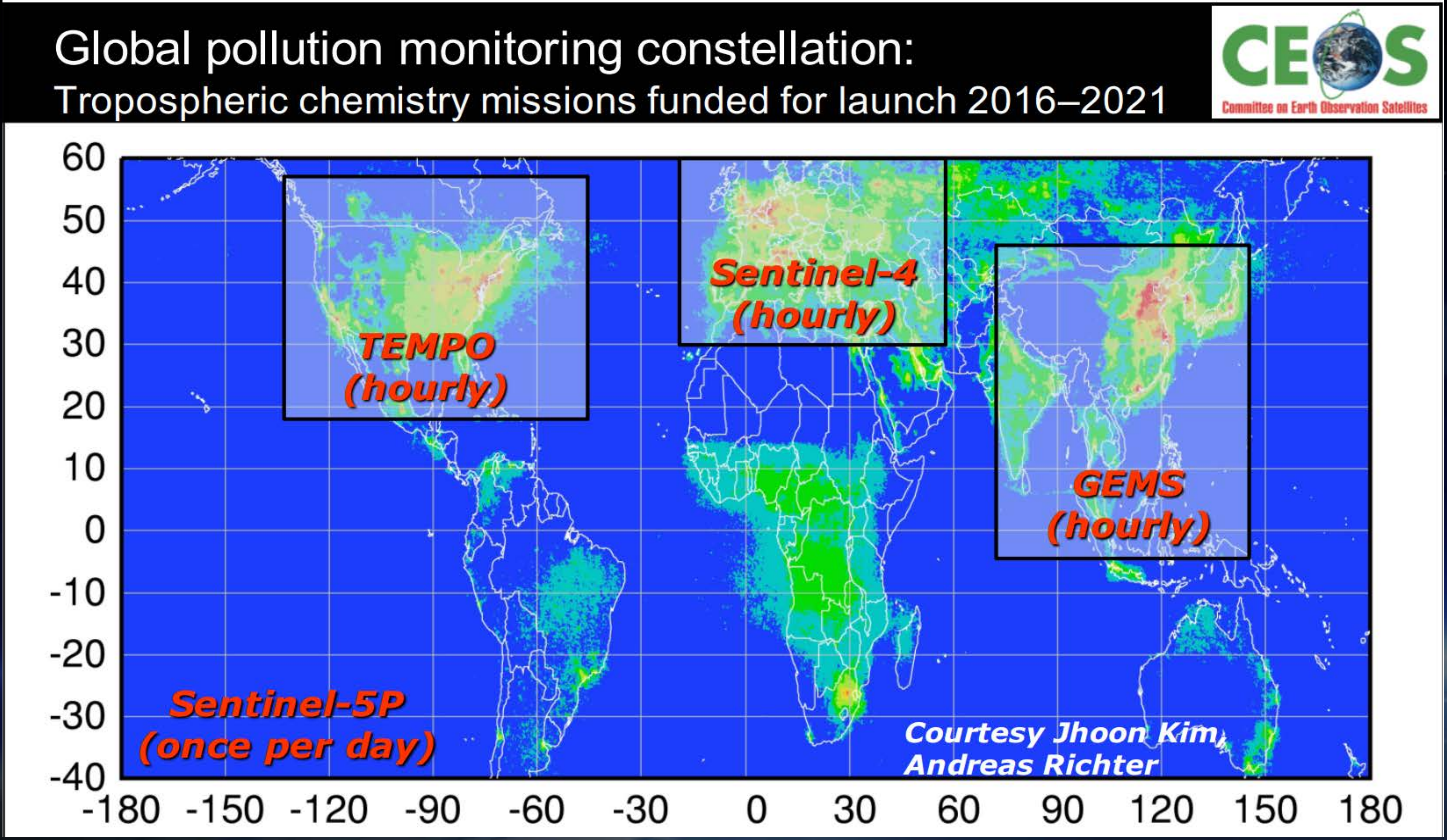
- Meteorological satellites revolutionized our understanding of dynamics
  - Now, 90% of data used in weather forecasting comes from satellites!

- What can a space borne perspective offer as compared to other atmospheric chemical datasets?
  - "Honest judge": uniform methods for daily, global snapshots
  - Copernicus Atmospheric Monitoring Service (CAMS) uses satellite data for global/regional air quality forecasts



TROPOMI

GEO + LEO Observing Strategy

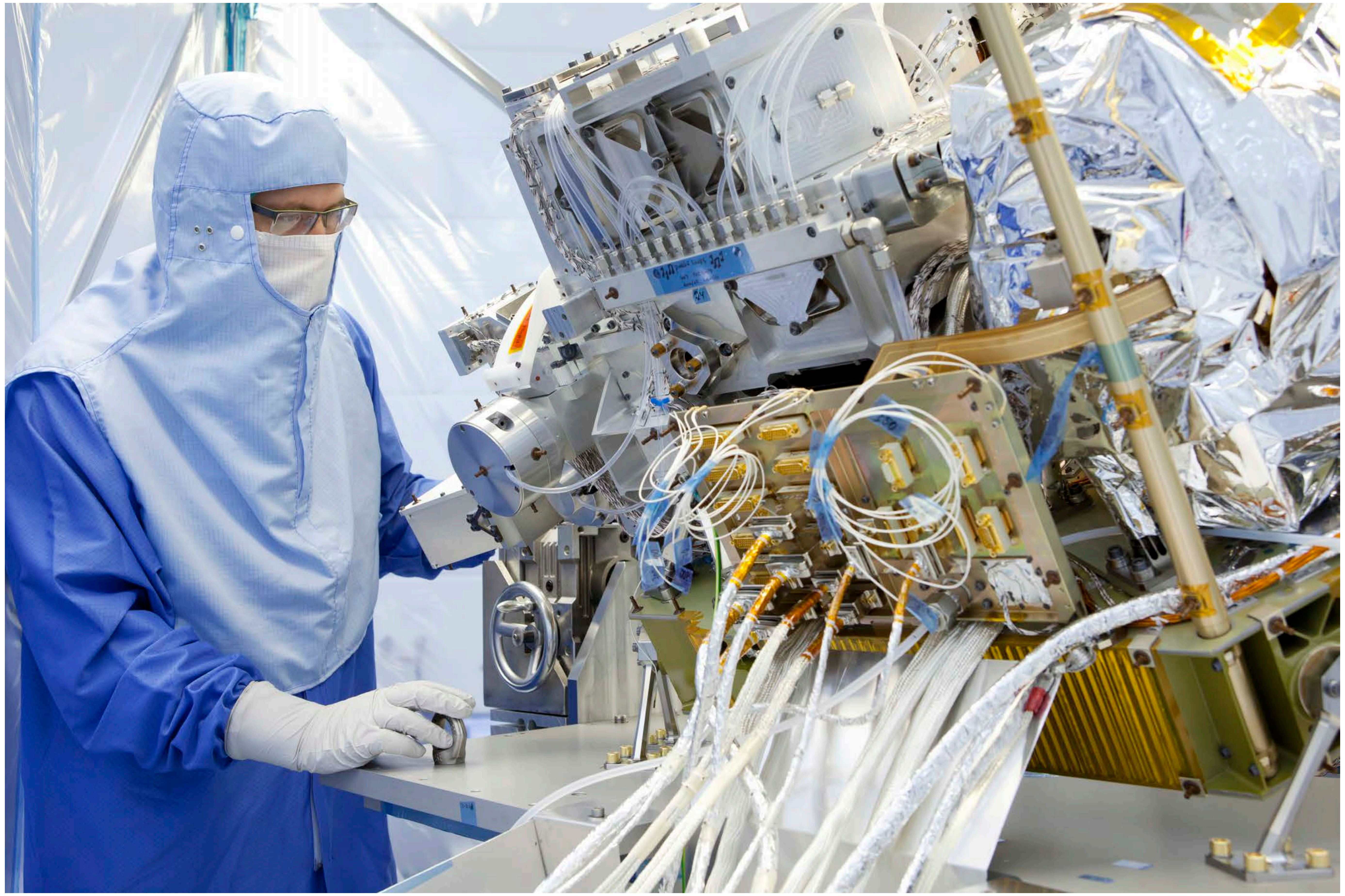


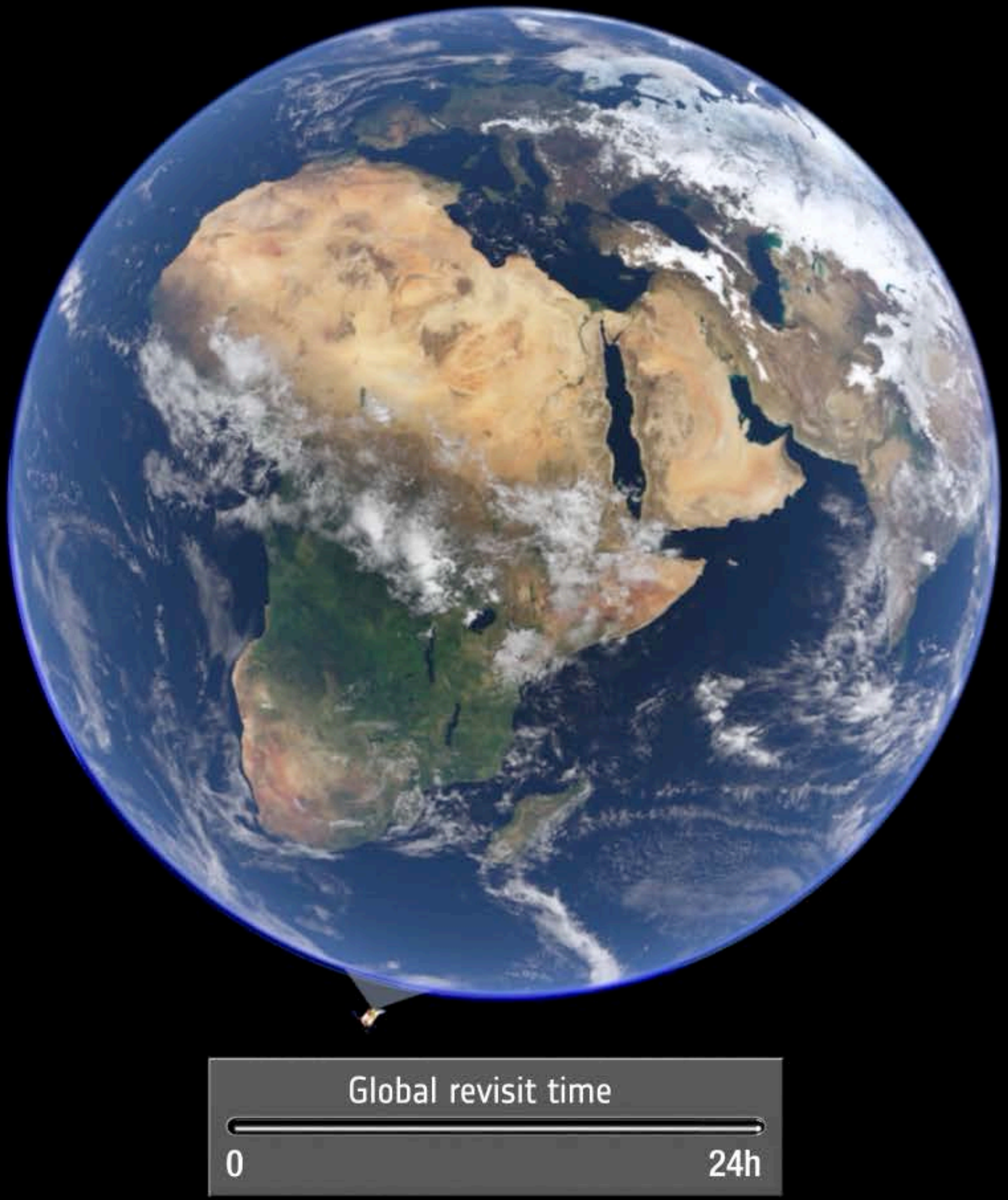
TROPOMI

Focus on TROPOMI:
TROPOspheric Monitoring Instrument

- Monitoring atmospheric composition, for:
  - Air quality
  - Climate change
  - Ozone layer

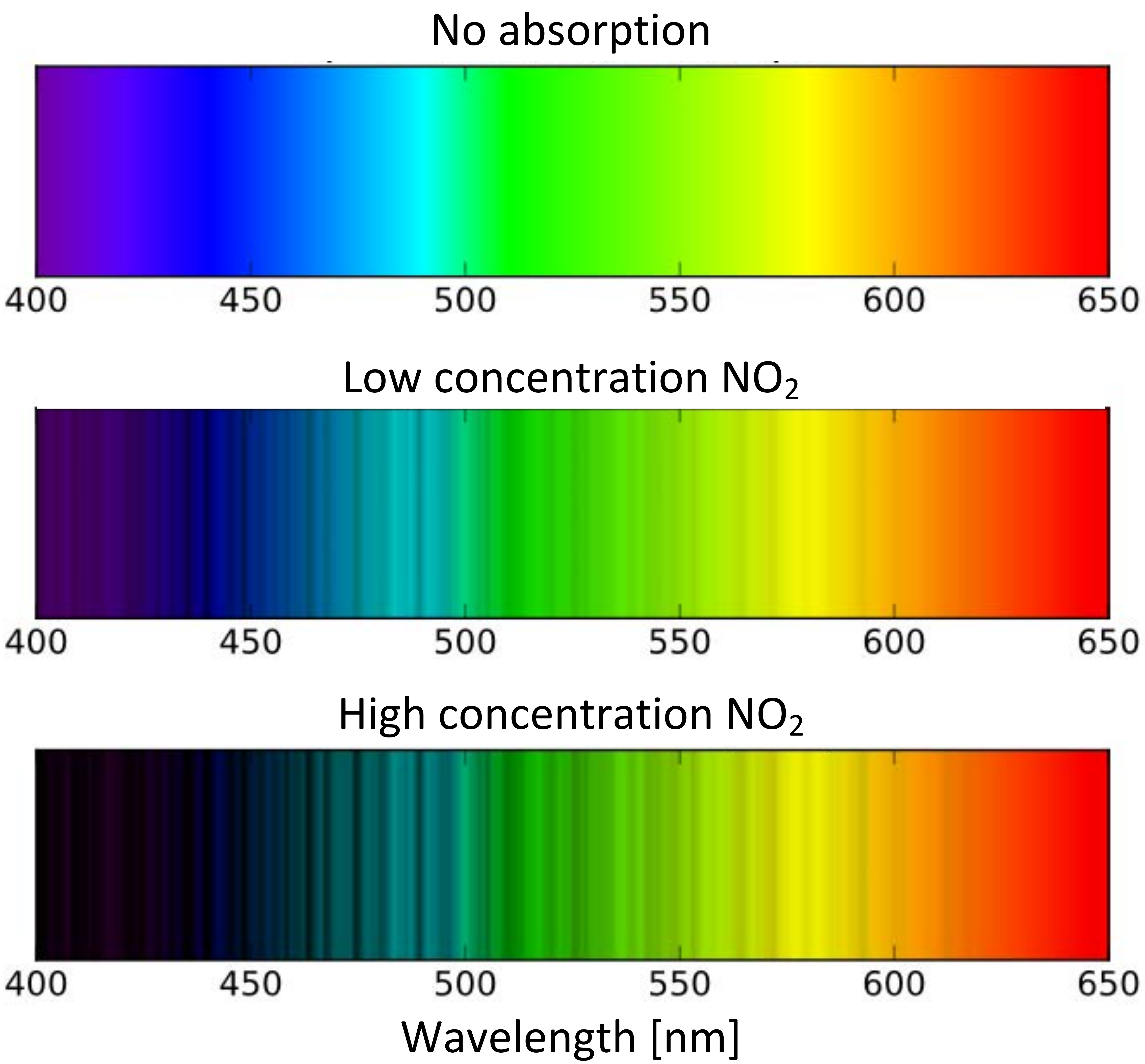
- TROPOMI details:
  - On Sentinel 5-Precursor Satellite (S5P)
  - Launched 13 October 2017
  - Polar-orbiting satellite
  - Overpass time ~13:30 LT
  - Data are free and open
  - www.tropomi.eu &
  - https://scihub.copernicus.eu/

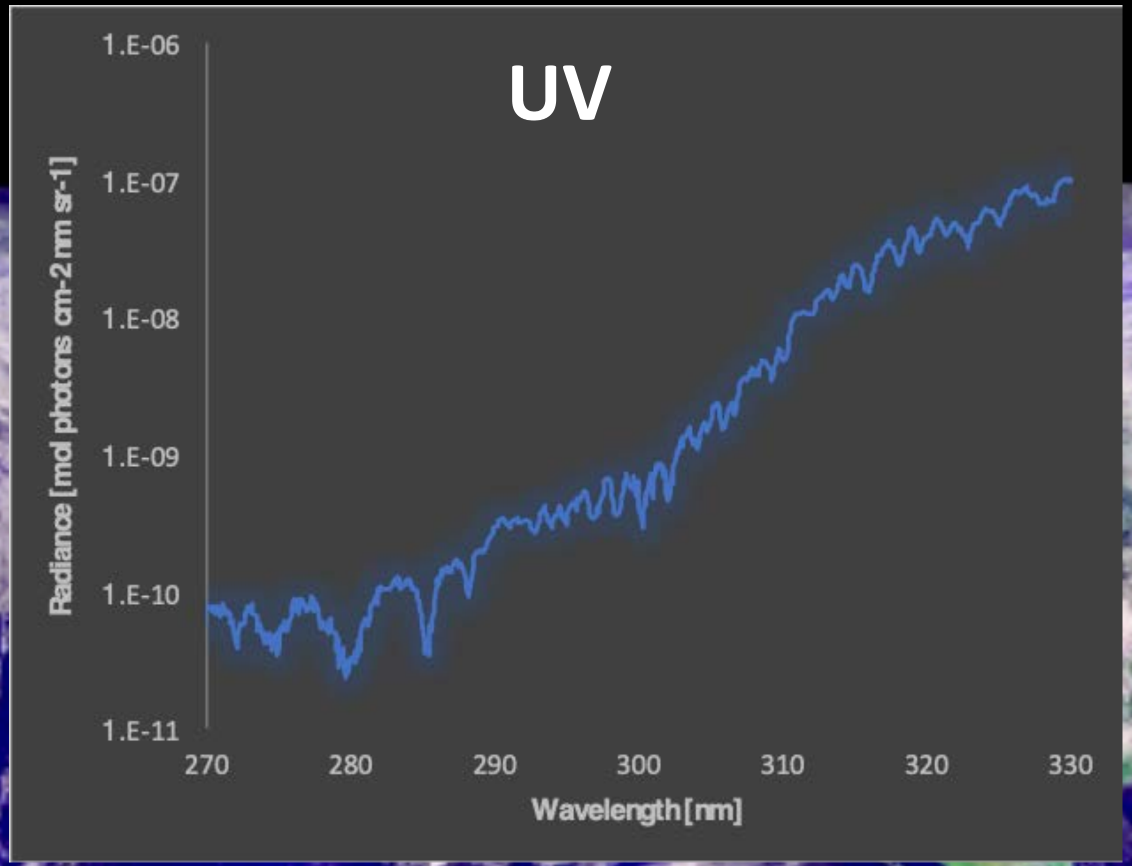


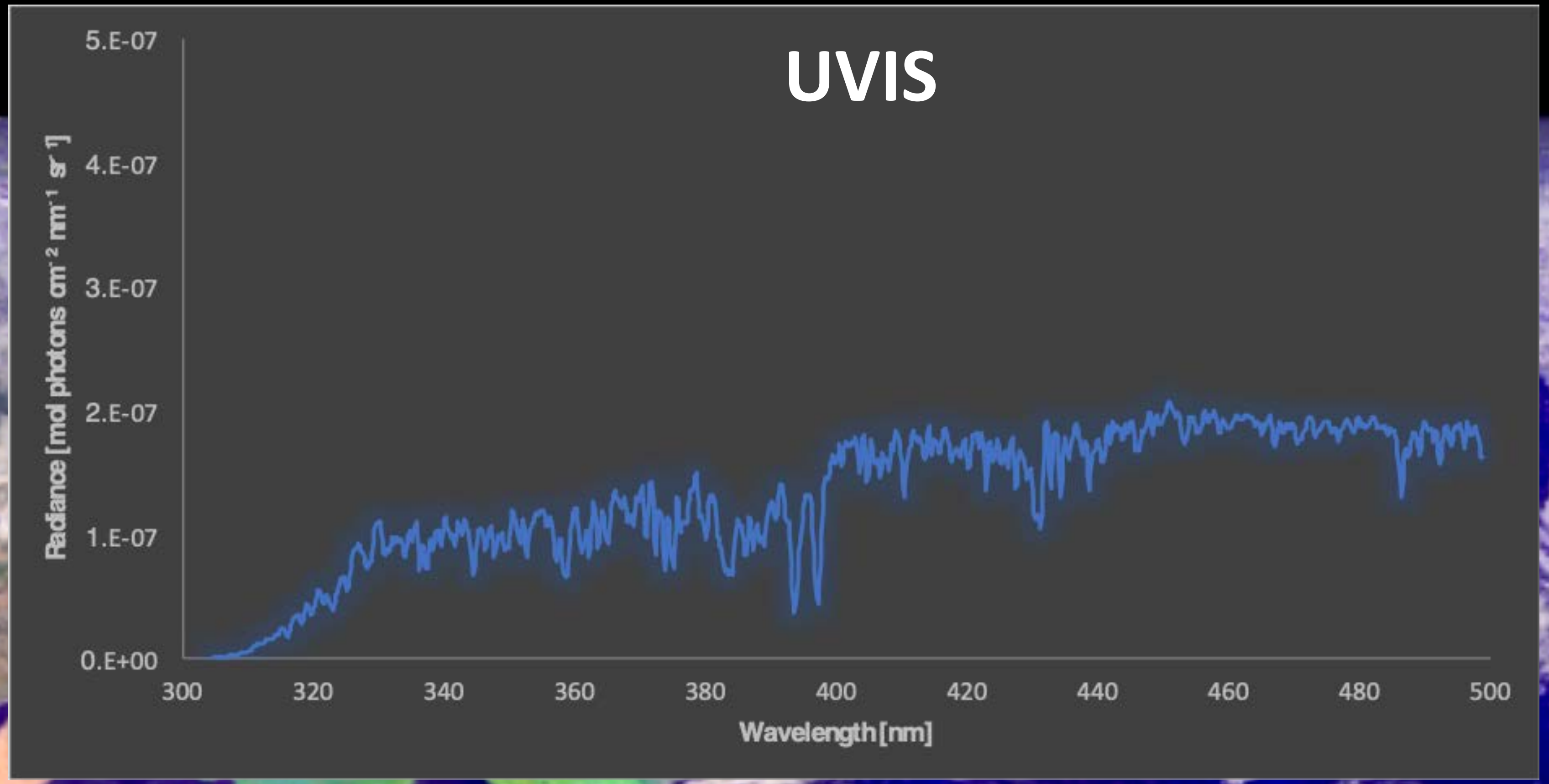

Global revisit time
0
24h


Wavelength
viewing direction
CCD detector

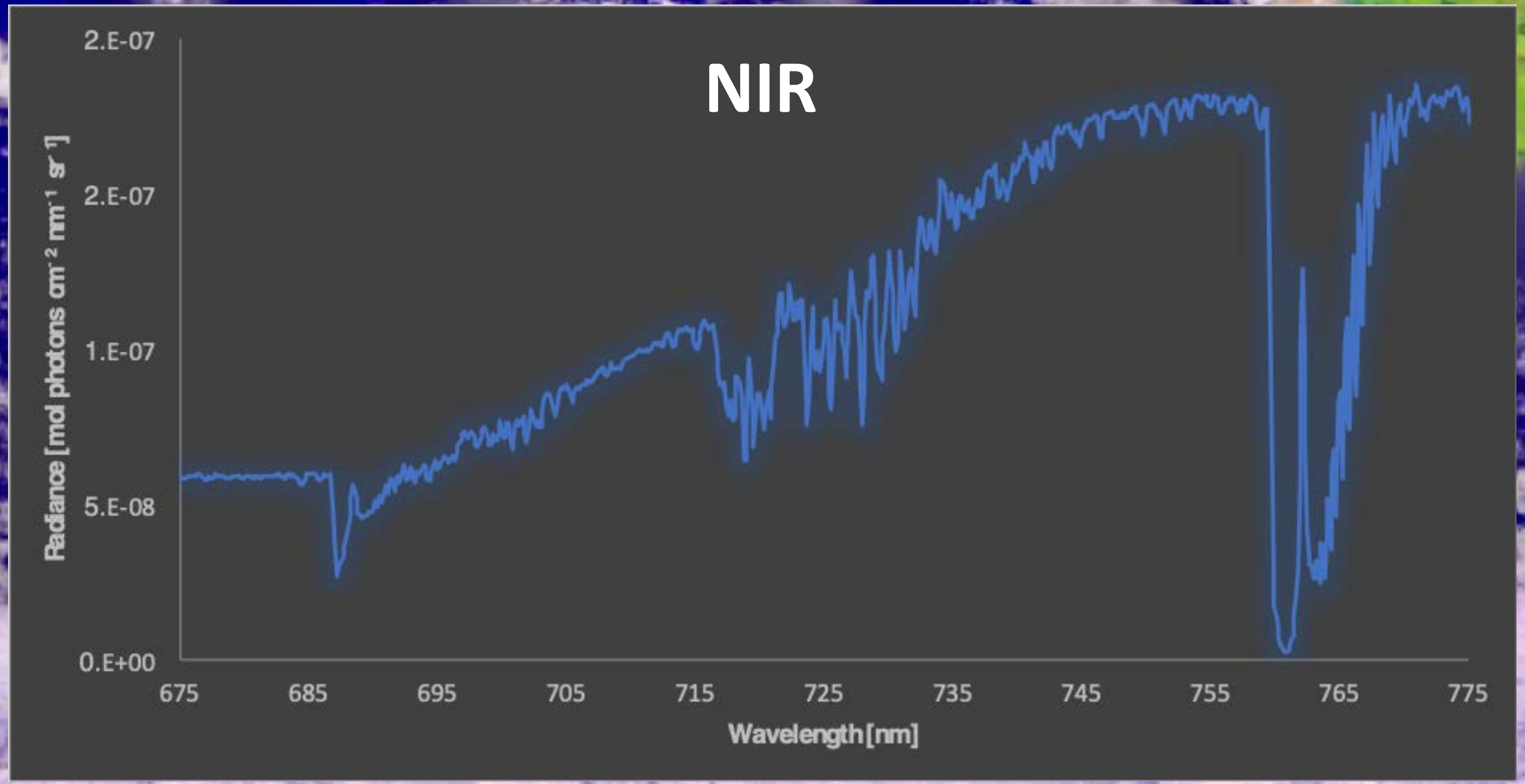
From spectra to concentrations

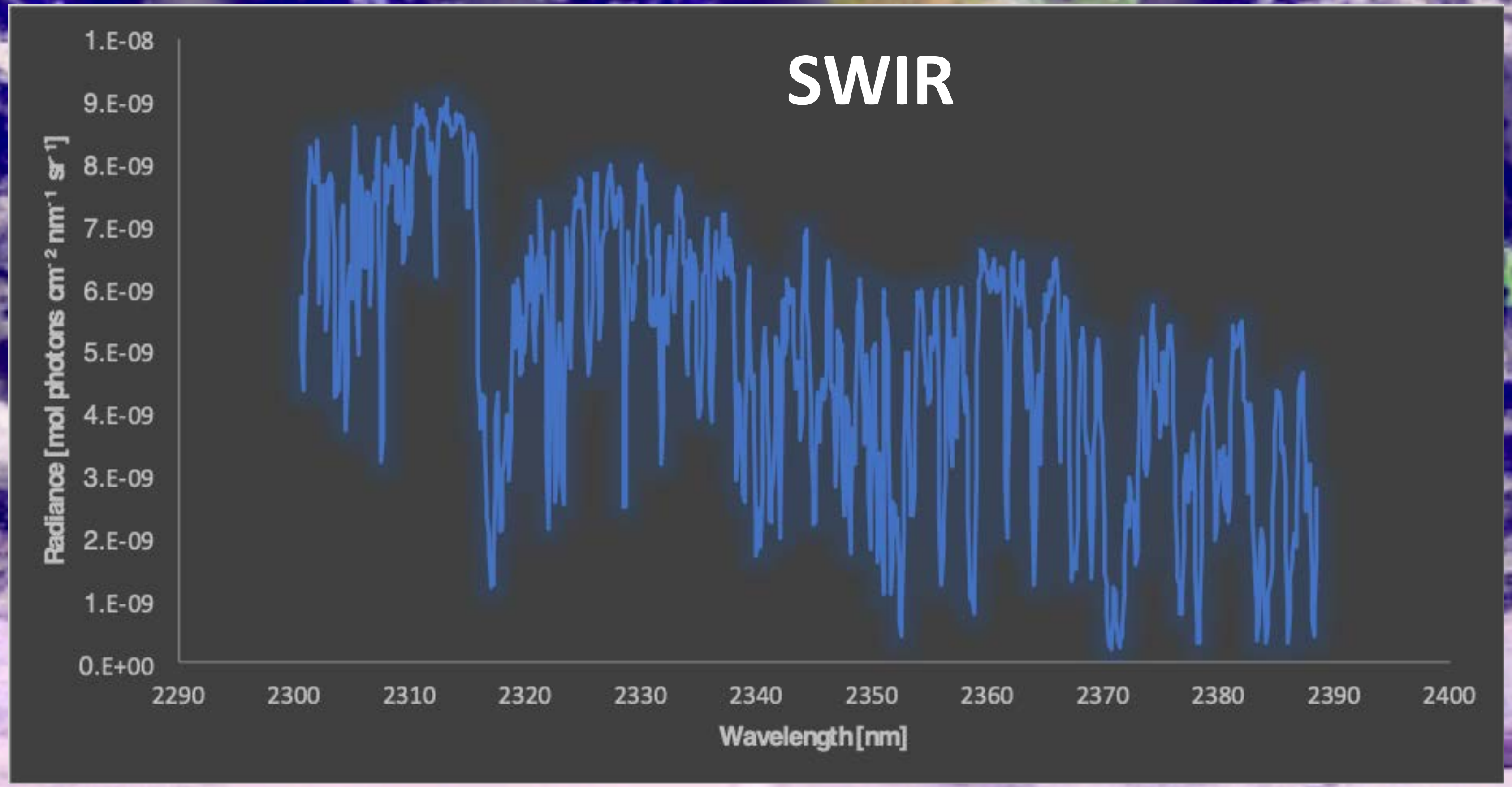






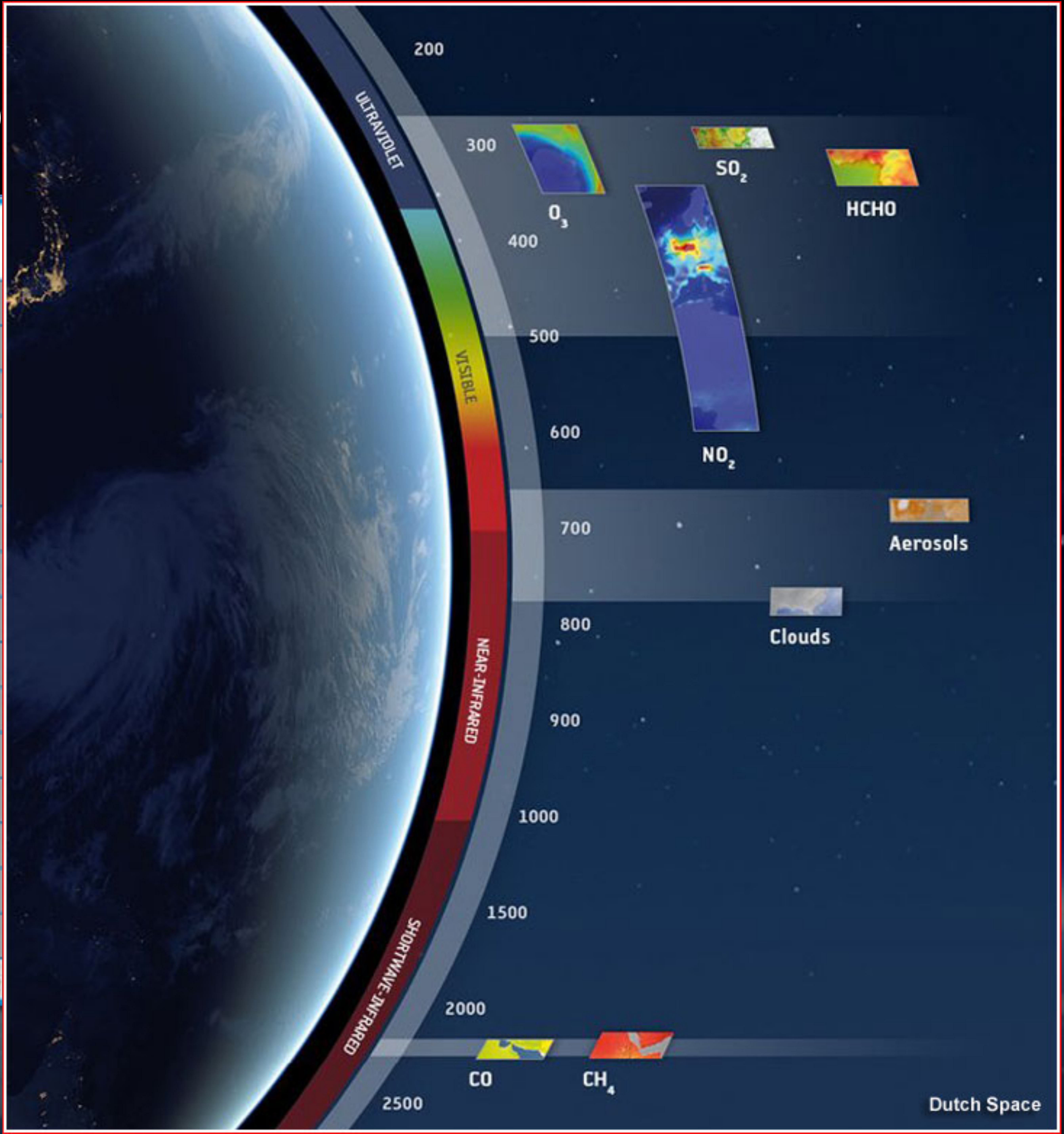
- 1 scanline per second
- 440 spectra per scanline
- 3000 scanlines per orbit
- 15 orbits per day
- 20 million groundpixels per day
- 225 Gbyte raw data per day
- 1 Tbyte L1b data per day





TROPOMI Level 2 Data Pro

Parameter	Data Product
Ozone	Ozone Profile
	Total Ozone
	Tropospheric Ozone
NO_2	Stratospheric NO_2
	Tropospheric NO_2
SO_2	SO_2 enhanced
	Total SO_2
Formaldehyde	Total HCHO
CO	Total CO
Methane	Total CH_4
Cloud	Cloud Fraction
	Albedo (Optical Thickness)
	Cloud Height (Pressure)
Aerosol	Aerosol Layer Height
	Aerosol Type
Surface UV	Provided by FMI in frame of the

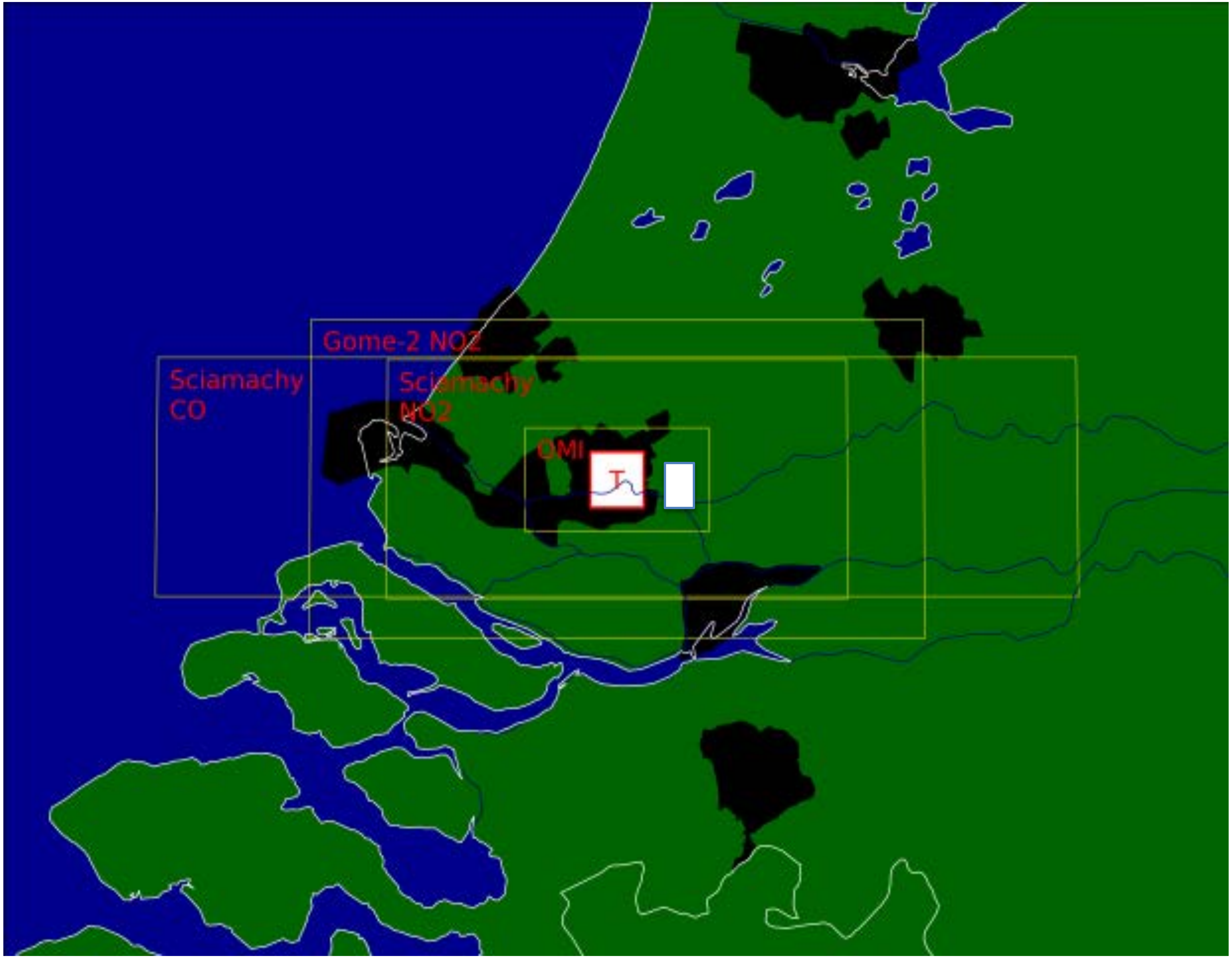


KNMI | DLR | BIRA-IASB | SRO

Spatial Resolution:

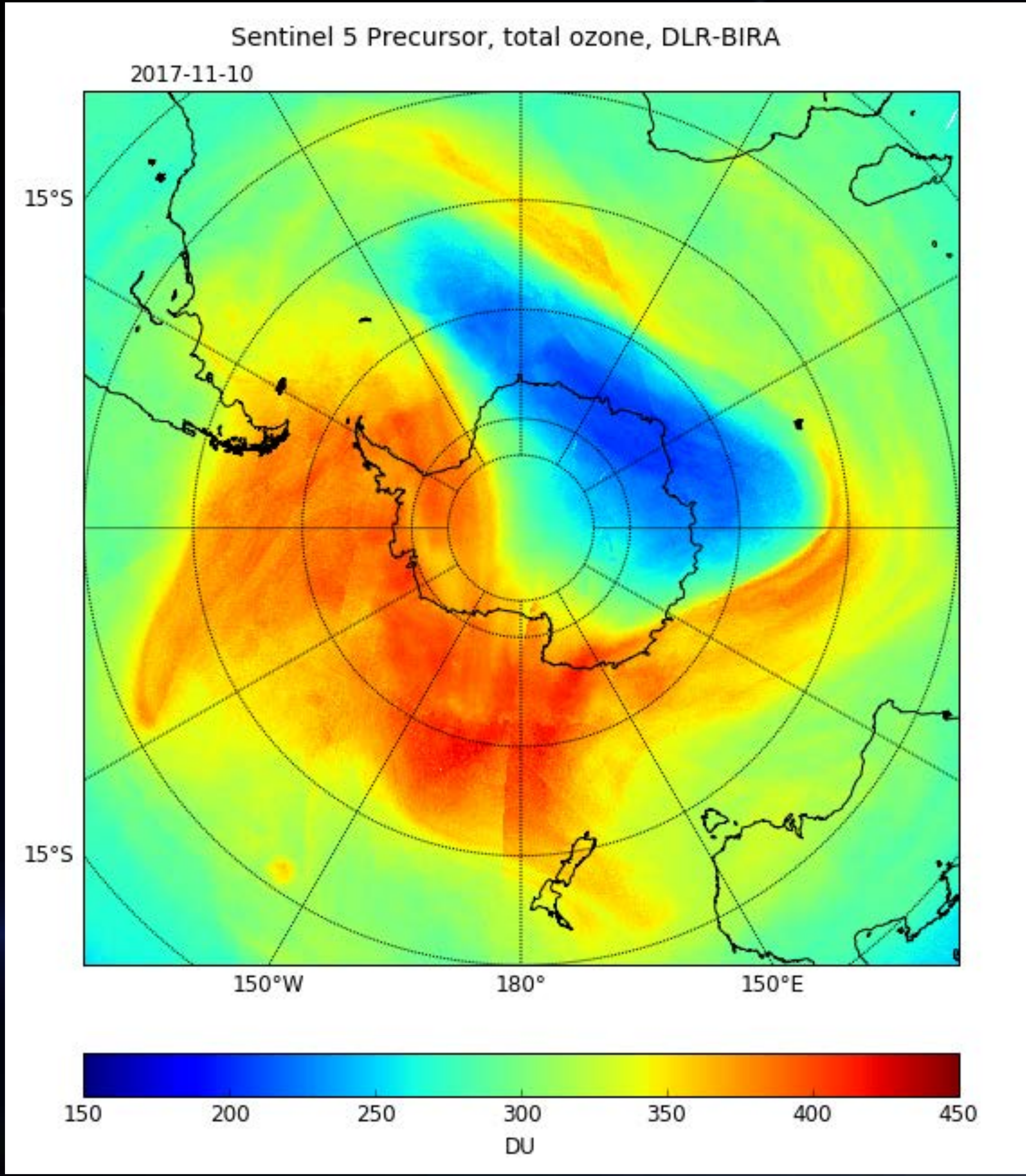
Further decreased to 3.5 x 5.5 km in August 2019

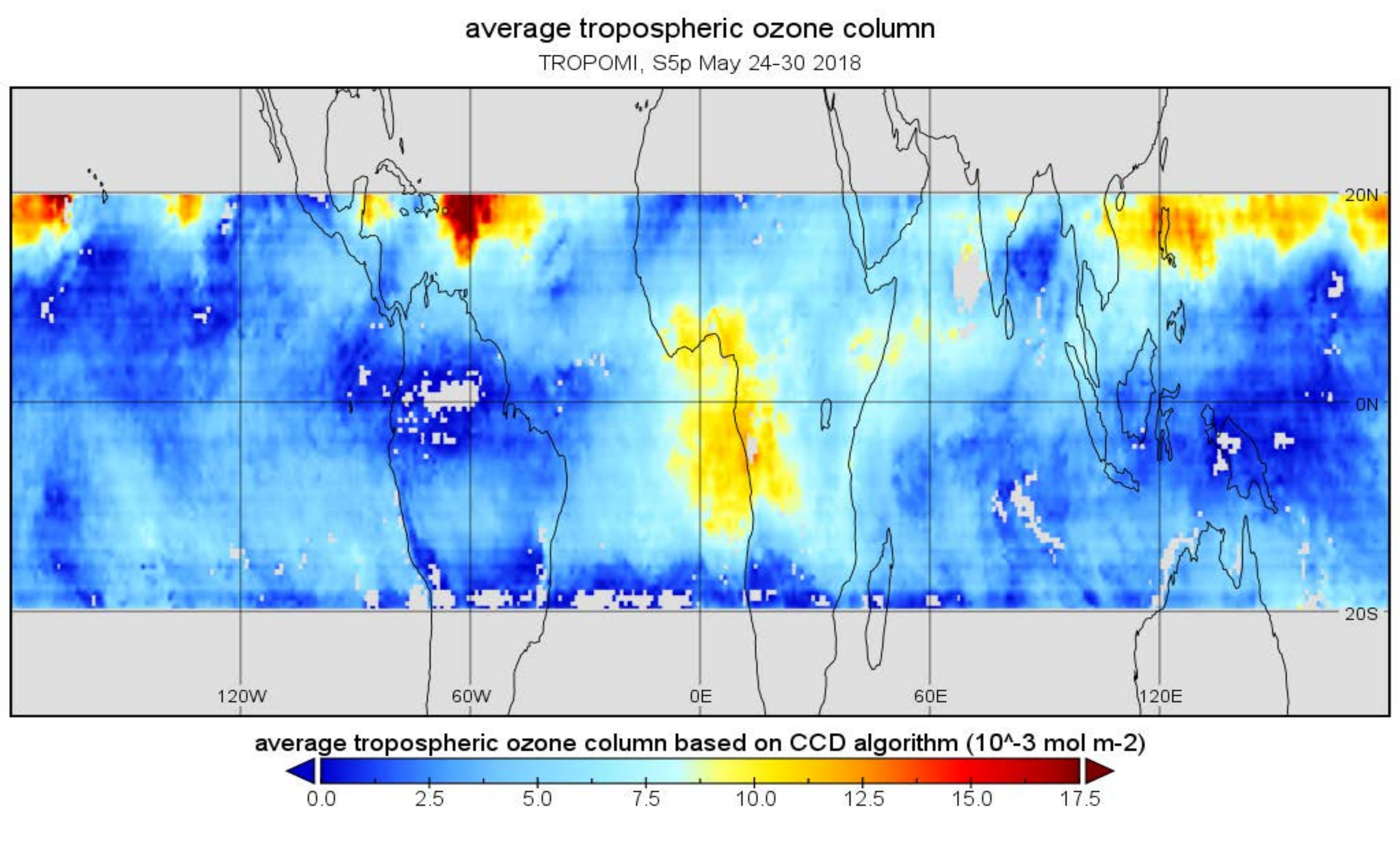
Individual source Identification, Intra-city variability



John Douros (KNMI)

TROPOMI Ozone data products: stratosphere & troposphere

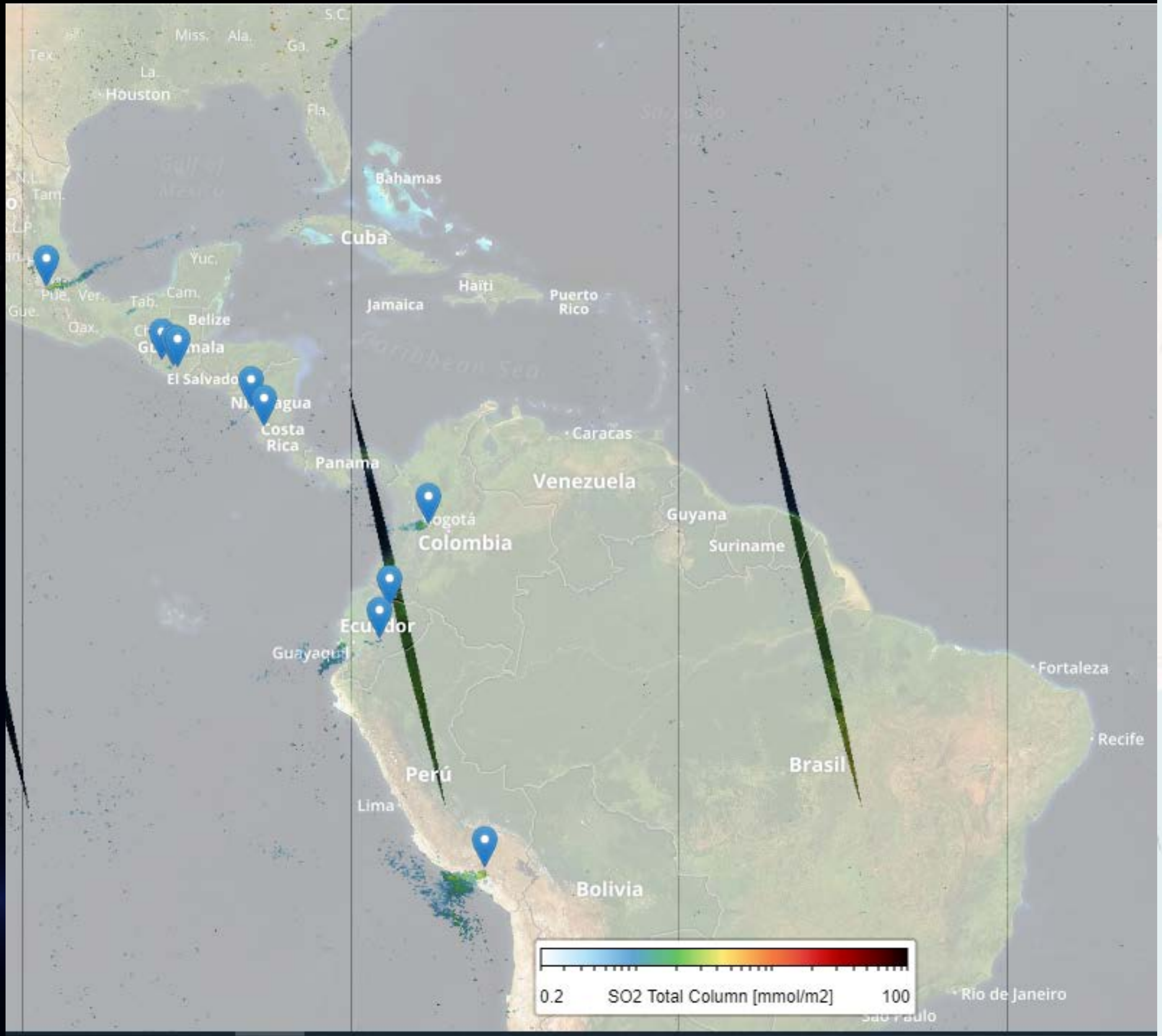




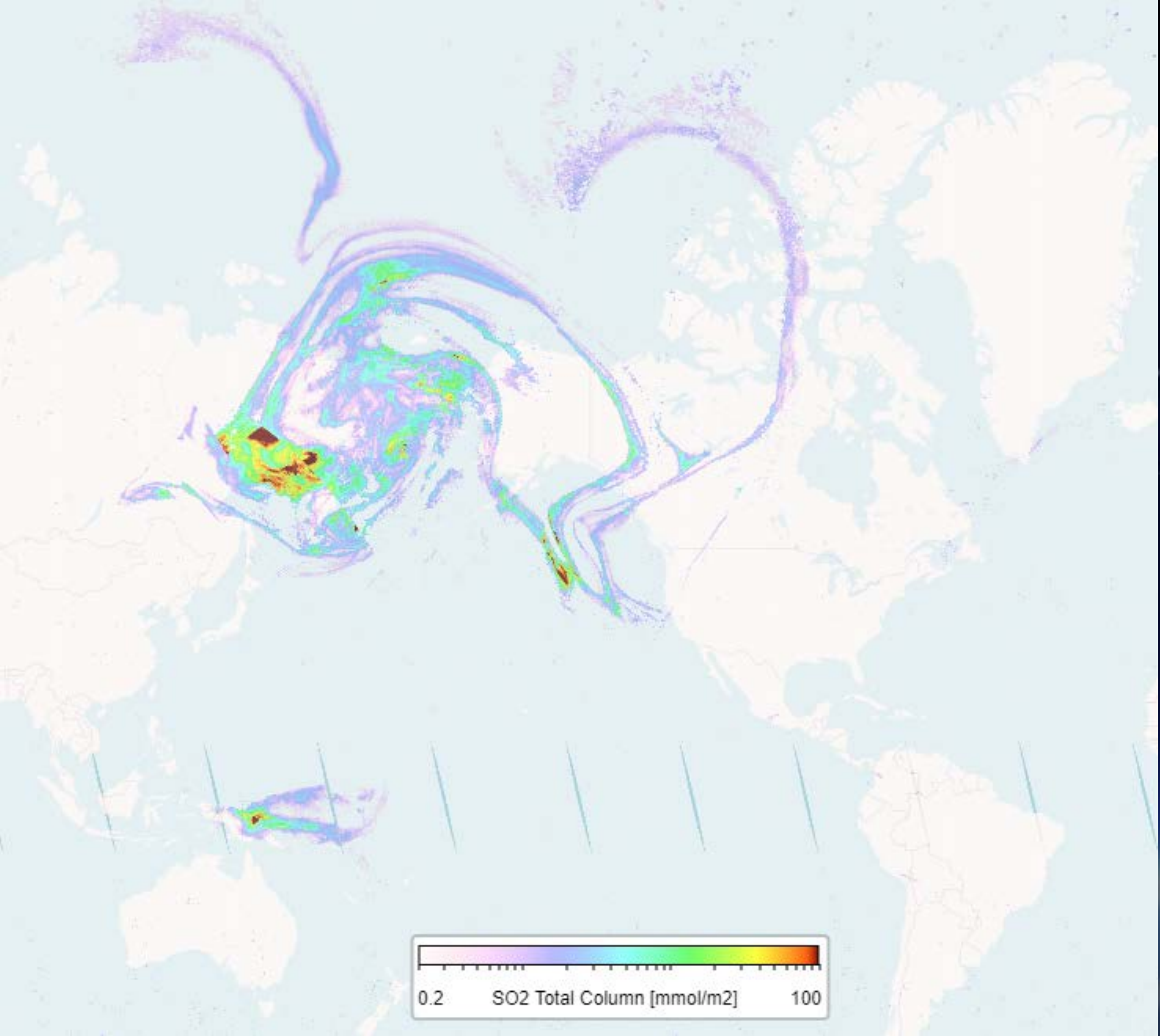
Carbon Monoxide

13 January 2020: Bushfire Smoke Transport to South America

Sulfur Dioxide (SO2): 2019 Volcanic Emissions, Small & Large sources

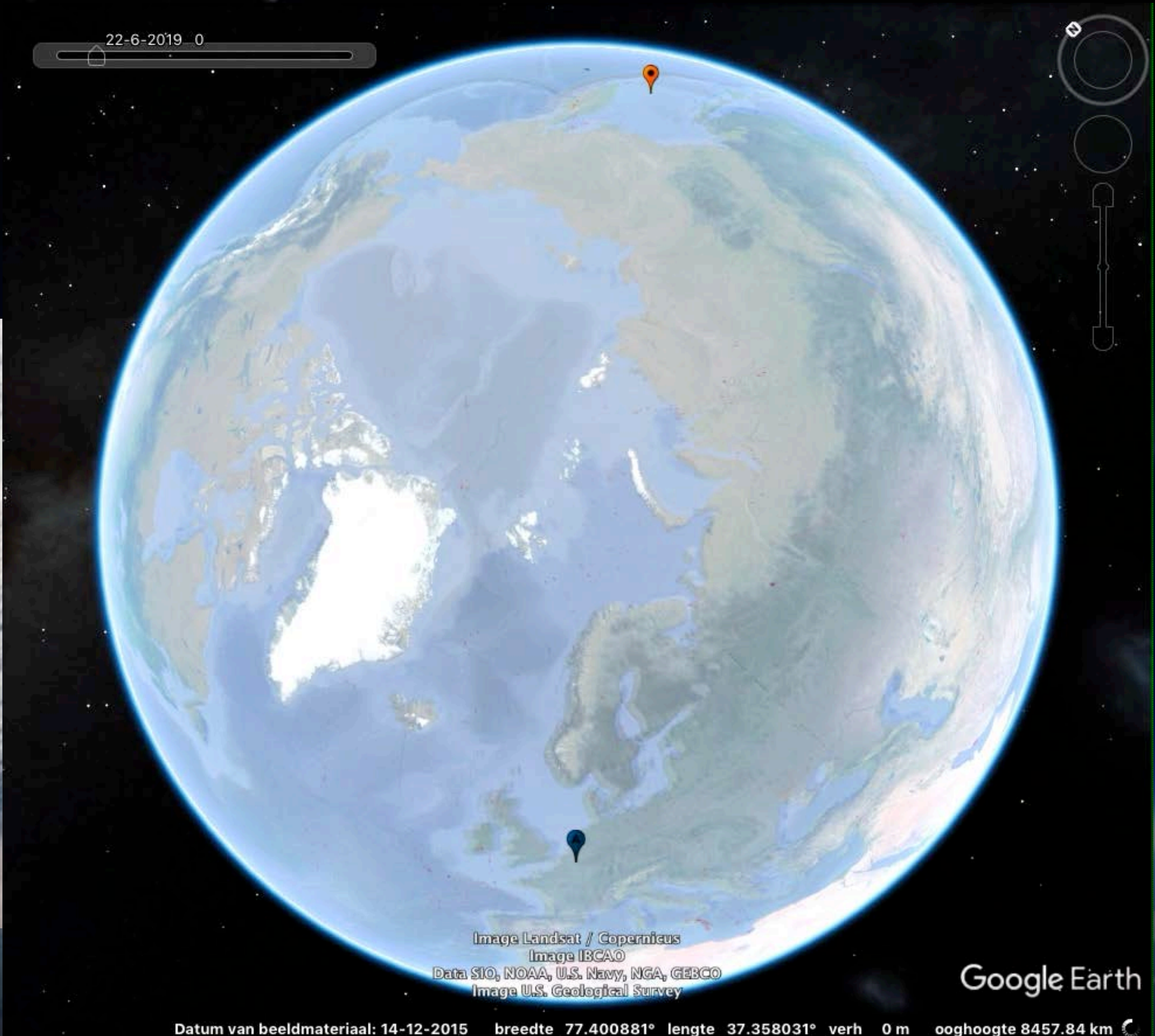


Popocatepetl & Sabancava, 19 Dec 2019



Raikoke 28 June 2019

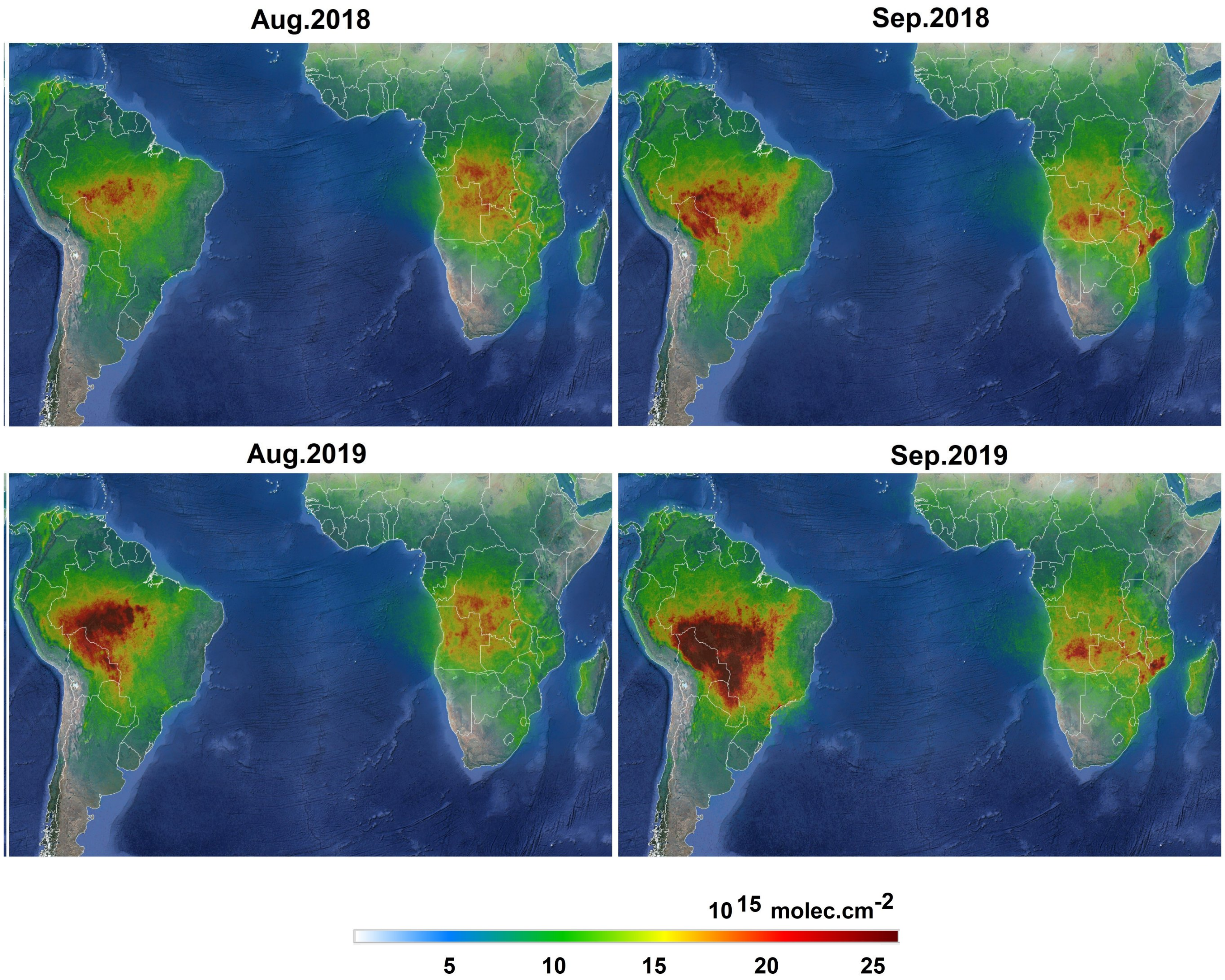
Raikoke Volcano
SO_2 in the stratosphere observed by TROPOMI



Formaldehyde:

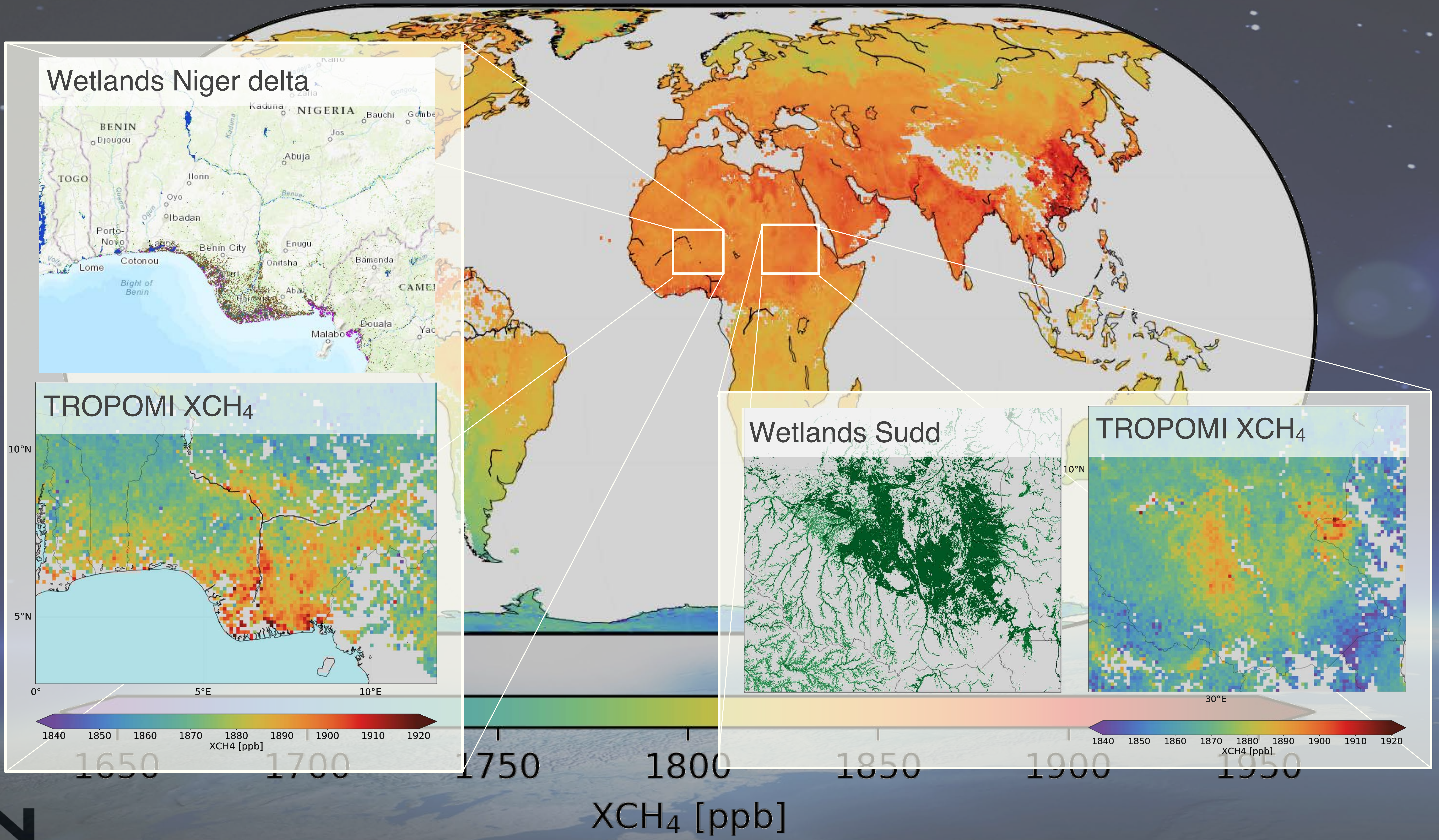
Temperature-dependent emission

Primarily Biogenic & Combustion sources



Isabelle De Smedt
BIRA-IASB

Methane (CH4): Wetland emission seen by TROPOMI



TROPOMI

SRON

Aerosol & Cloud: Key for correcting trace gas retrievals

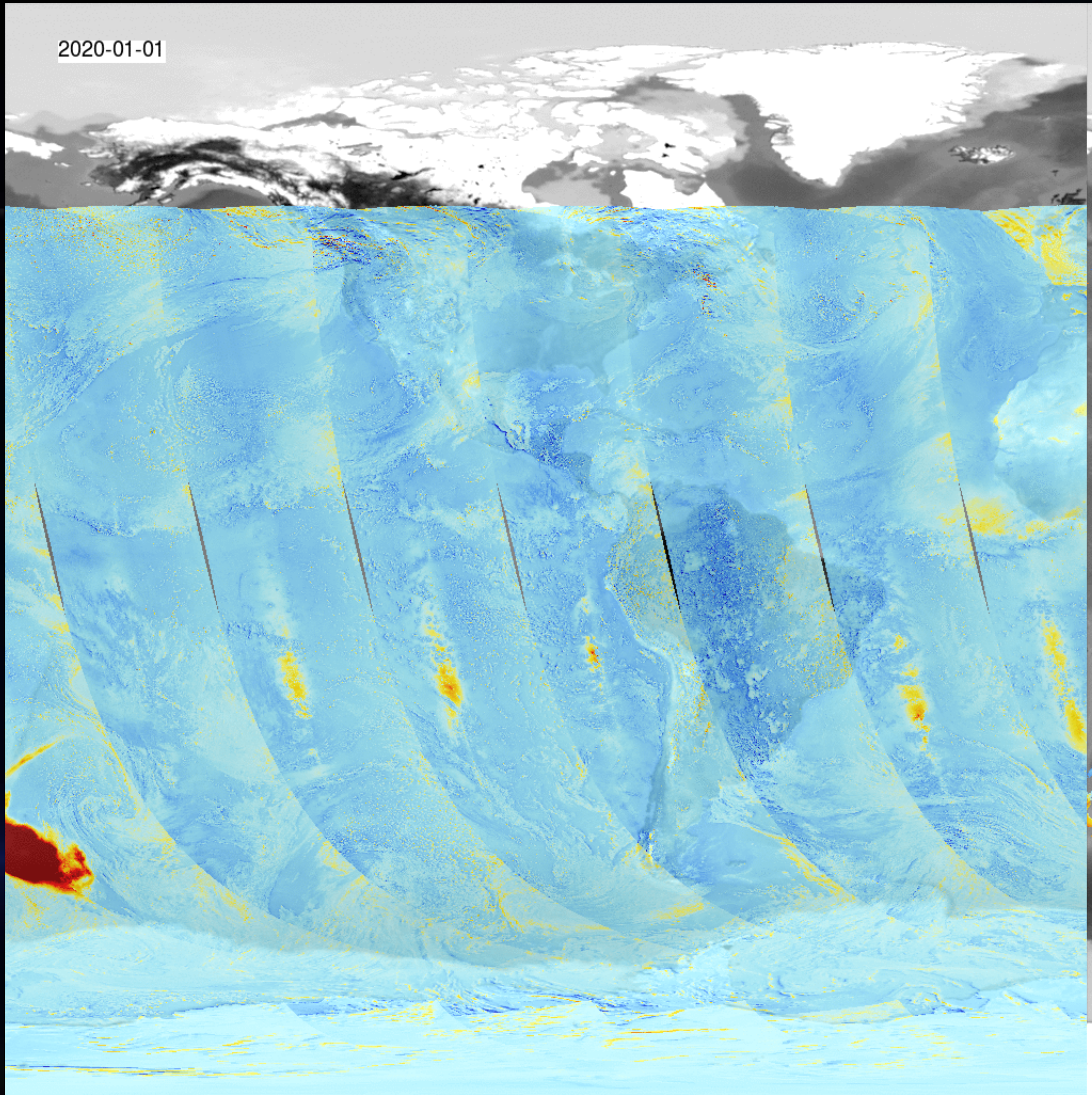
NO2 tropospheric column, cloud filtered
01 Octob

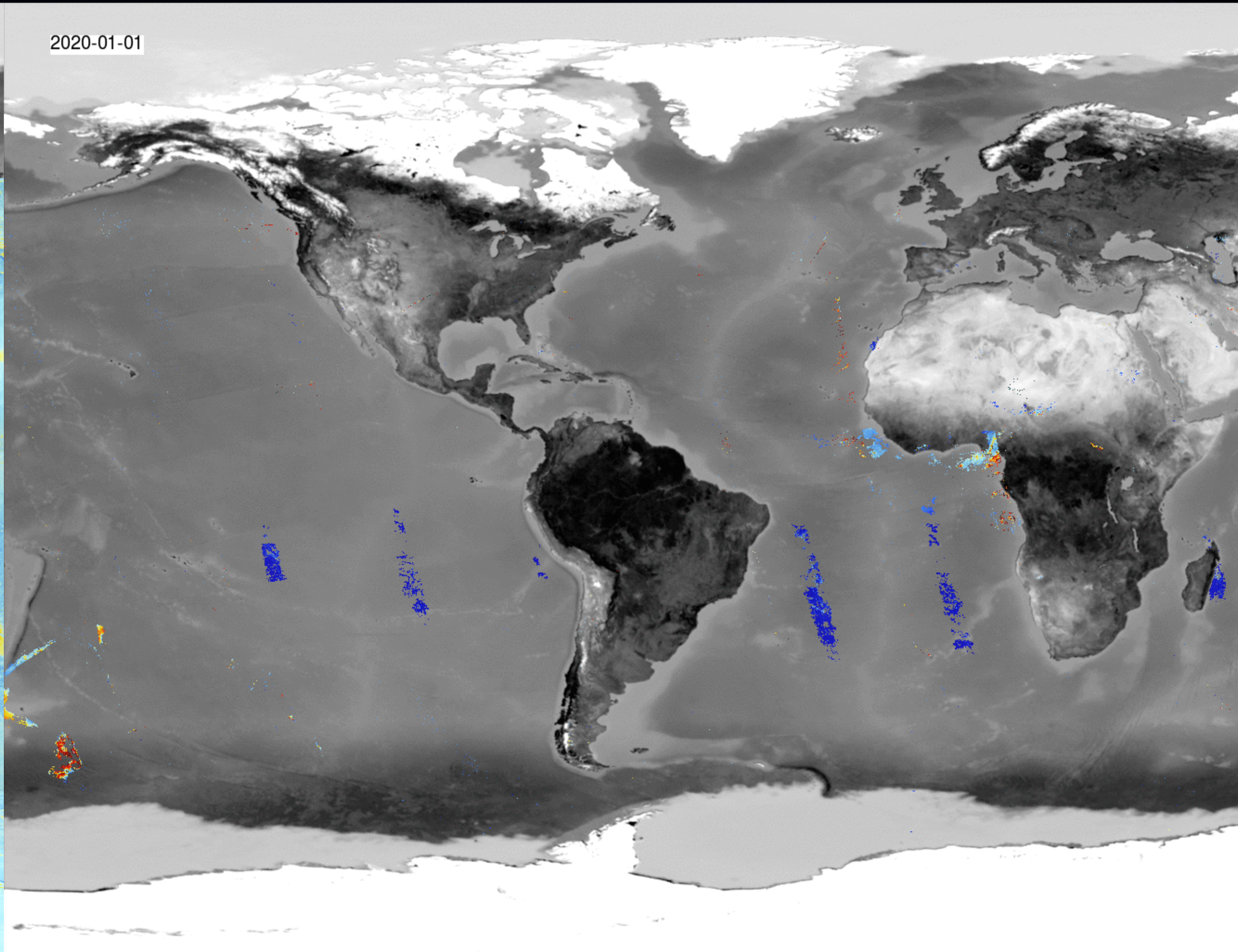
Cloud Fraction & Cloud Height

Aerosol Index used to filter out thick smoke in CO, 7 Jan 2020

Plume Tracking: Aerosol Index and Aerosol Layer Height

TROPOMI

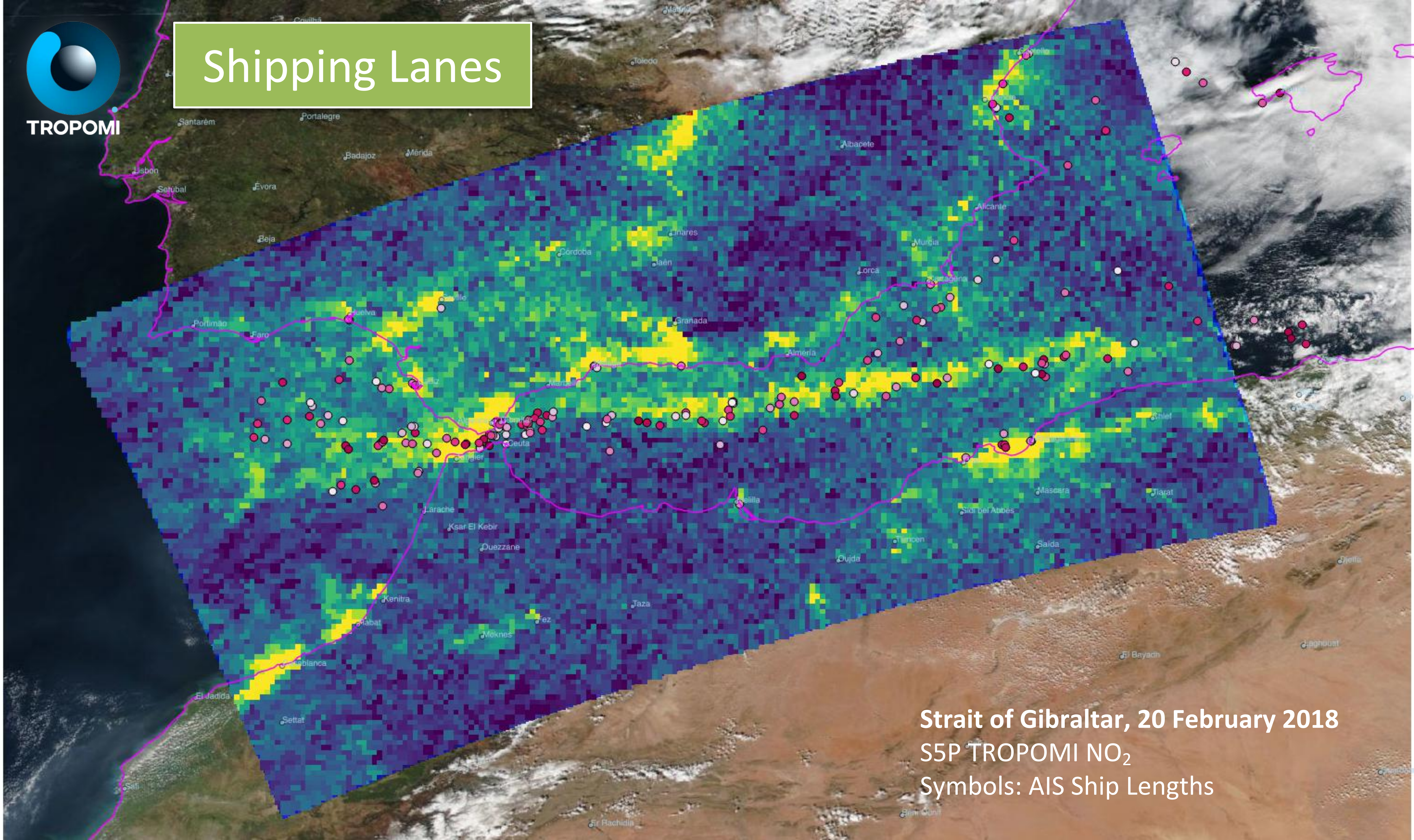





Oil & Gas
Activity
Biomass
Burning
Coal-fired
Power Plants
Shipping Lanes
S5P NO2
April 2018 - Maart 2019

TROPOMI

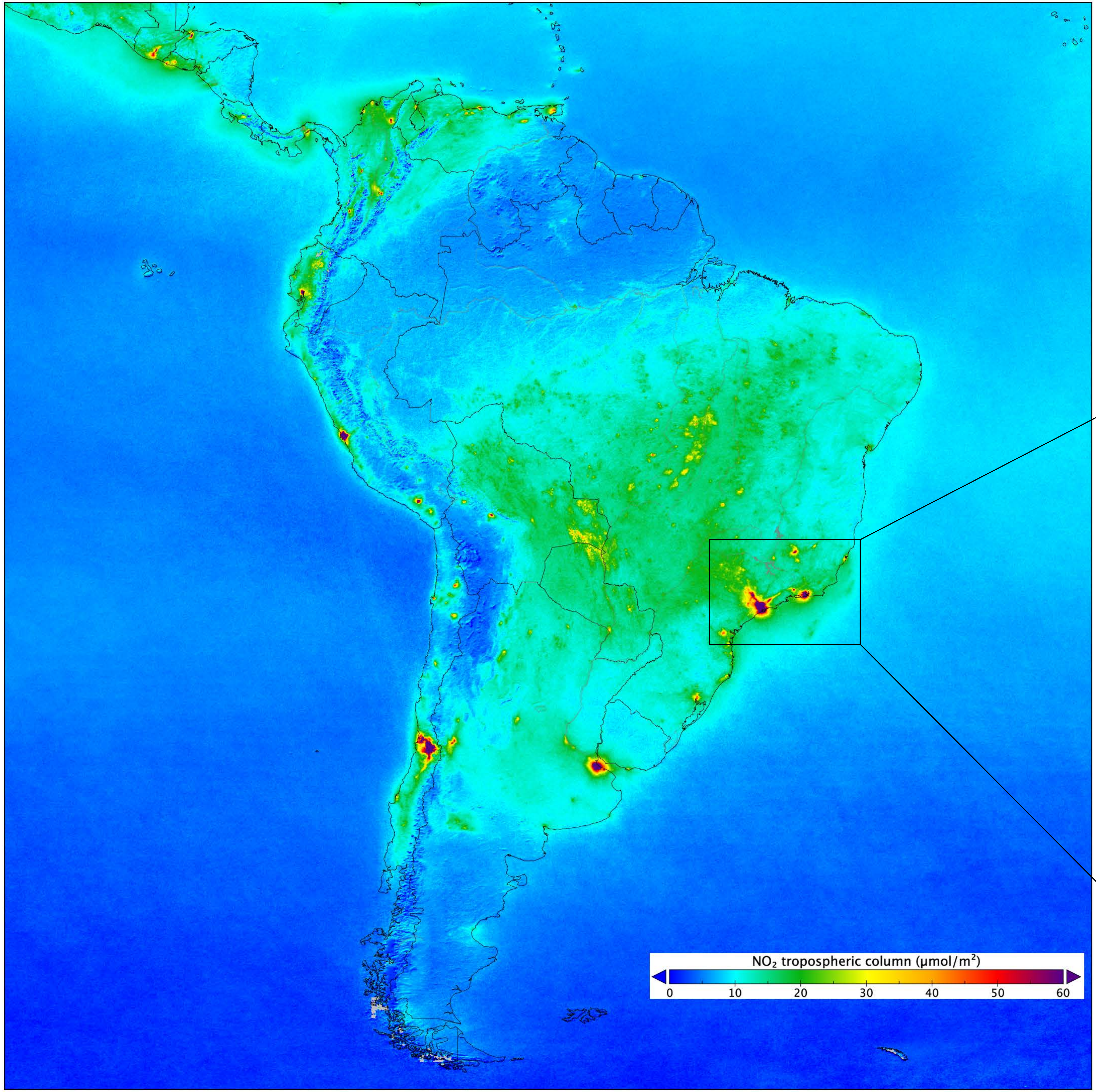
Shipping Lanes

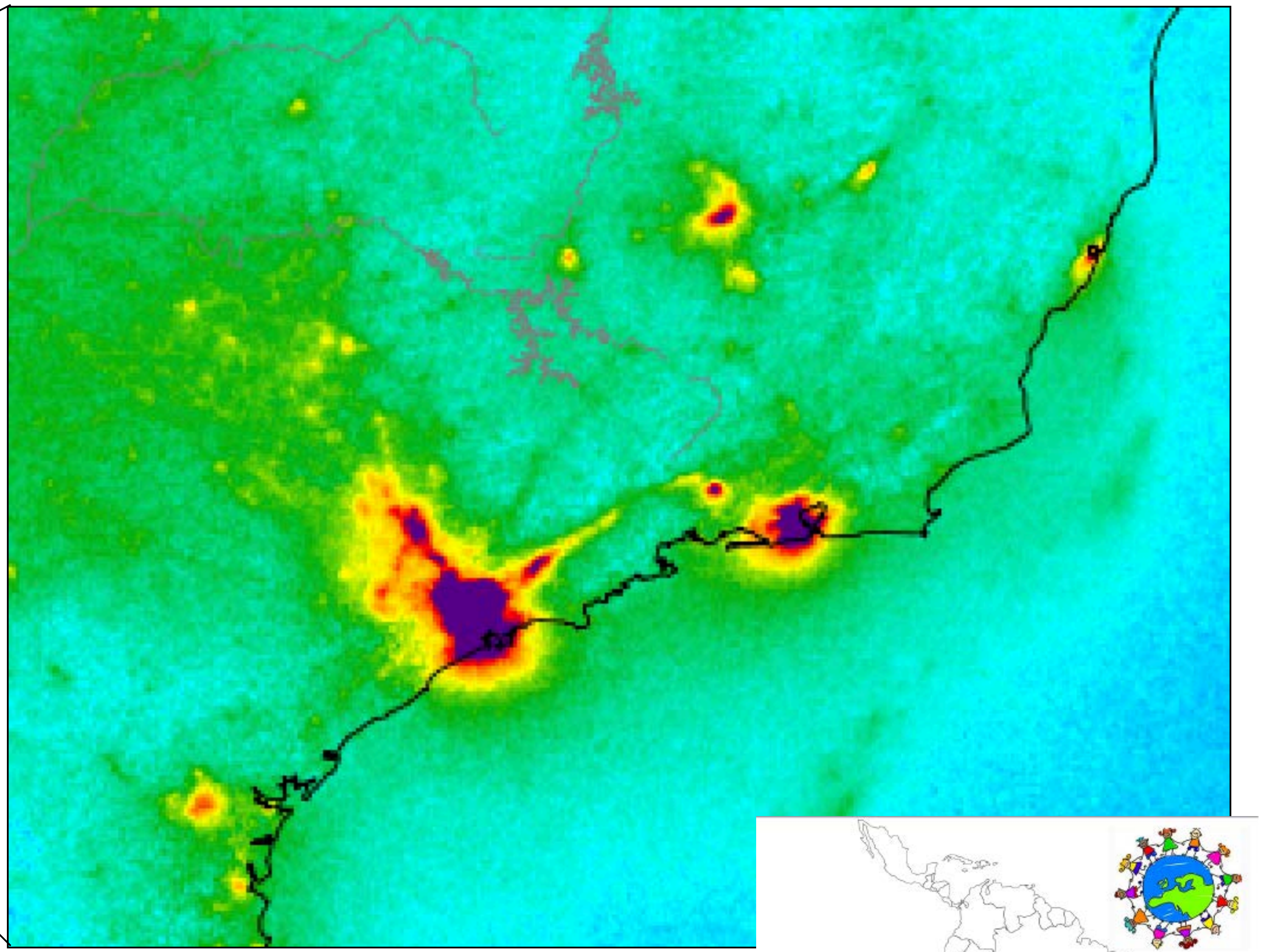


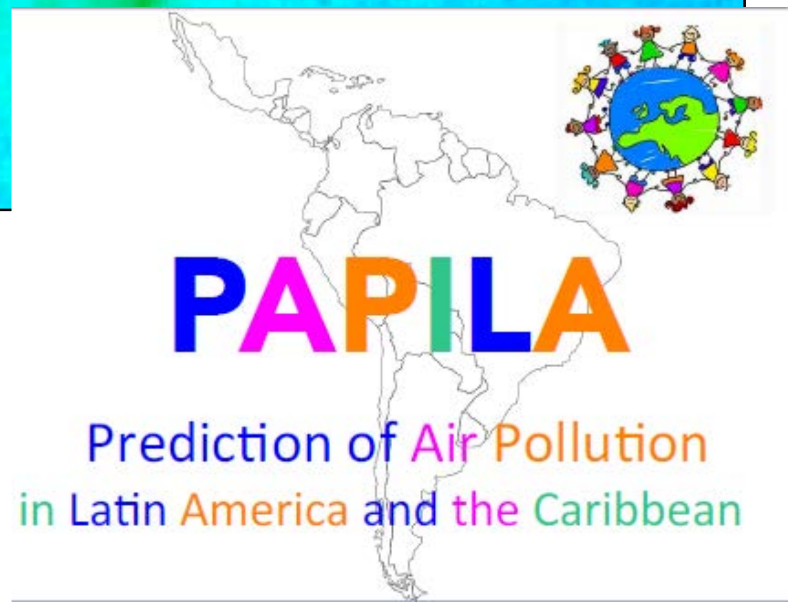
Strait of Gibraltar, 20 February 2018
S5P TROPOMI NO_2
Symbols: AIS Ship Lengths

Sentinel-5P TROPOMI
NO_2 tropospheric column

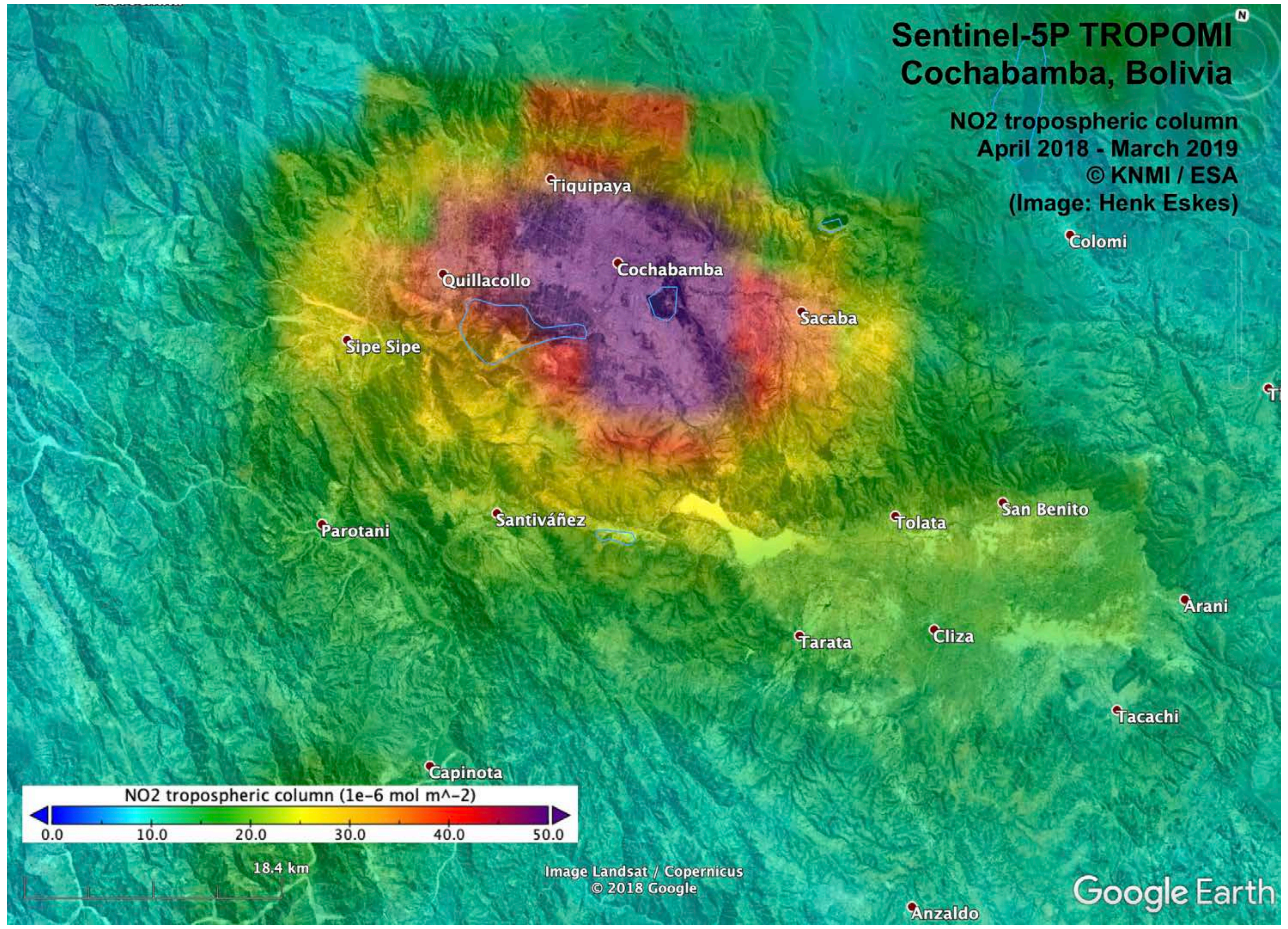
Annual Average 2019



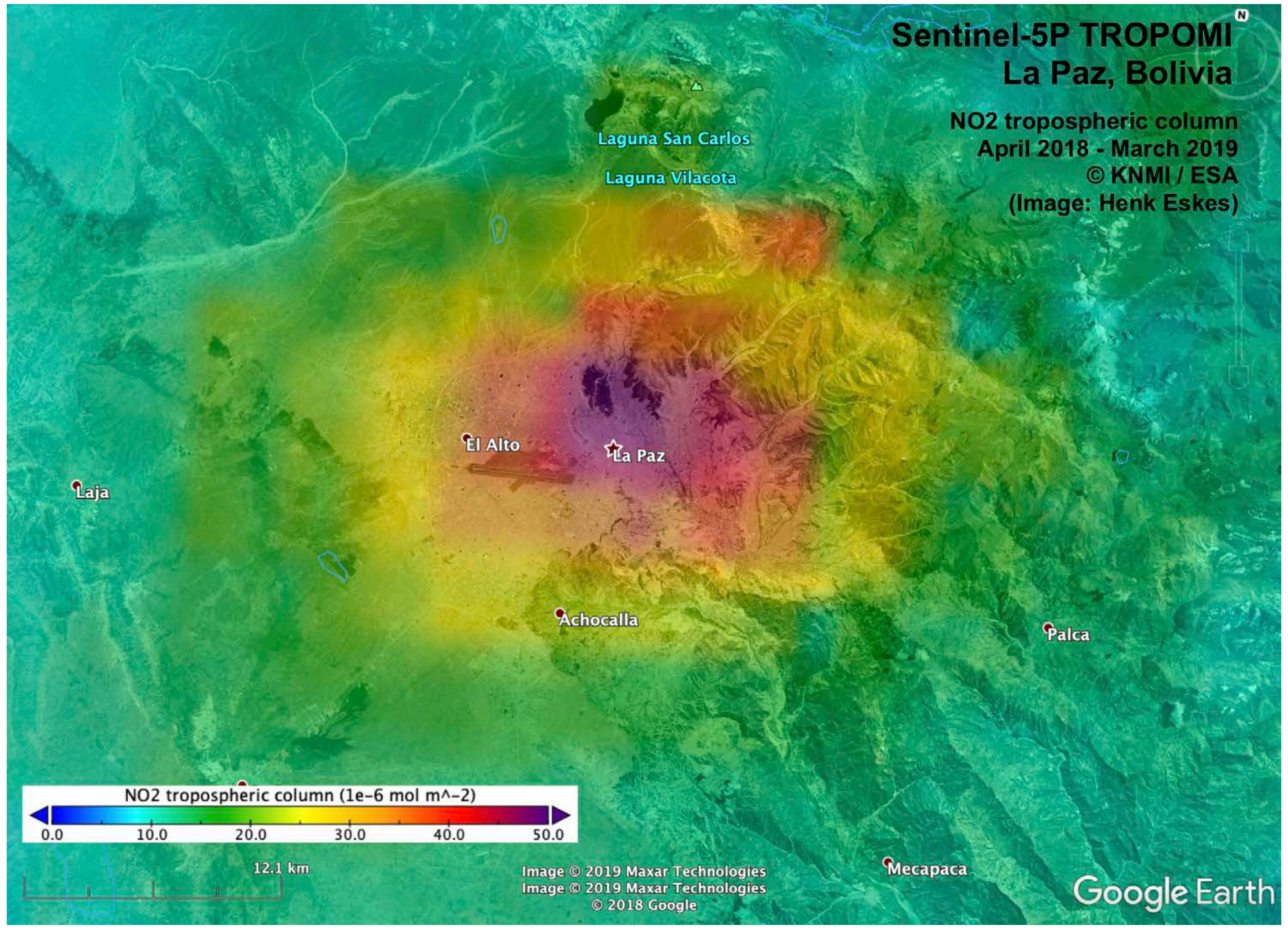




Zoom images of NO_2: City footprints, Annual average

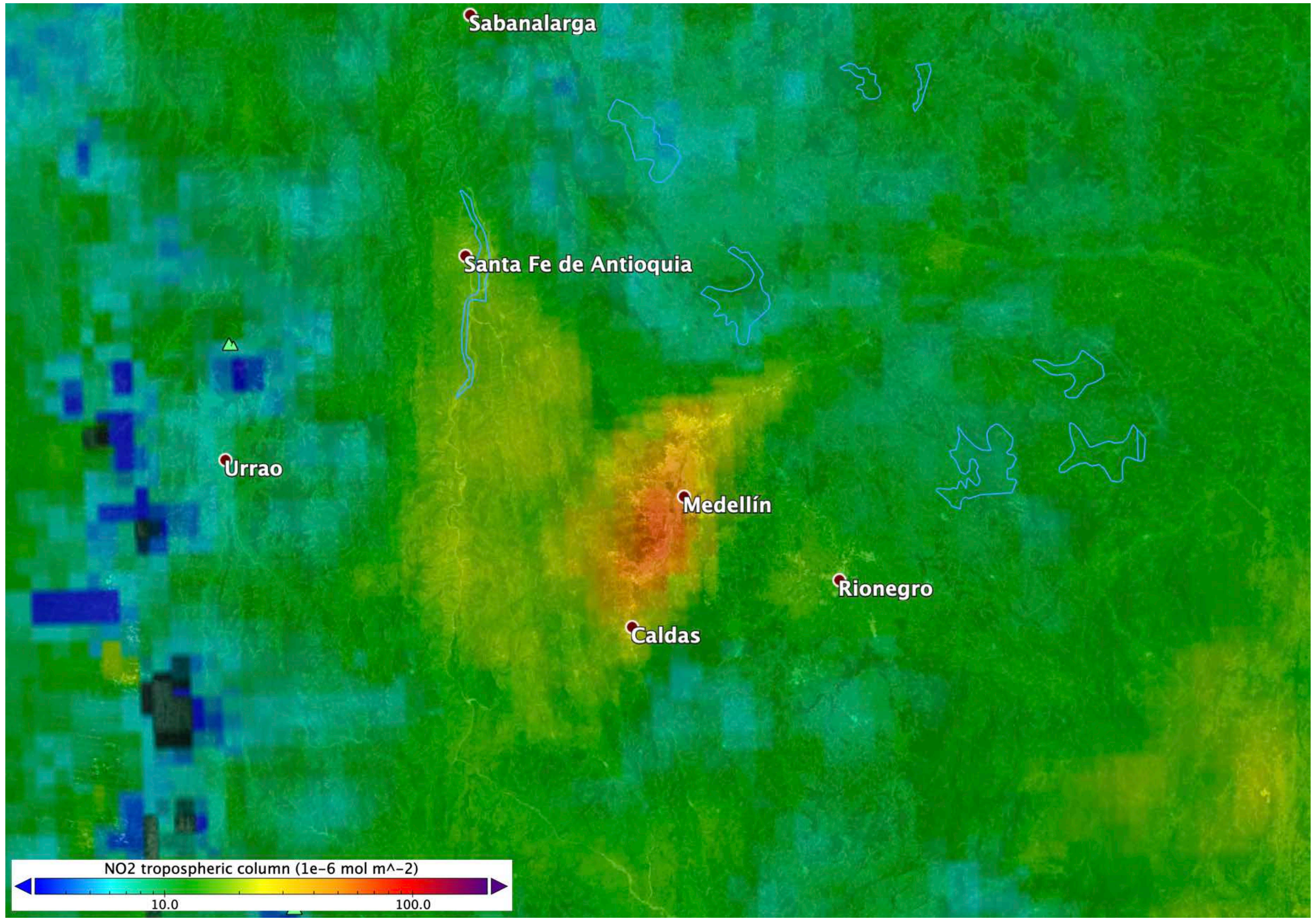


Cochabamba, Bolivia

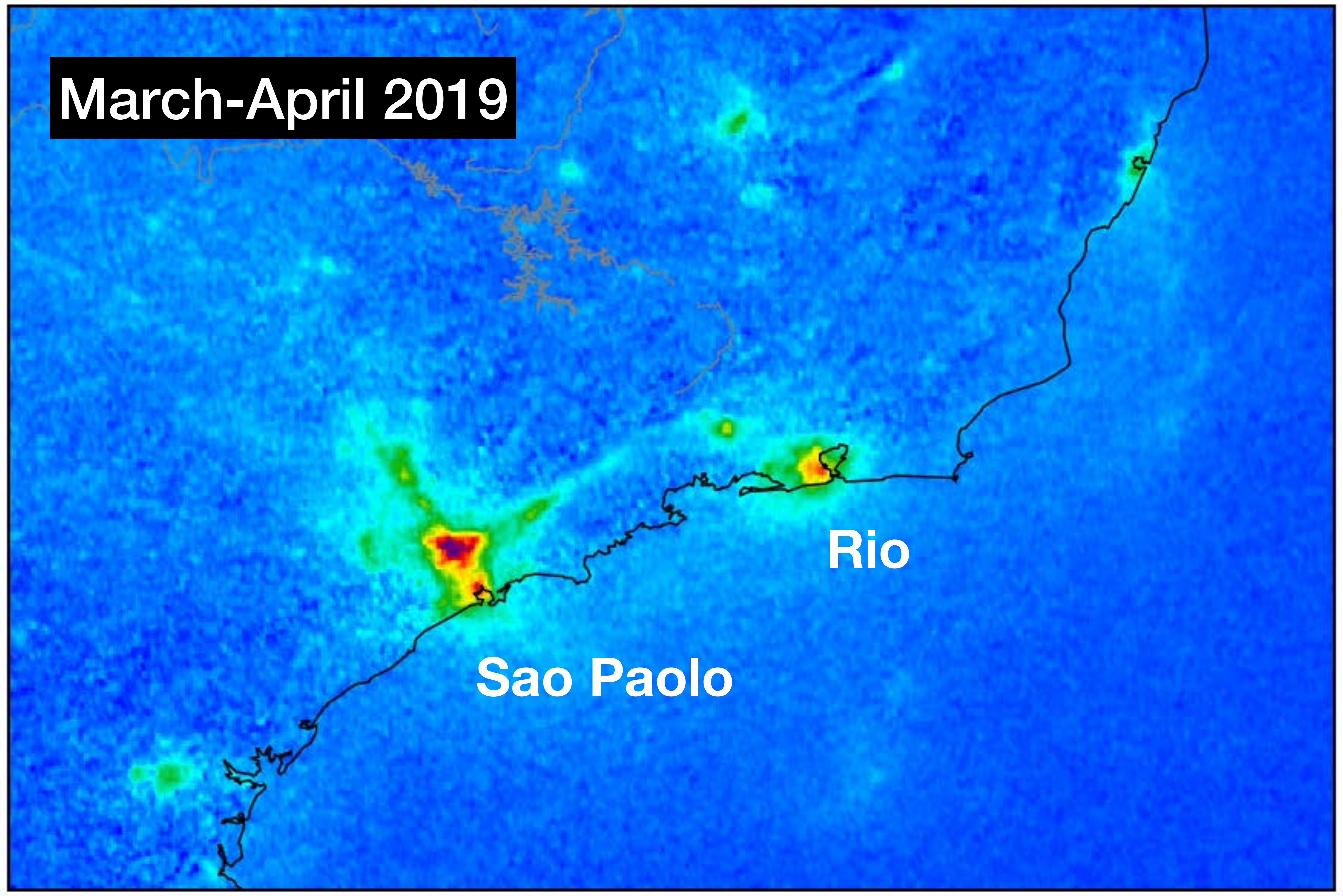


La Paz, Bolivia

Medellin, Colombia



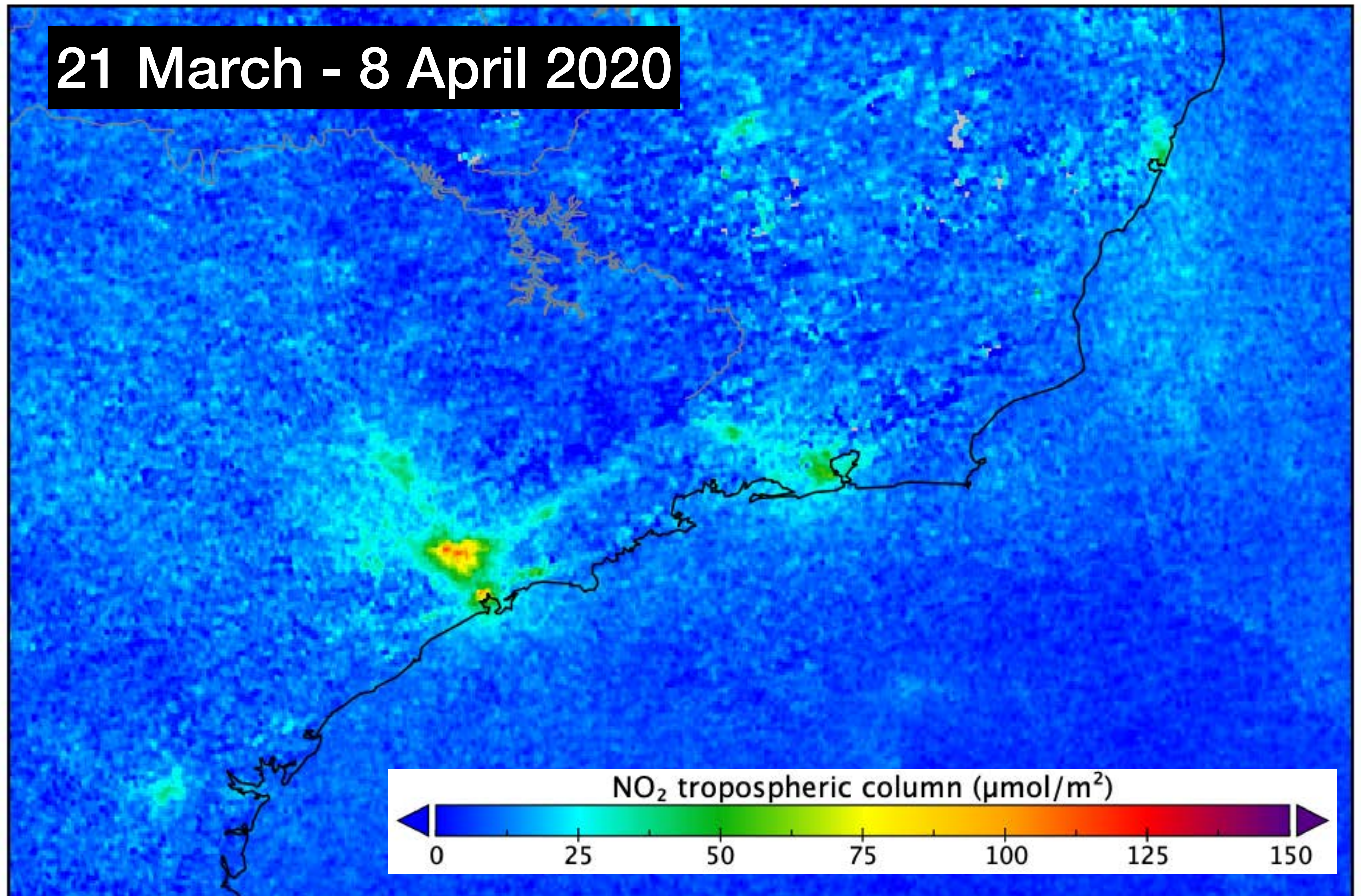
Reduction in NO2 in Brazil related to Covid-19 measures

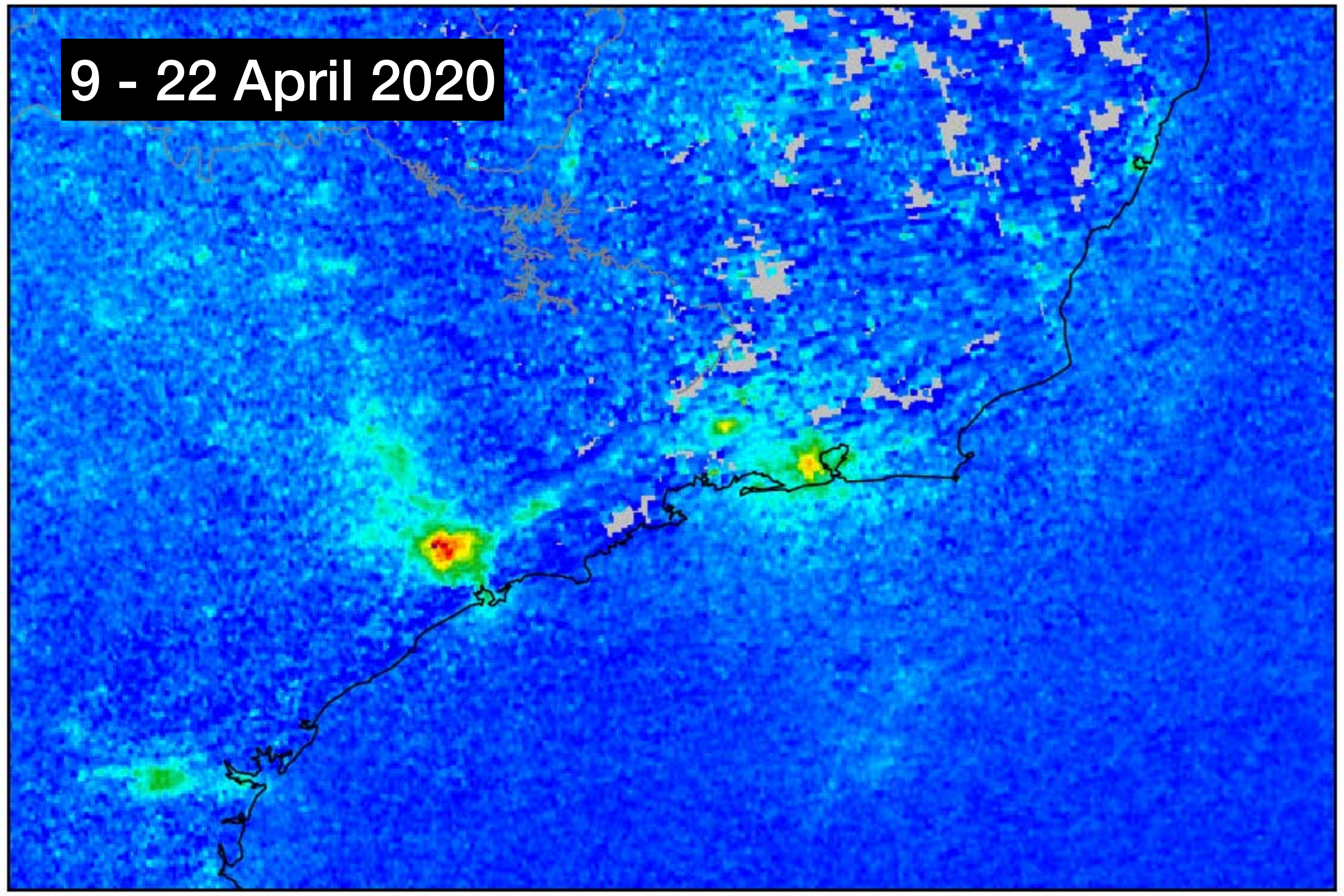


2019

First weeks after lockdown

The two weeks after that:
Indication of increasing emissions.
Traffic?






Wavelength
viewing
CCD detector

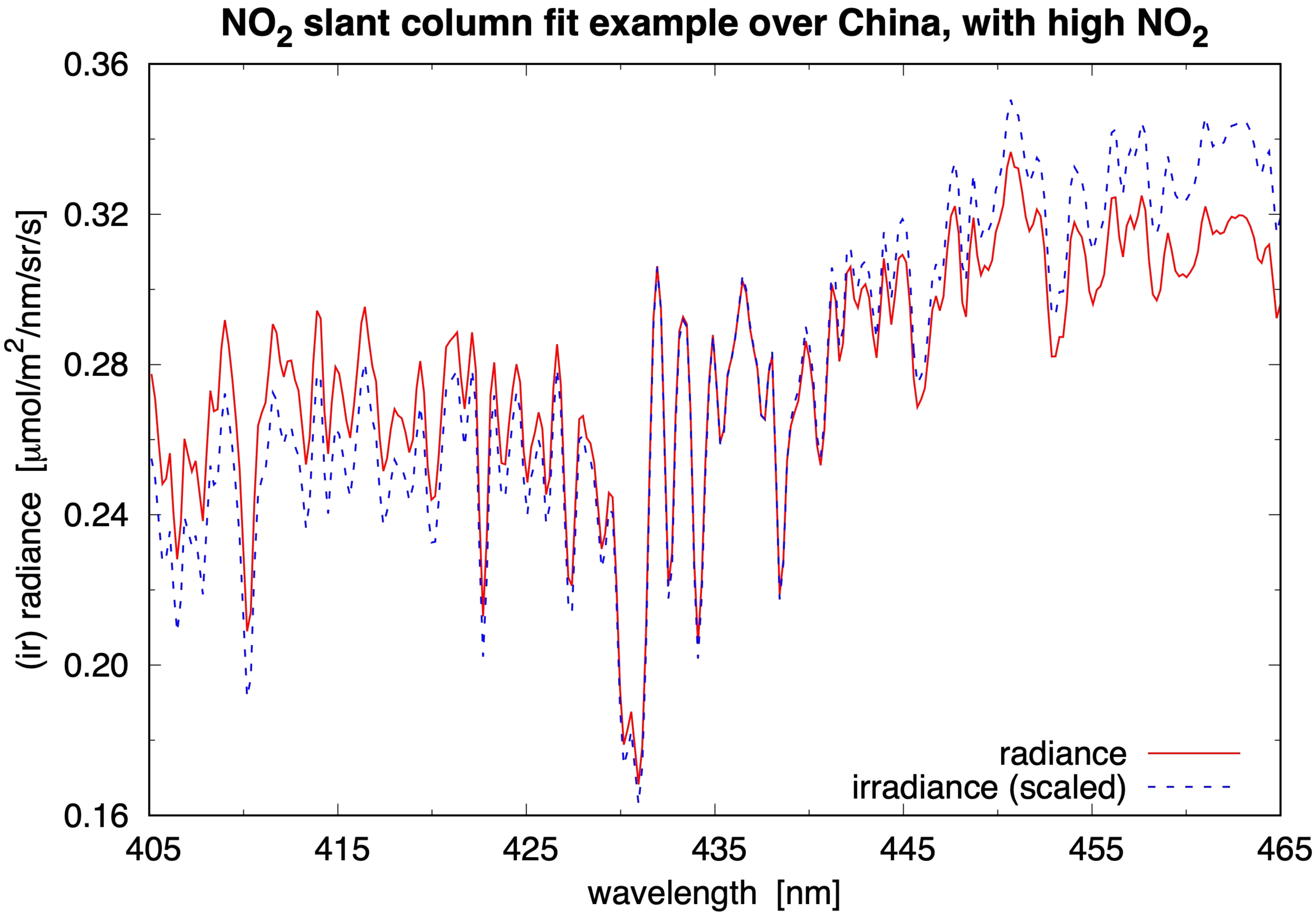
Spectral observations in the wavelength range for NO_2

TROPOMI observations

405-465 spectral range

When looking at the Earth the main spectral features observed are in the solar spectrum

Jos van Geffen, KNMI



Comparison of Reflectance: ‘Clean’ Pacific vs. Urban Paris

TROPOMI observations

405-465 spectral range

Reflectance is a

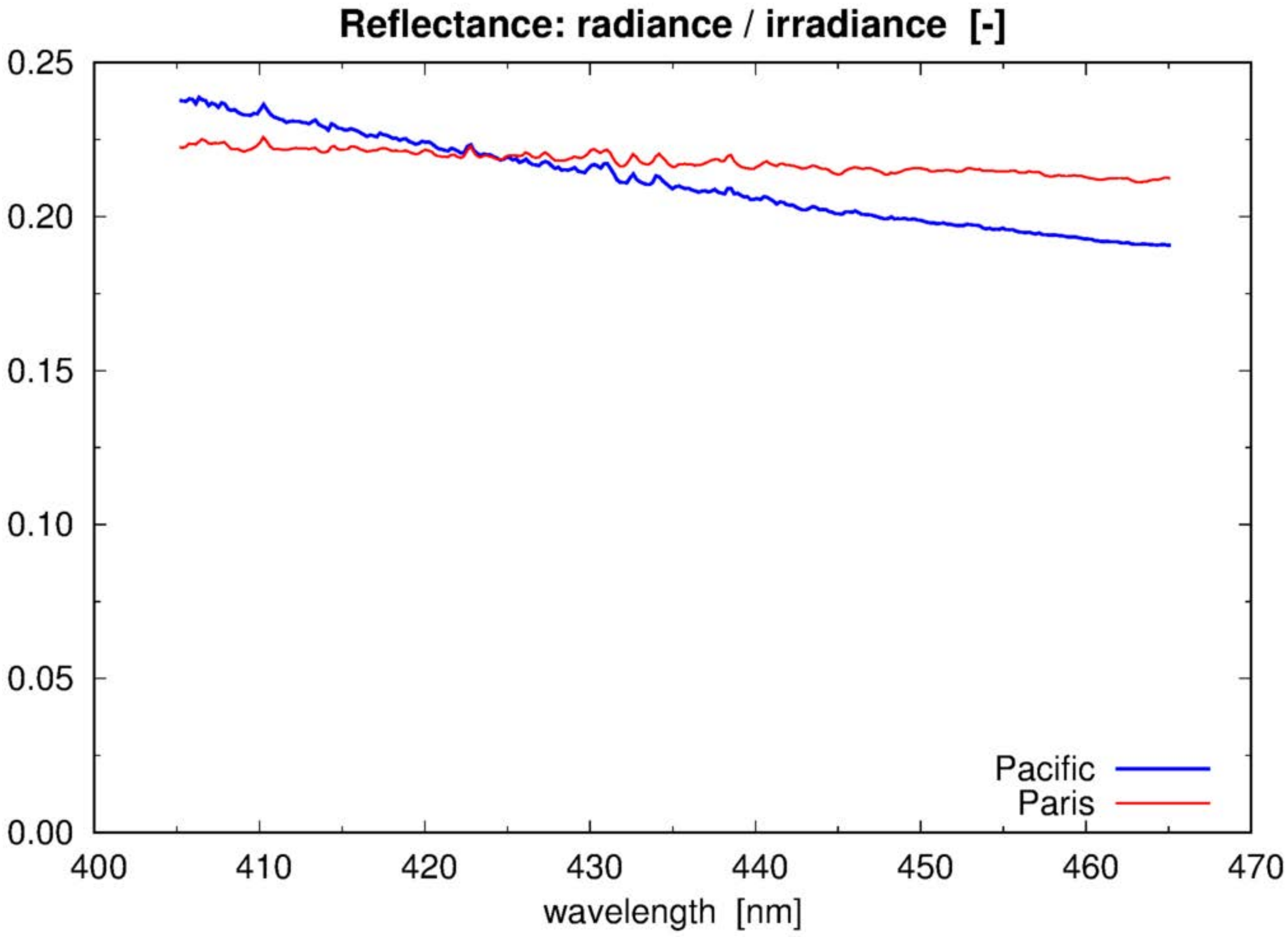
“nearly” straight line

Note:

NO2 concentration

typically 1 molecule per

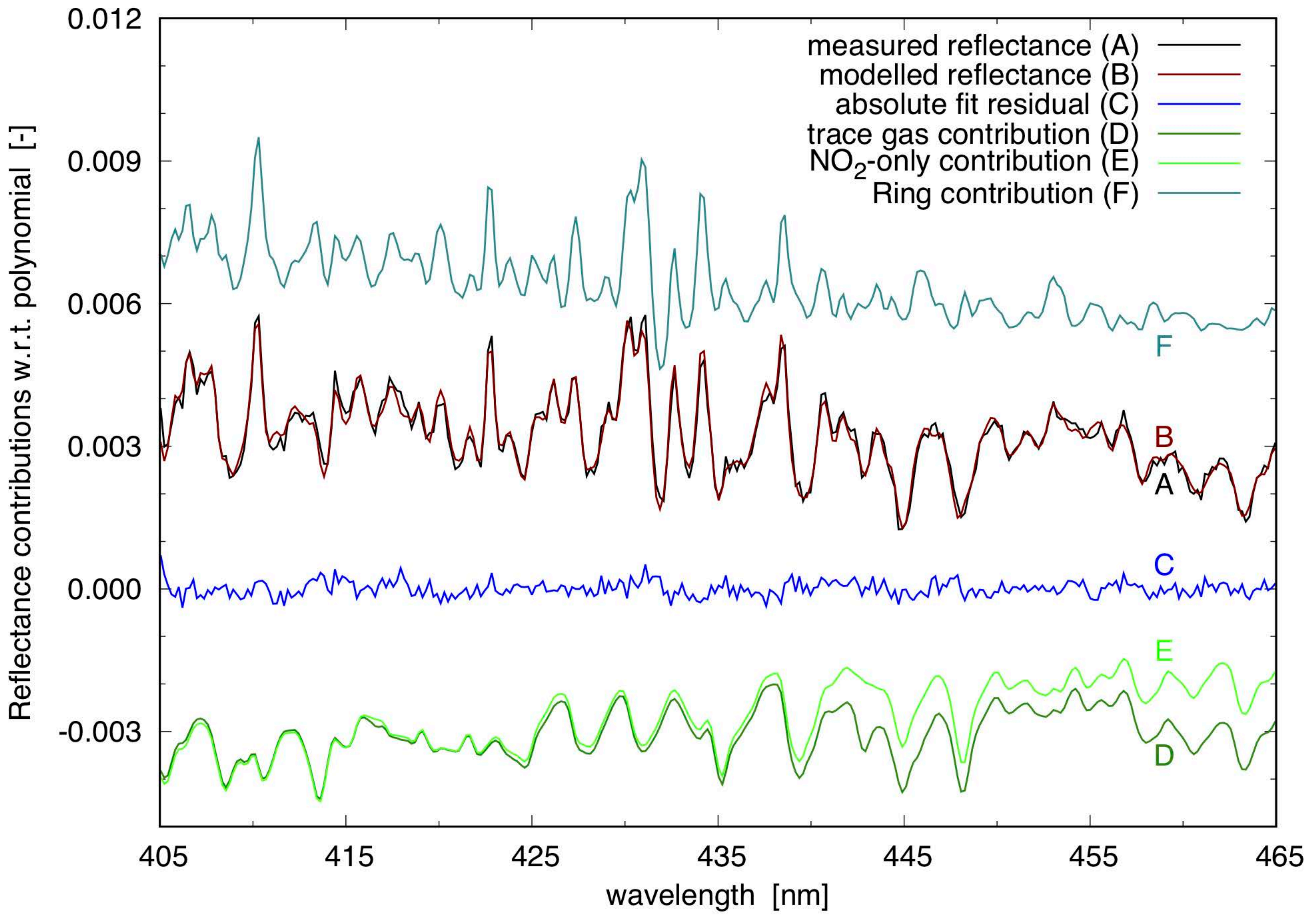
10^9 air molecules



Reflectance: Separating NO_2 contribution from other spectral features

Also in the reflectance the solar spectral features are still dominant

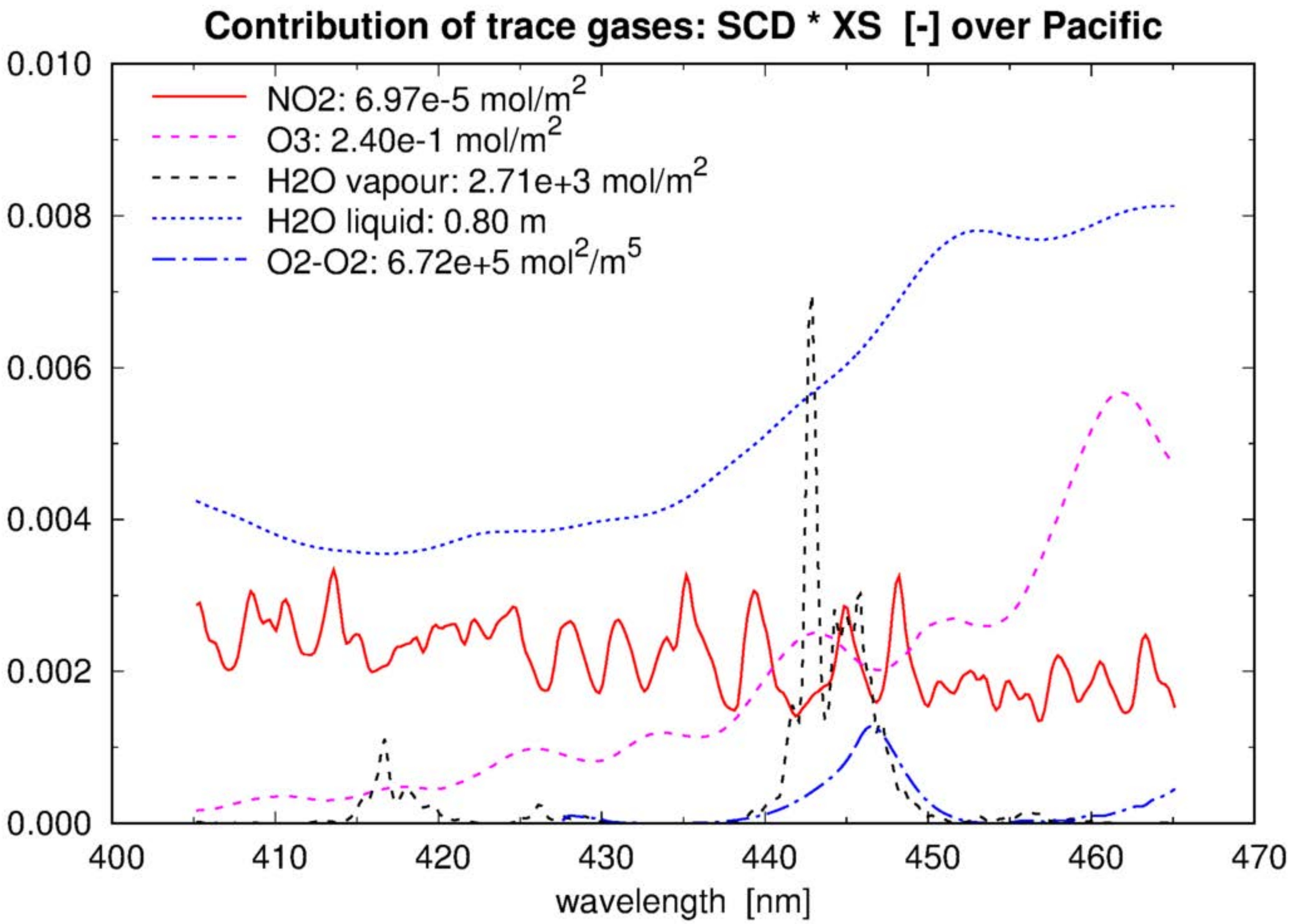
Ring effect = inelastic Raman scattering of sunlight in the atmosphere



Accounting for other trace gas absorbers

Other absorbers accounted for:

- Ozone
- Water vapour
- Liquid water
- O2-O2



Summary: DOAS (slant column) observations, End Part 1

Instrument:

- Need high signal to noise, typically 1000.
- Need very accurate calibration of Earth and solar spectra.

Conclusions related to the DOAS fits in NO2 window:

- We understand the Earth radiance in great detail, residuals ~1e-4
- NO2 has a very distinct spectral fingerprint and the slant column can be quantified accurately.

General Conclusion:

- TROPOMI is a great instrument, with good L1b calibration and high SNR and is well suited for not just NO2 but air quality & climate-relevant measurements of trace gases, cloud & aerosol
- Will play an important role in continuing the data record and linking geostationary measurements for assimilation in global & regional models

Part 2:

But … this was only the “easy” part of the retrieval

Easy part = most certain part, part with smallest error

What did we measure?

The amount of NO_2 along the path of the light through the atmosphere

What is still unknown?

Where did the light go?

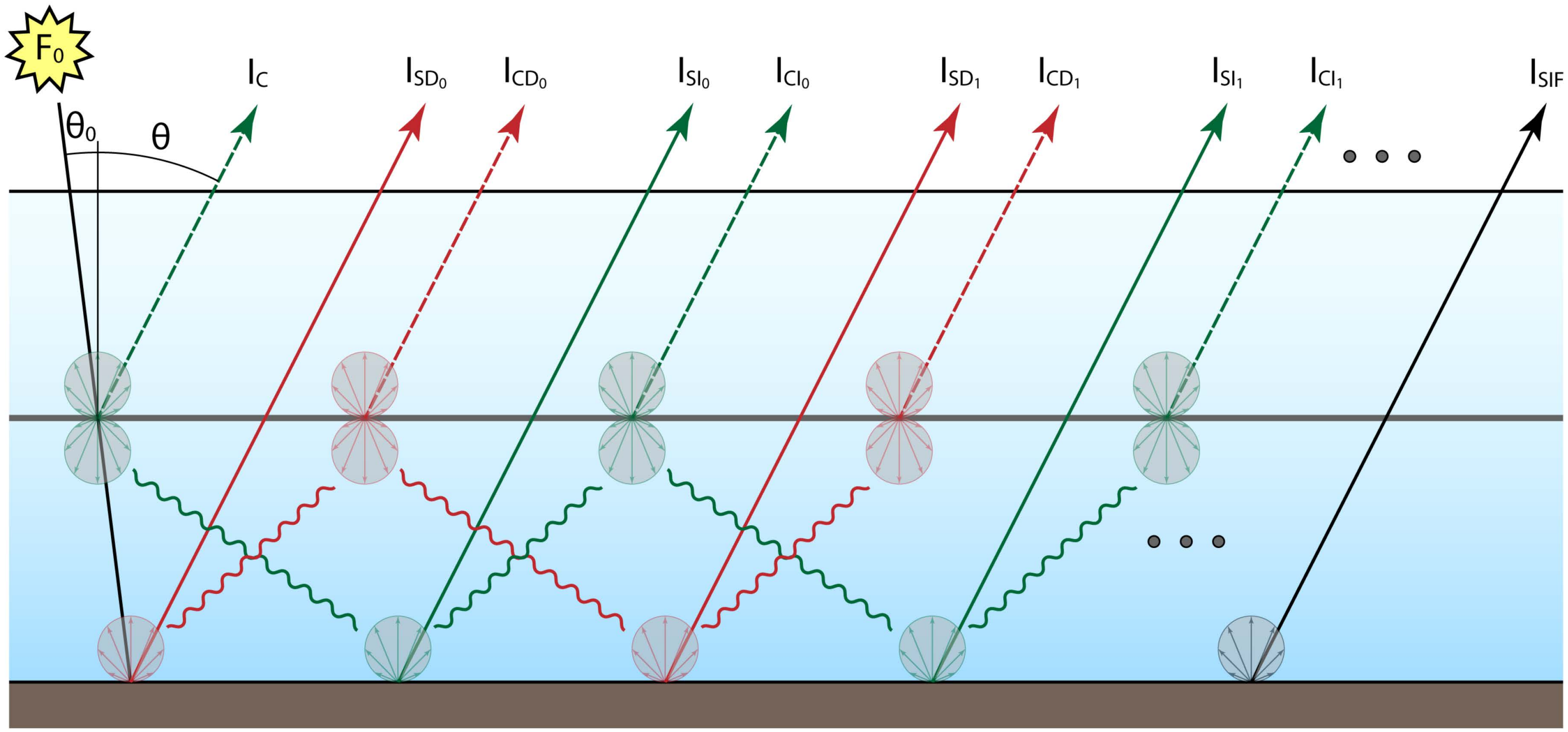
Where is the NO2 located? (At what altitude? Vertical distribution?)

Quantify both of these unknowns using an ***air mass factor***

Where did the light travel?

Input needed from Radiative transfer models

Depending on
geometry,
clouds,
surface albedo,
aerosols



Air-mass factor

Where did the light travel?

Aspects that influence
the light path:

Surface properties (reflection)

Aerosols

Clouds

Air-mass factor

Filtering to remove clouds: using the *qa_value*

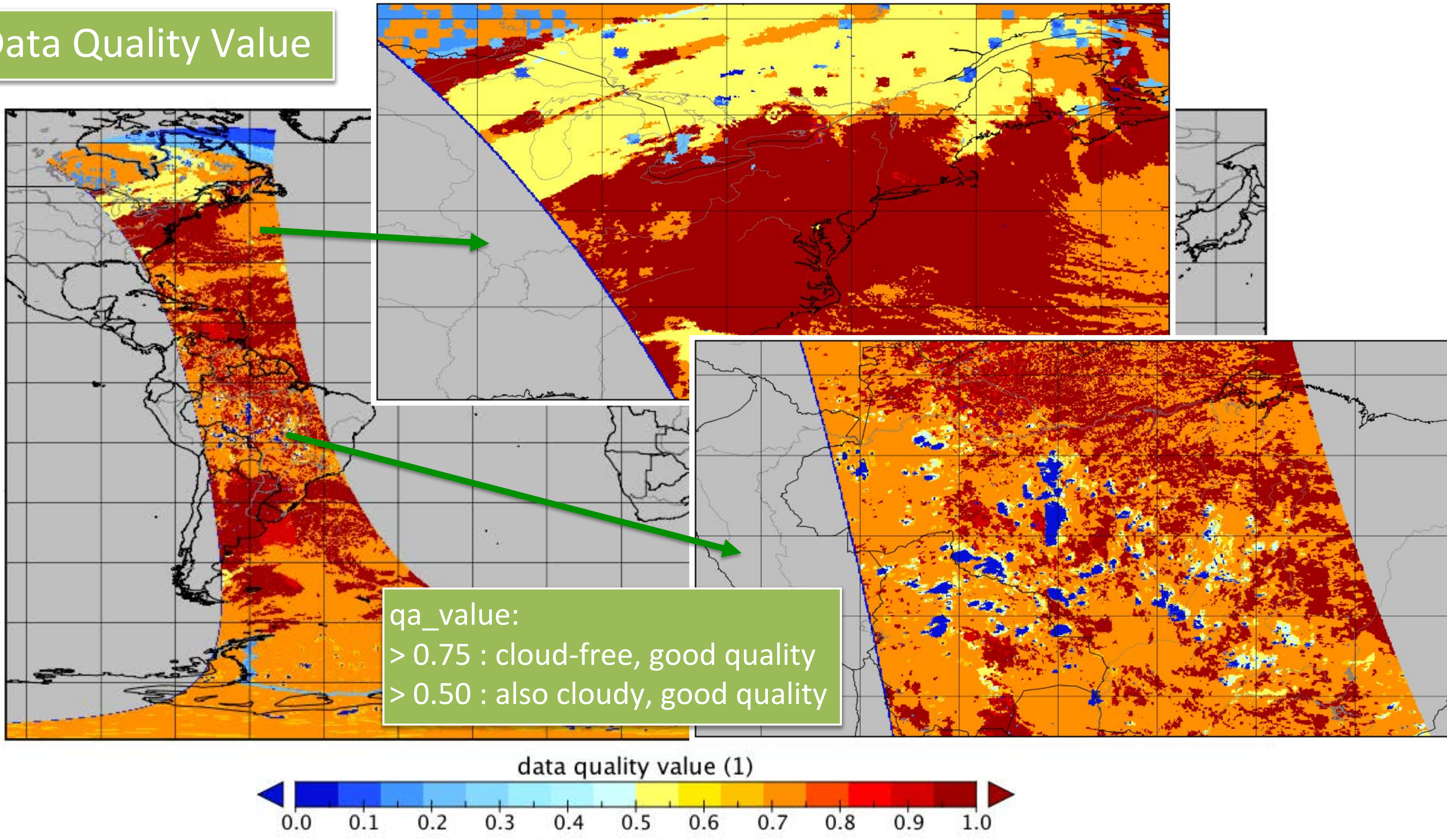
- `qa_value > 0.75`

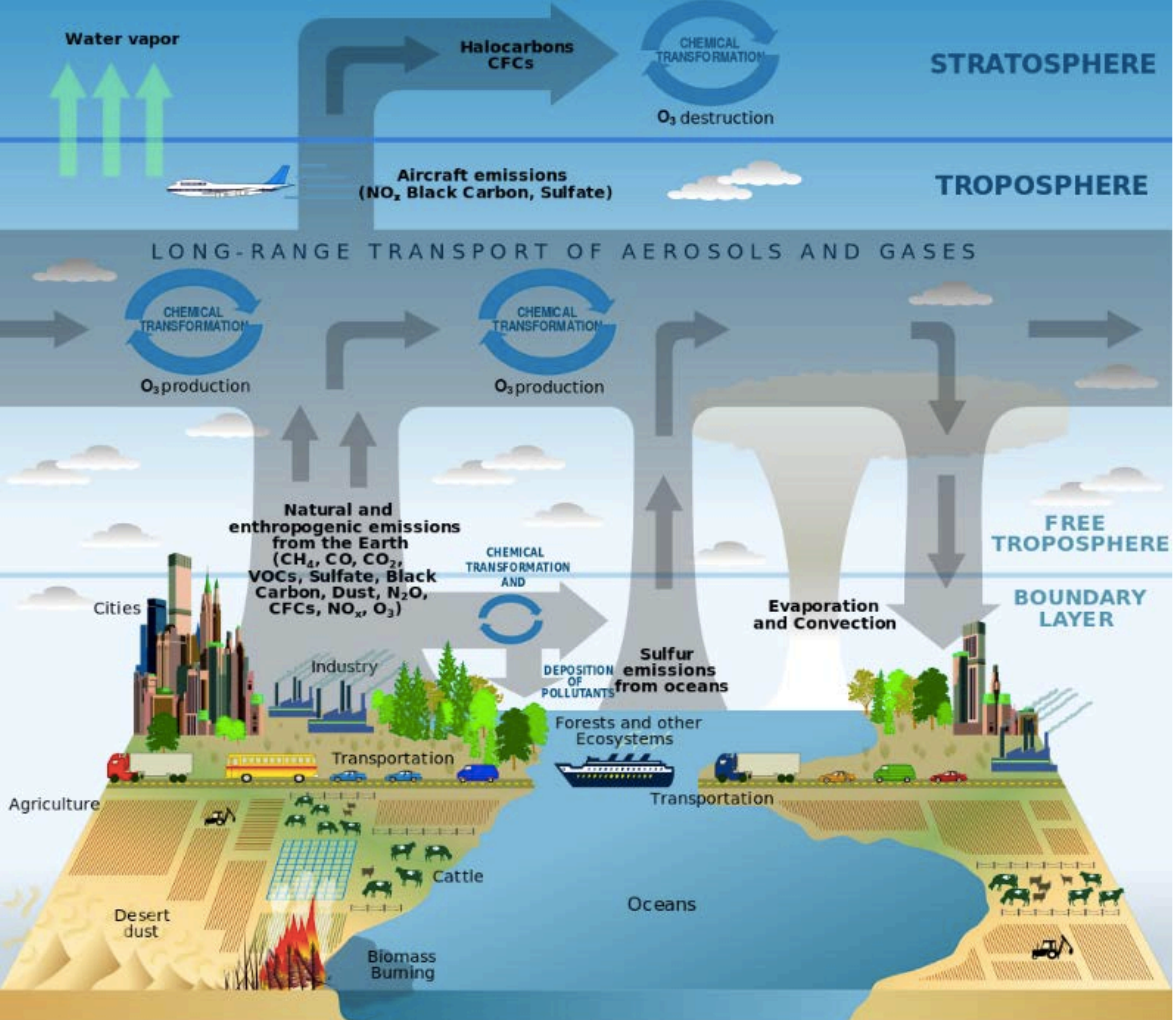
  This is the recommended pixel filter. It removes cloud-covered scenes (cloud radiance fraction > 0.5), partially snow/ice covered scenes, errors, and problematic retrievals.

- `qa_value > 0.50`

  Compared to the stricter filter, this adds the good quality retrievals over clouds and over scenes covered by snow/ice. Errors and problematic retrievals are still filtered out. In particular, this filter may be useful for assimilation and model comparison studies.

Data Quality Value

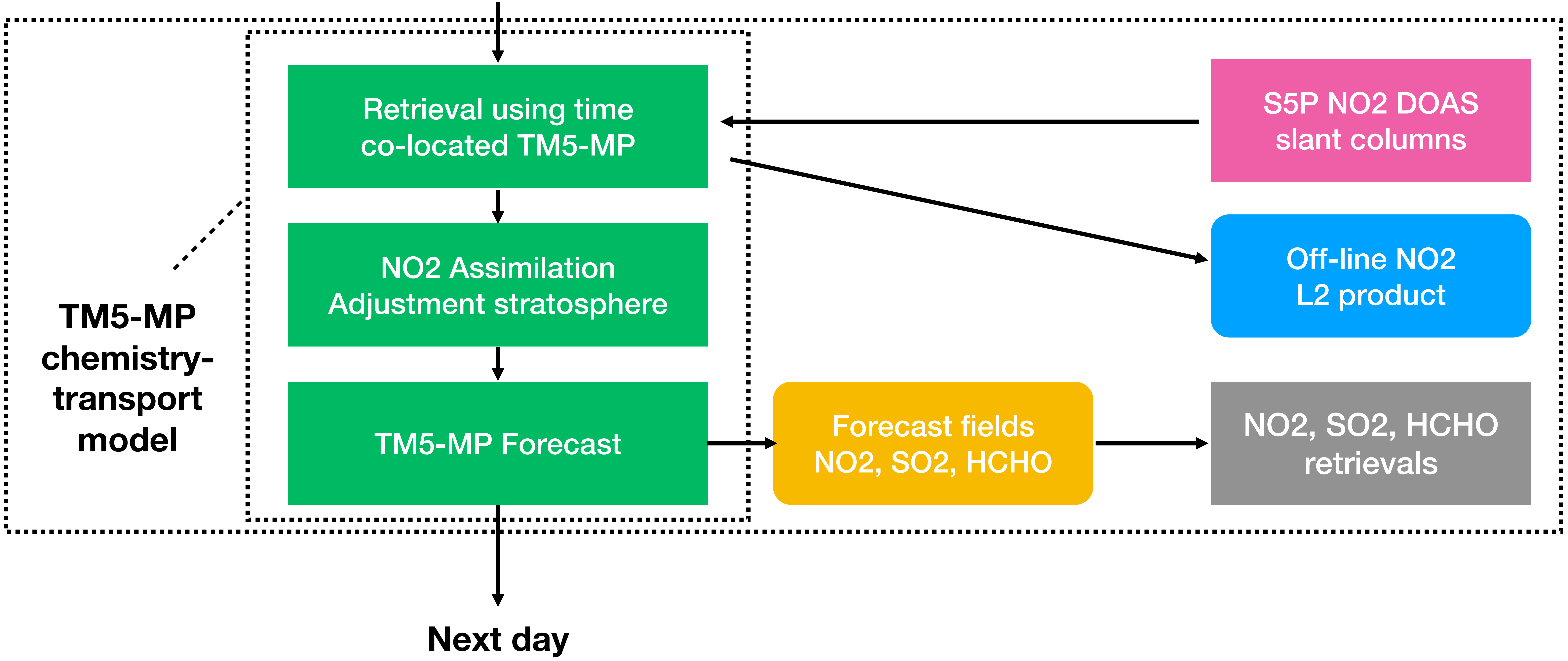




Where is the NO_2?

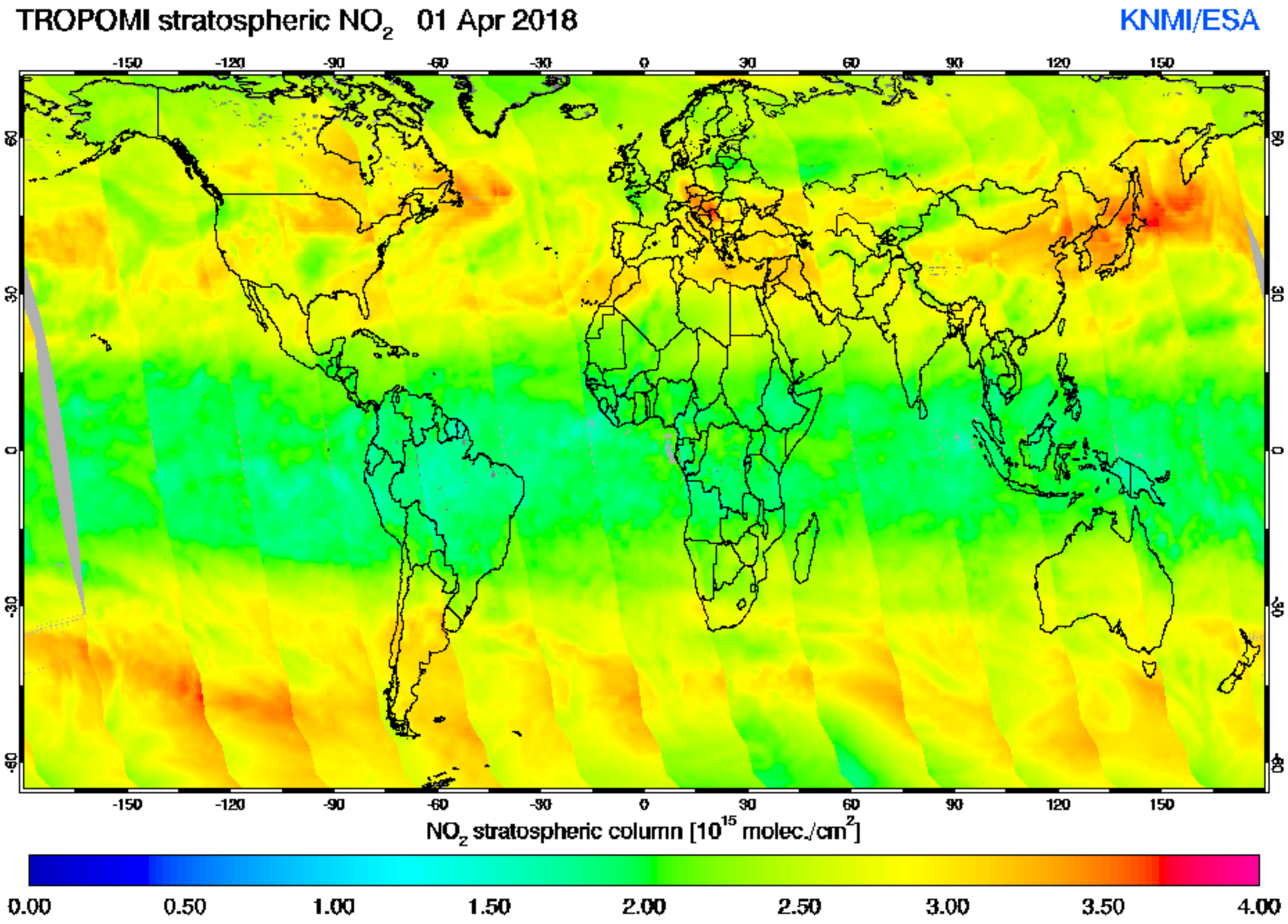
General circulation models including chemistry

TROPOMI NO2 processing chain (DOMINO setup): Adding information from models



The TM5 model provides a priori information about NO2 vertical profile

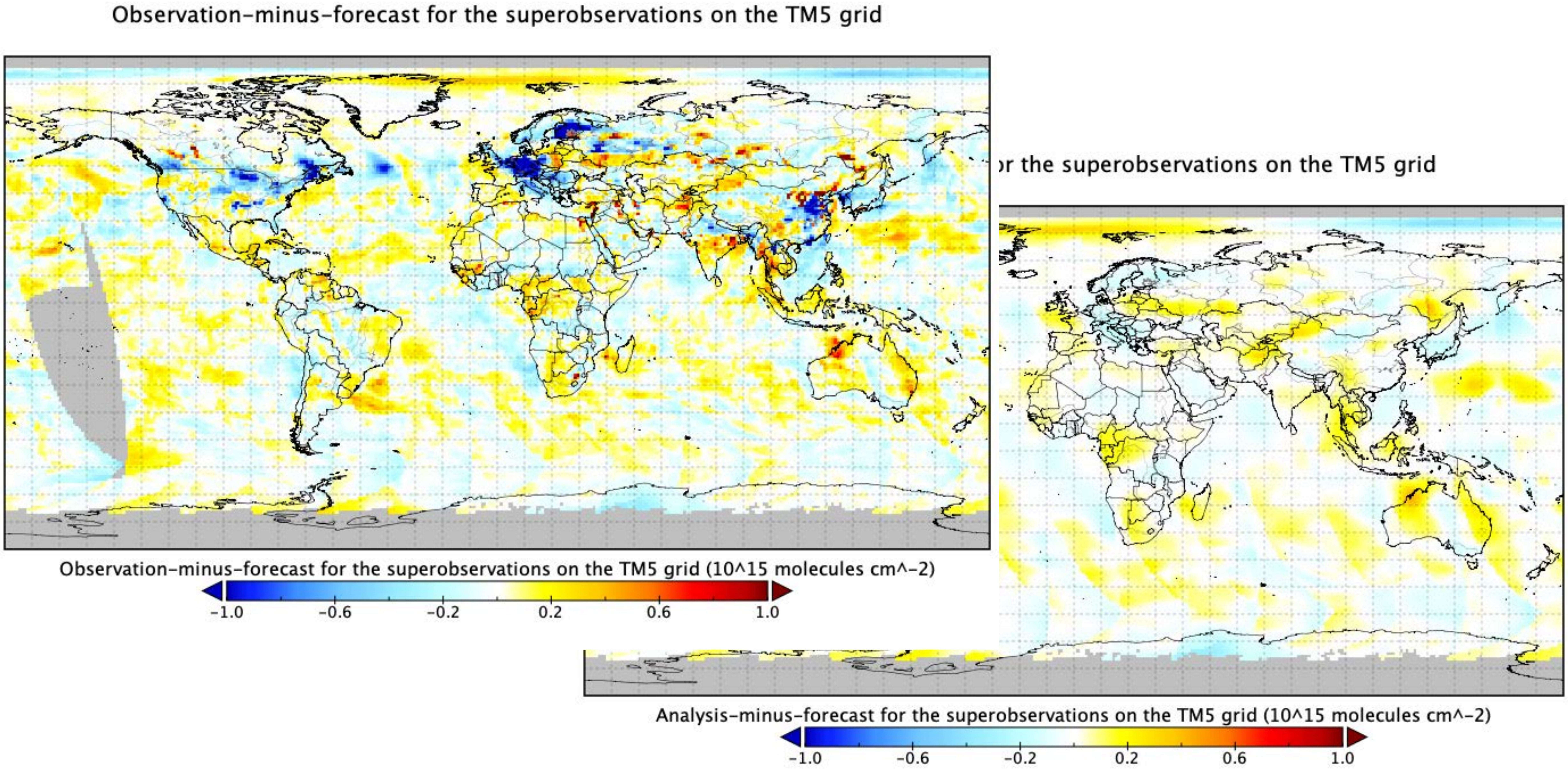
Stratosphere: from assimilation in TM5-MP



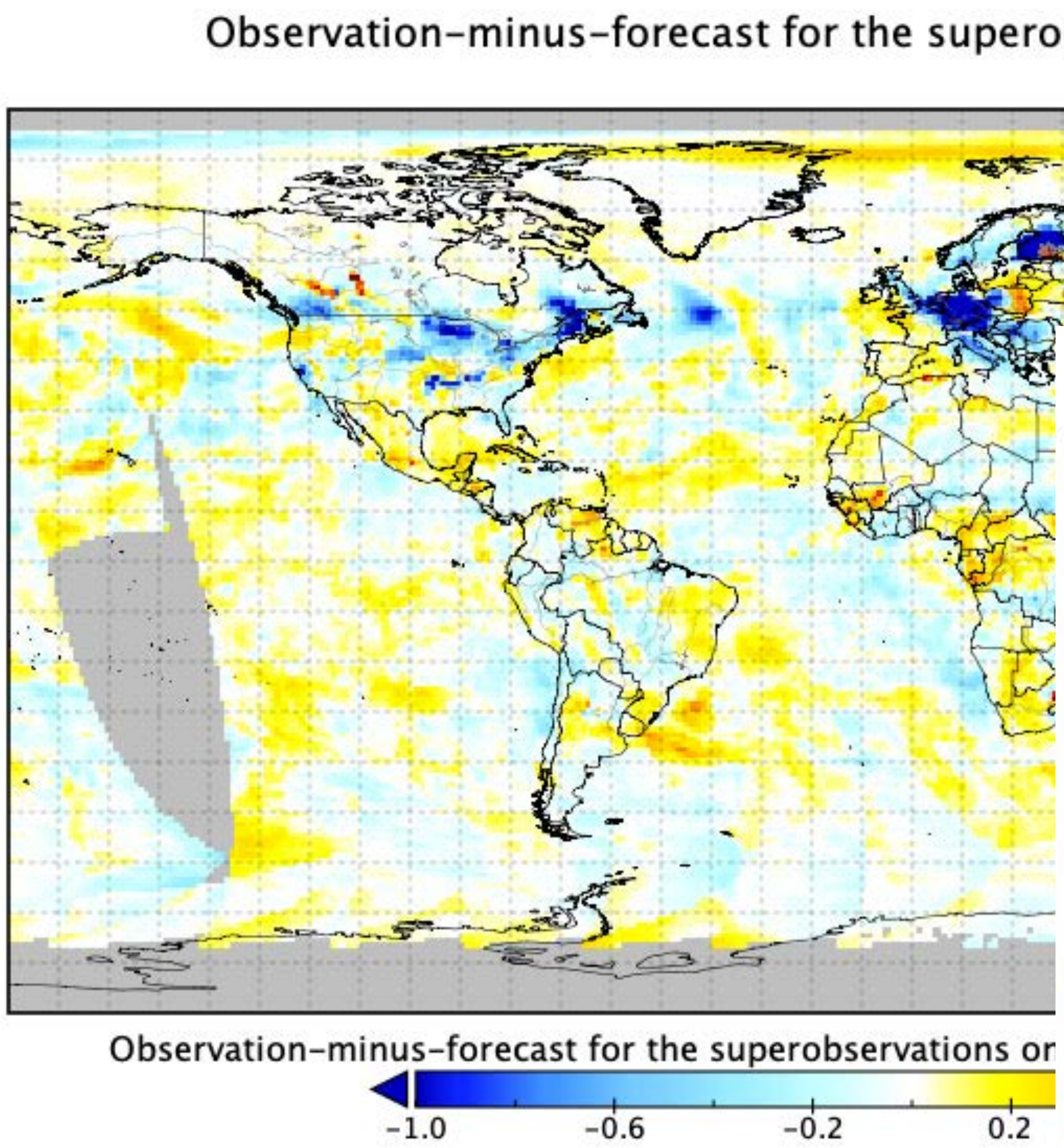
Tropospheric column = Total column minus stratospheric column

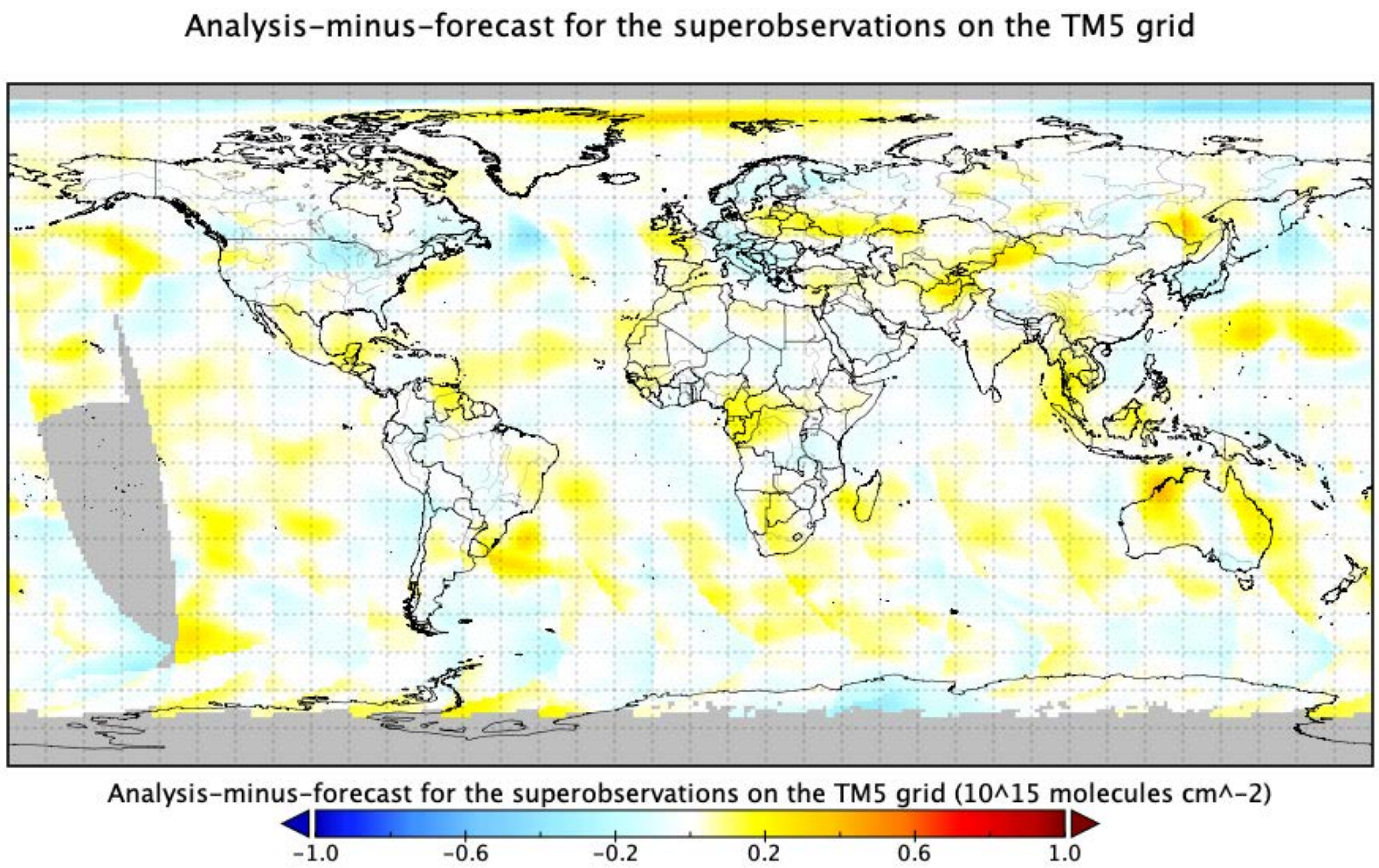
Stratospheric column determined by:
-> Atmospheric dynamics
-> Diurnal cycle (chemistry)

Stratosphere: from assimilation in TM5-MP



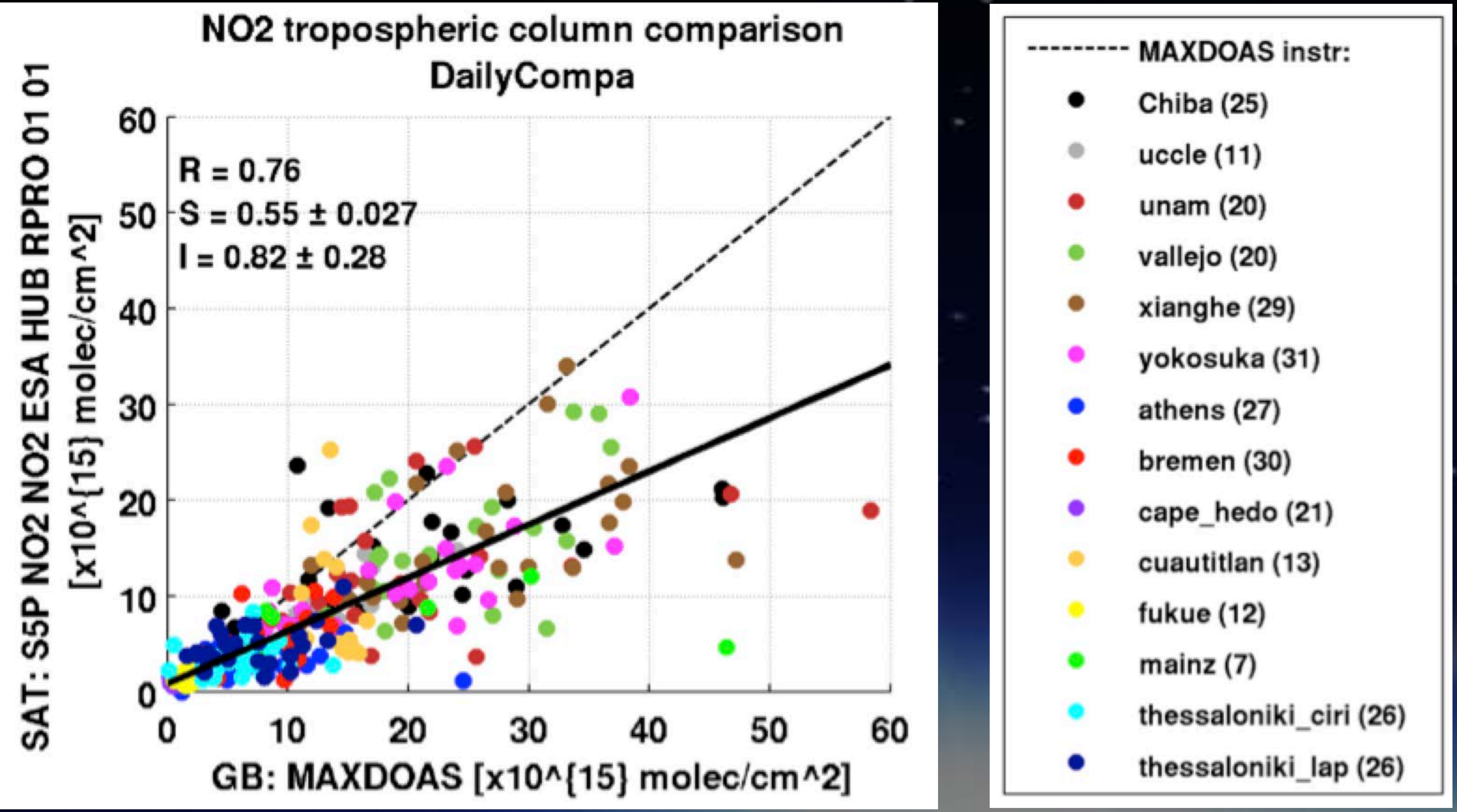
Stratosphere: from assimilation in TM5-MP





Validation is crucial to identify biases

TROPOMI vs. MAXDOAS



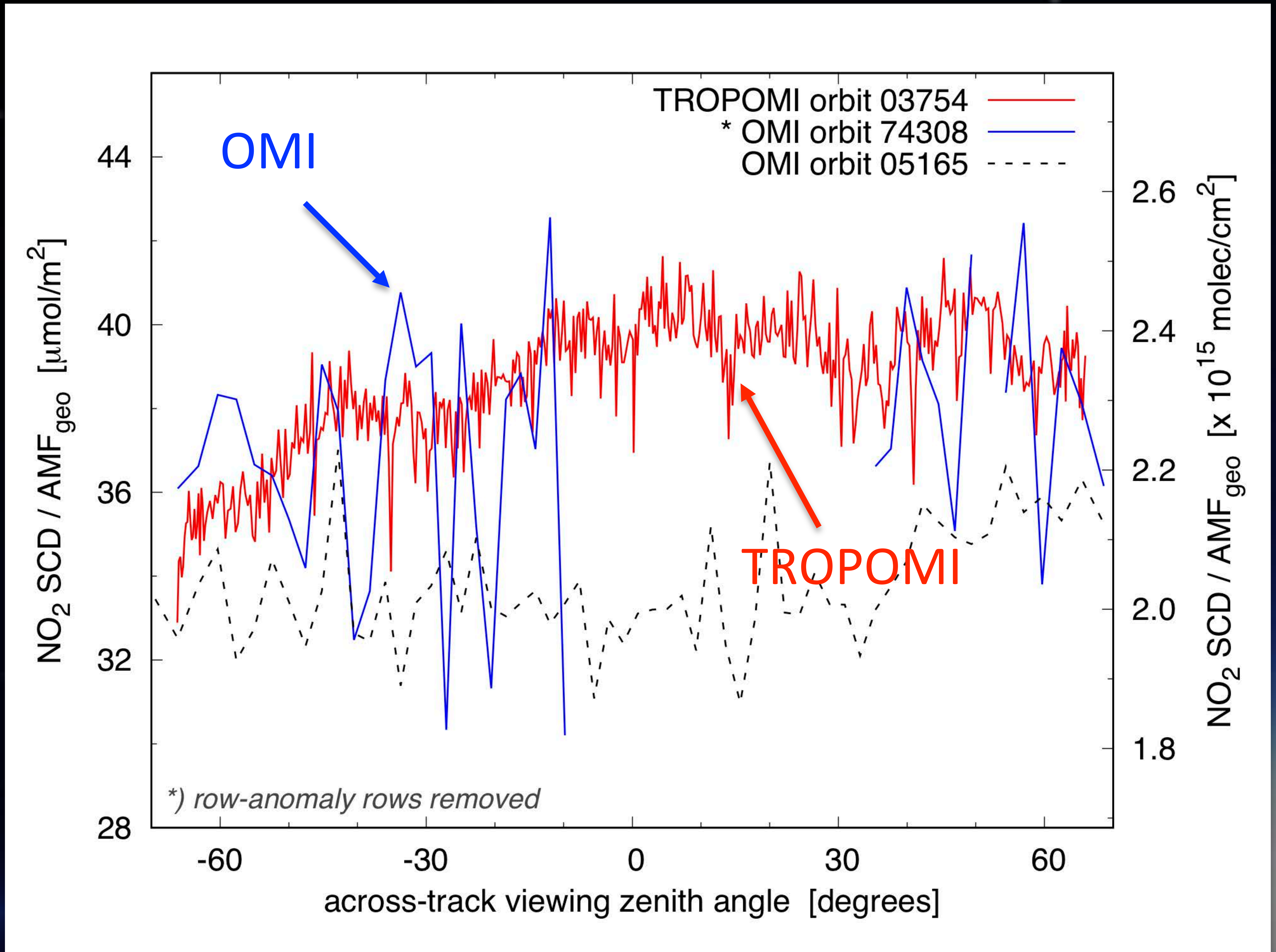
TROPOMI 30% lower than MAXDOAS

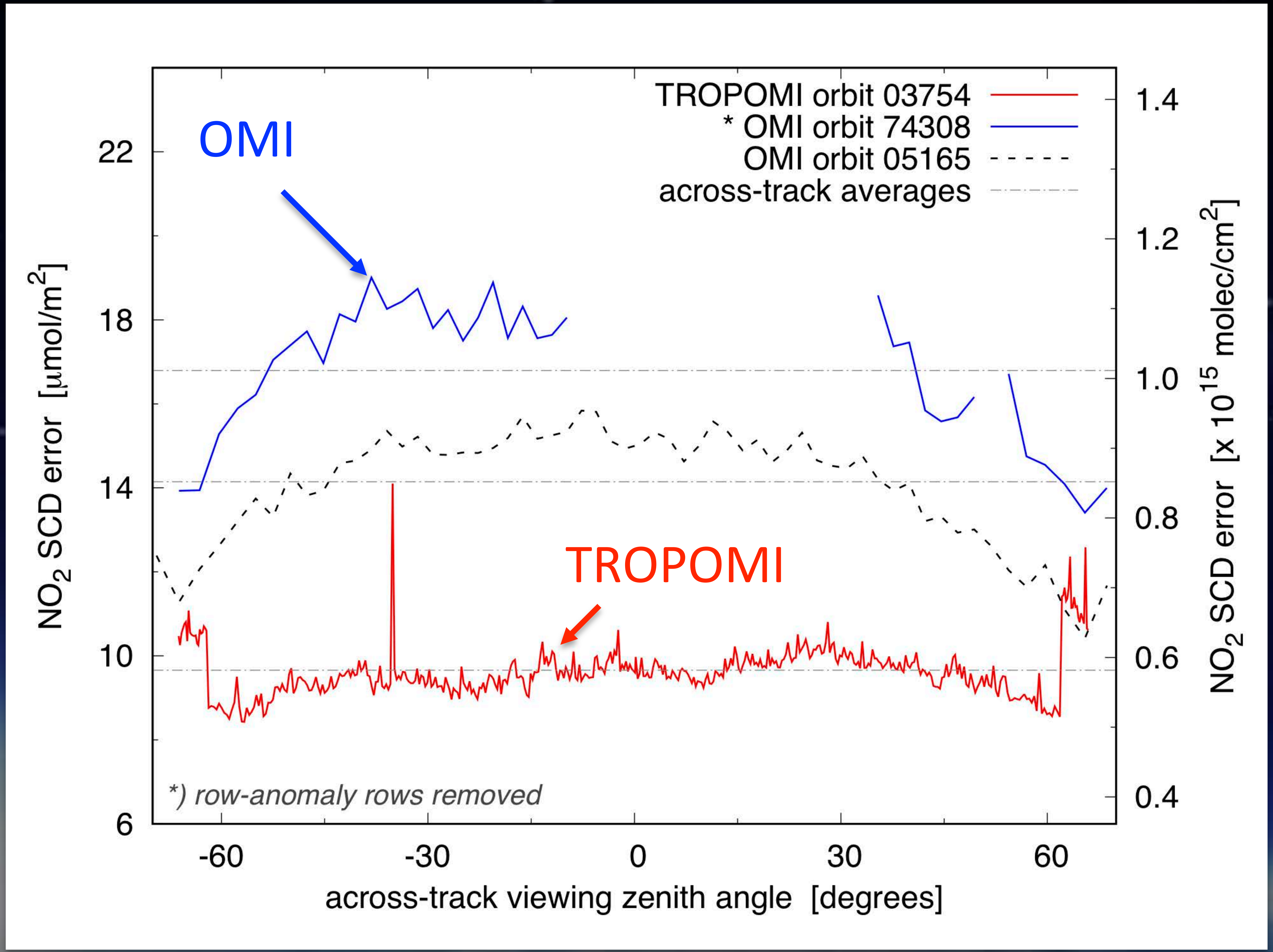
Bridging the gap ?

- Profile shape
- Clouds
- Local situation
- Kernel difference

Steven Compernolle, Tijl Verhoelst, Gaia Pinardi, José Granville, Jean-Christopher Lambert (BIRA-IASB), Kai-Uwe Eichmann (IUP-B)

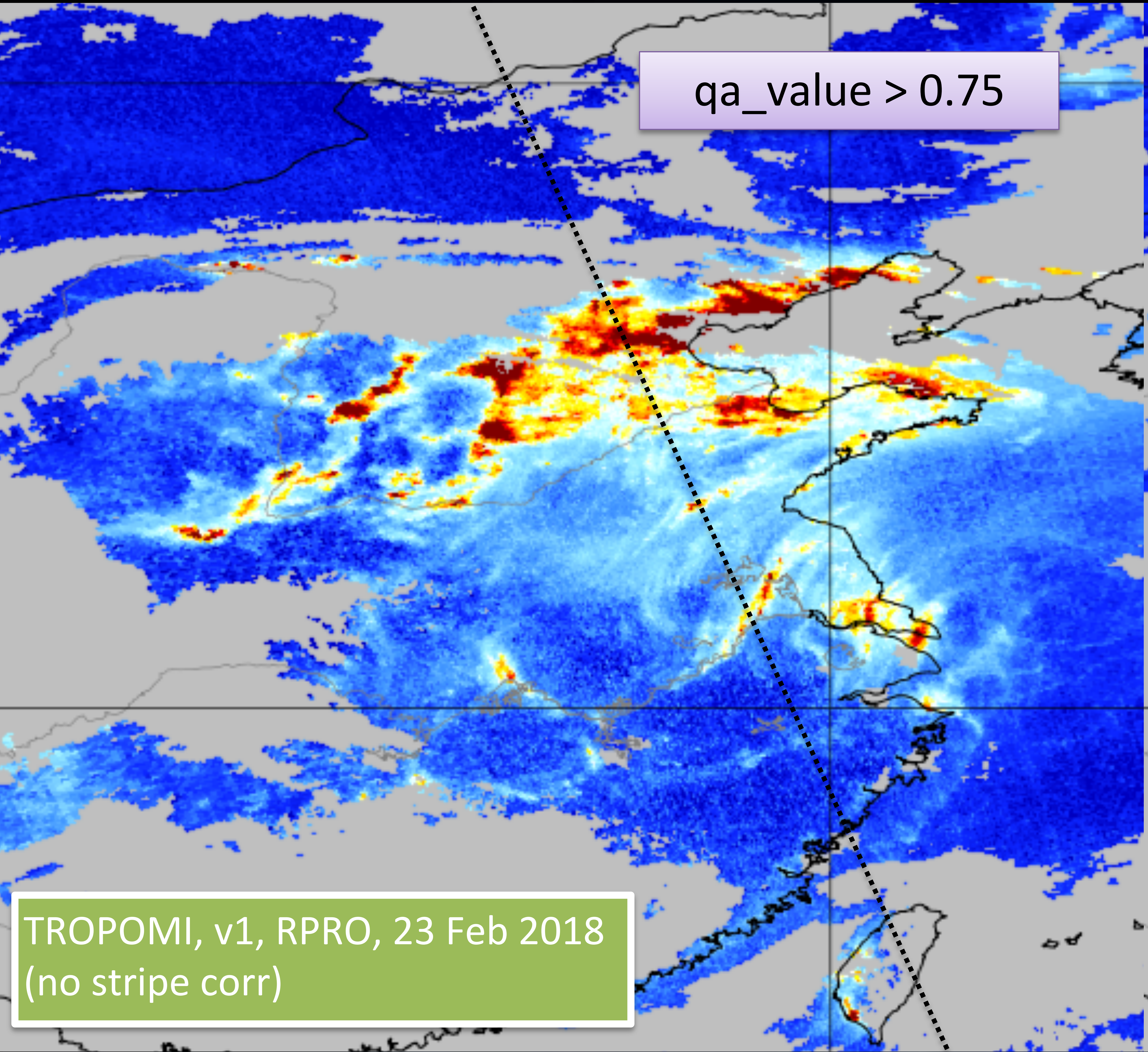
Comparison to other satellites: OMI vs. TROPOMI for DOAS slant column fits

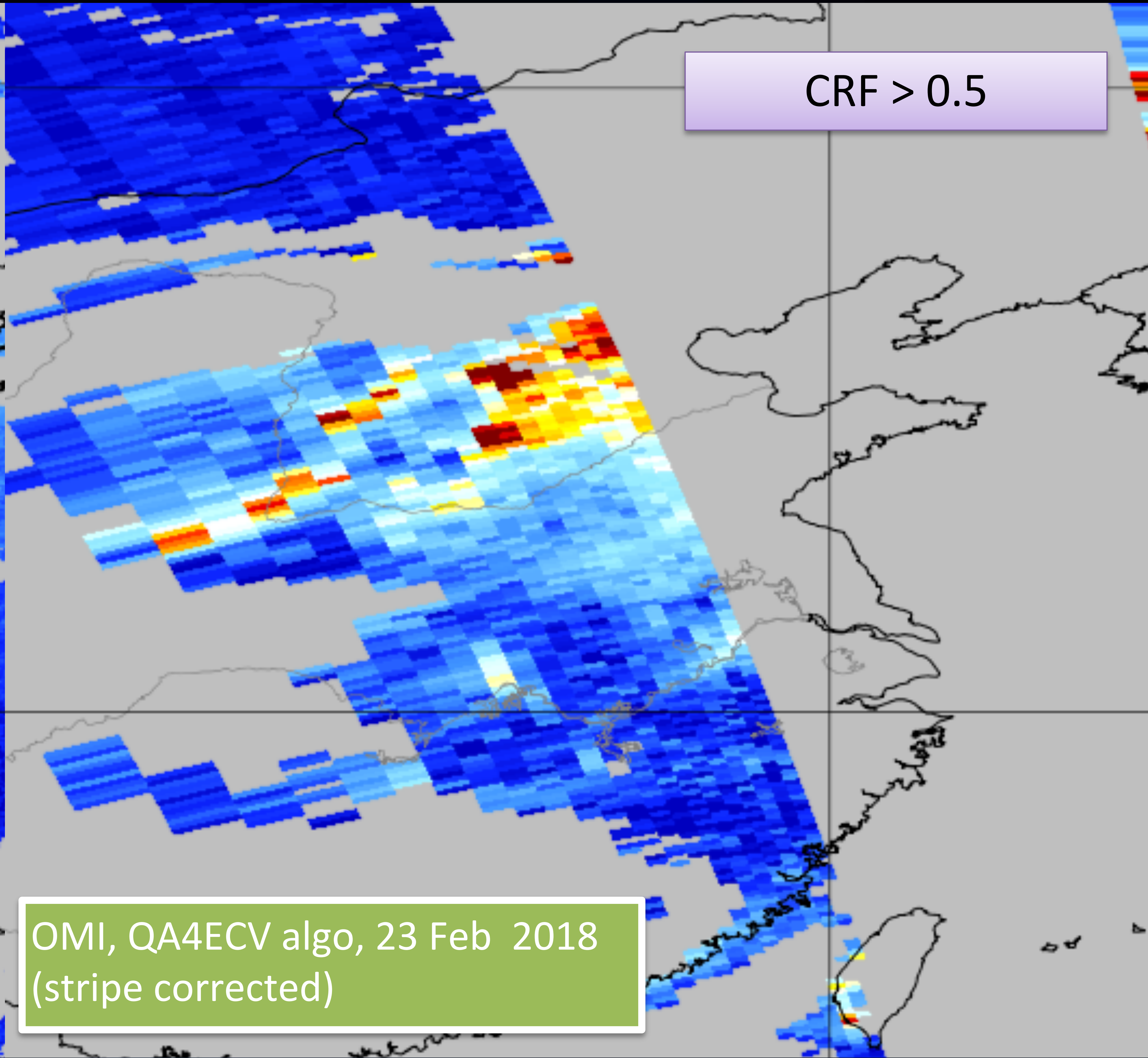




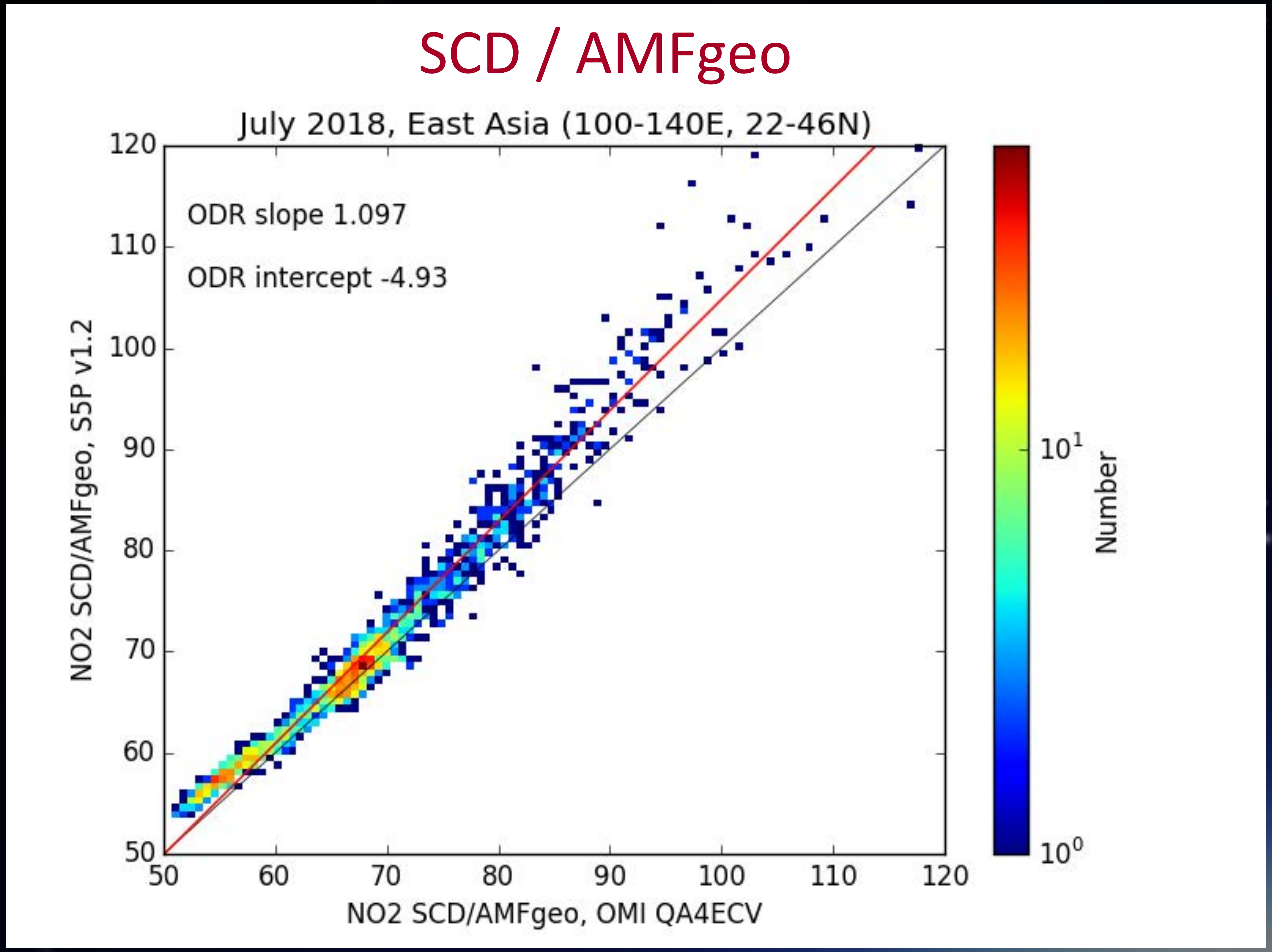
TROPOMI 10x more (smaller) pixels than OMI
But each pixel 1.5-2 times lower error bar

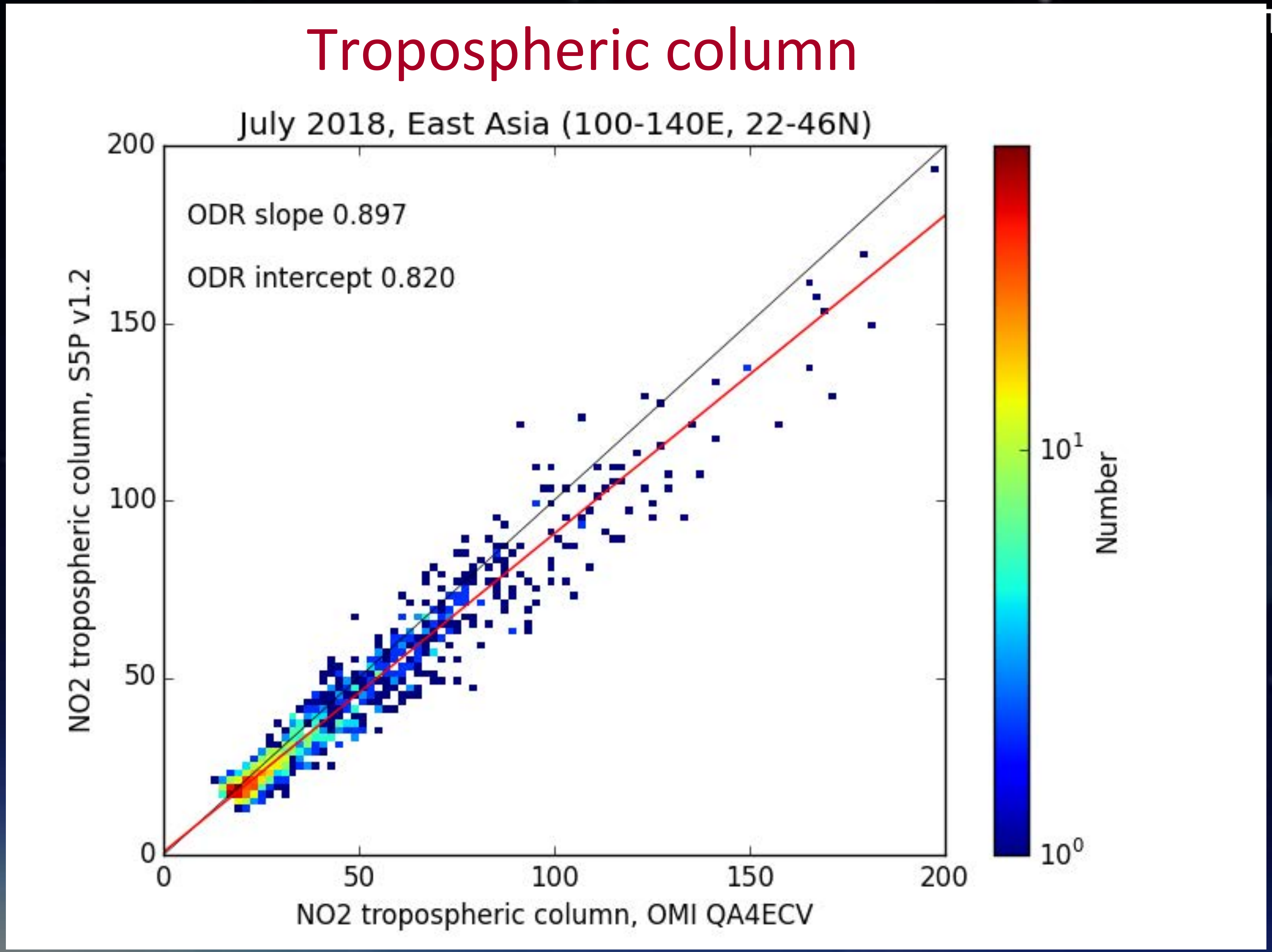
TROPOMI comparison with OMI - China





Comparison with OMI

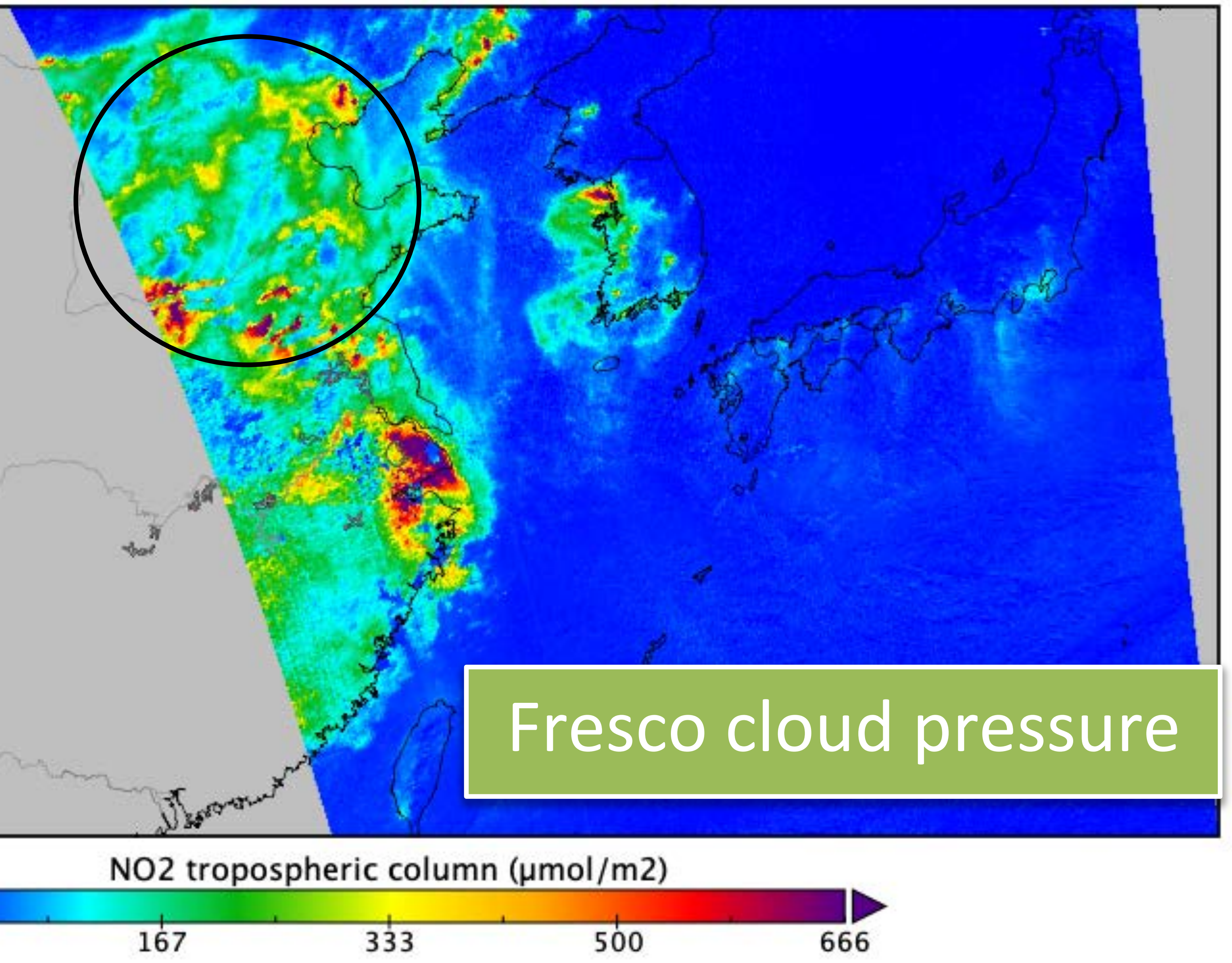


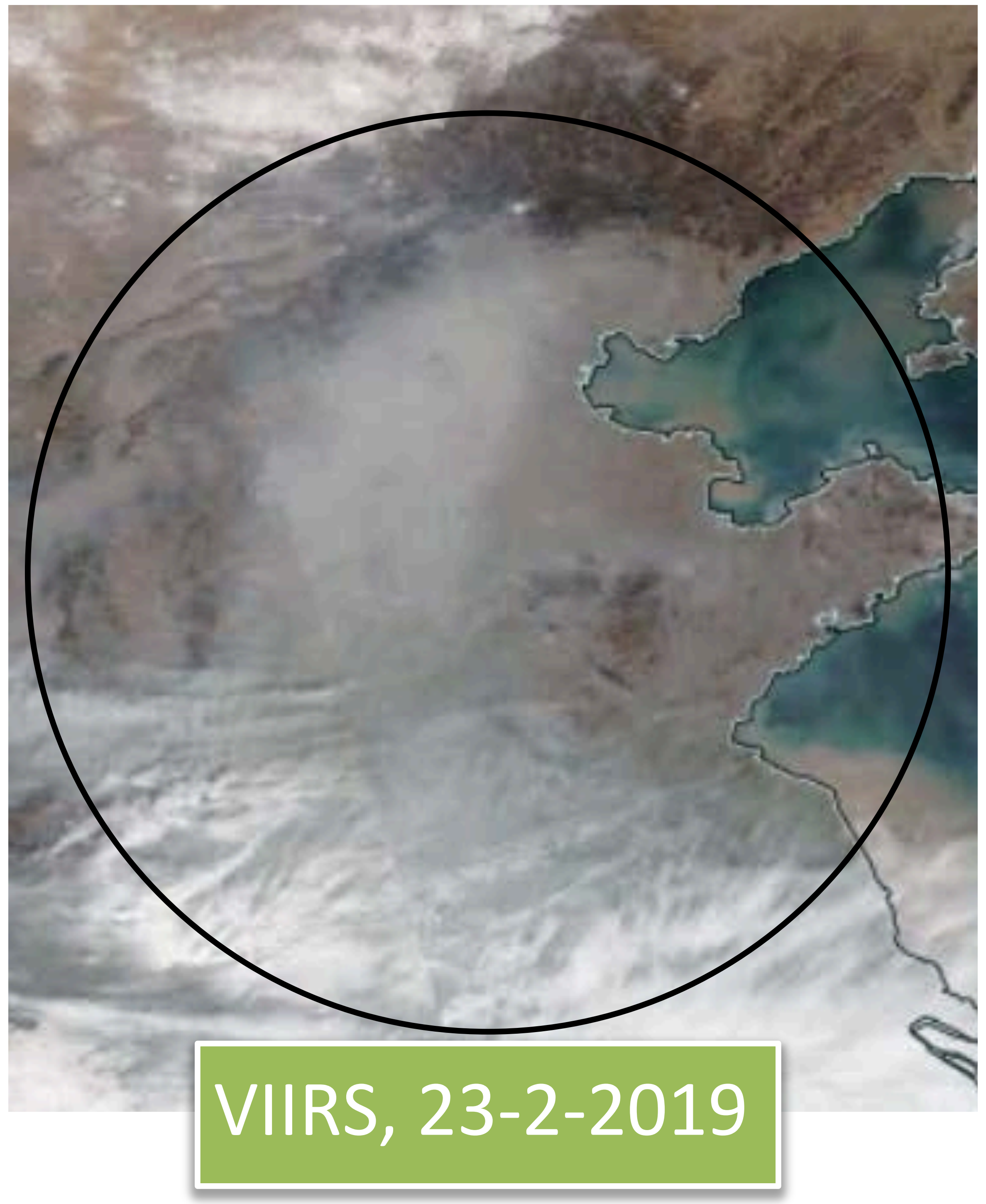


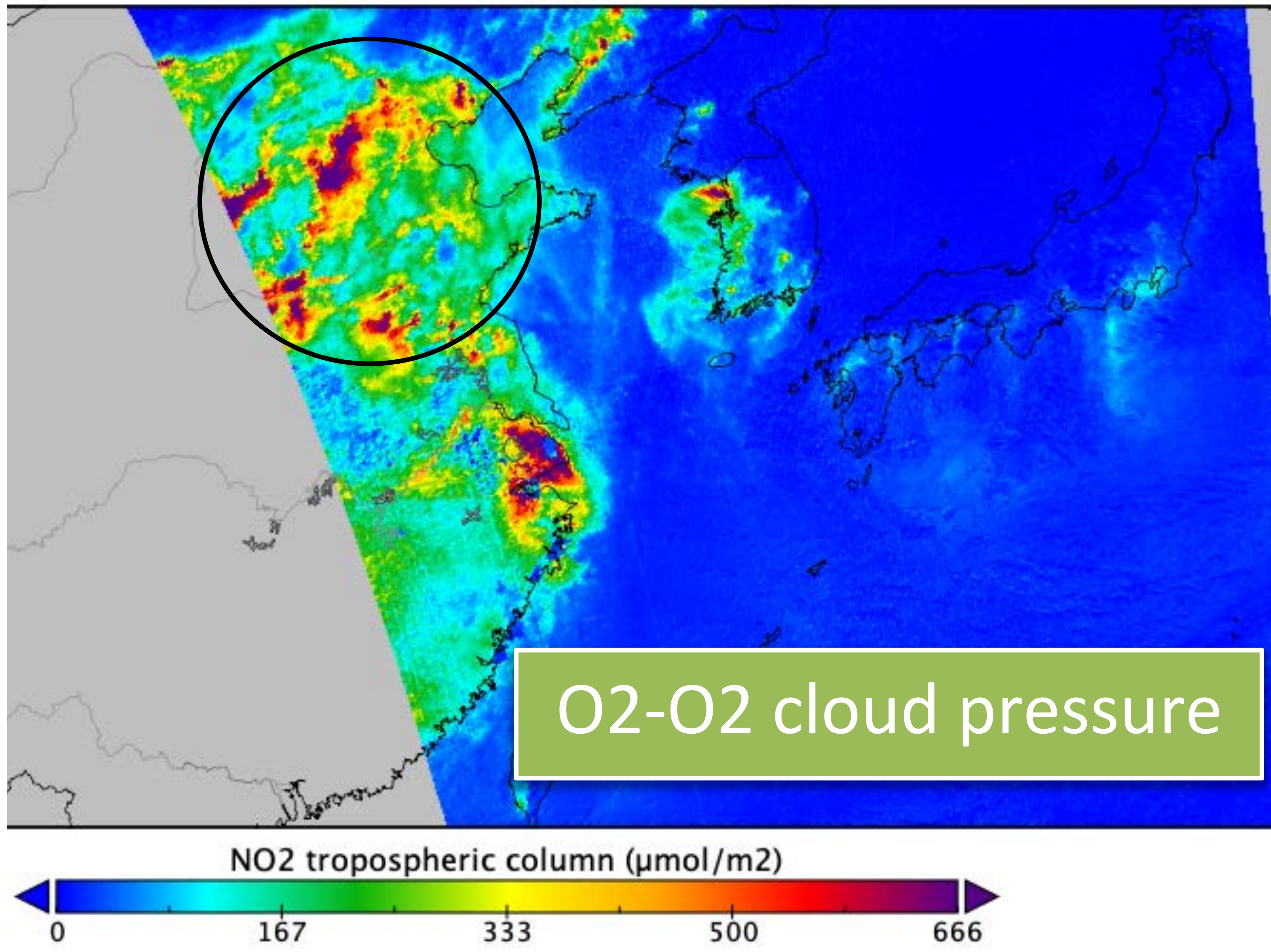
Differences in AMF ?

- Cloud product is different: Fresco (compare with O2-O2)

Dependence on cloud retrievals: Fresco vs O2-O2







Retrieval very sensitive to cloud height over area's with thick aerosol pollution or (broken) low clouds

Averaging kernels

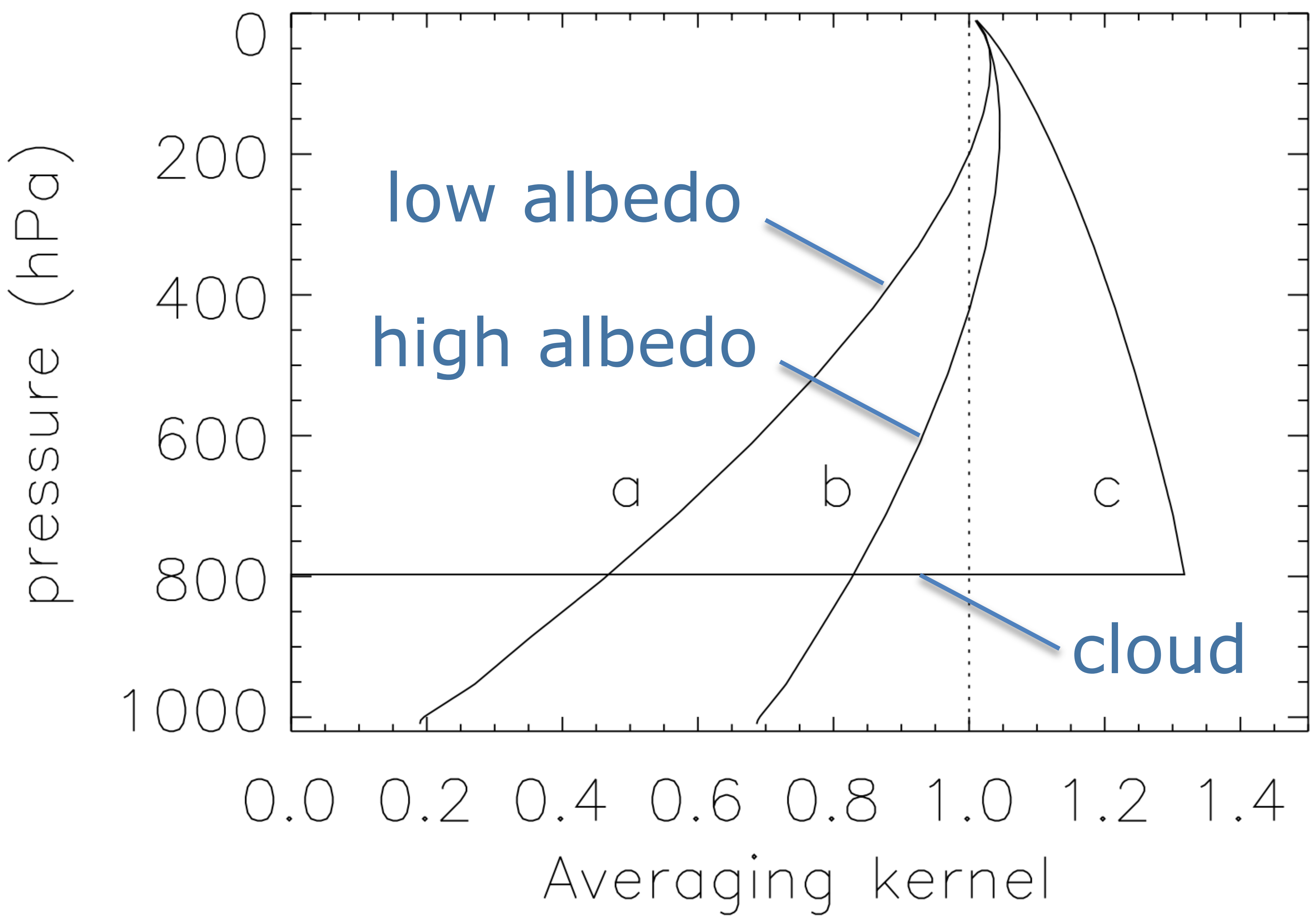
Atmos. Chem. Phys., 3, 1285–1291, 2003
www.atmos-chem-phys.org/acp/3/1285/
Atmospheric Chemistry and Physics

Averaging kernels for DOAS total-column satellite retrievals

H. J. Eskes and K. F. Boersma

In 2003 we showed how the DOAS retrieval may be re-formulated using Rodgers Optimal Estimation formalism.

DOAS averaging kernels profiles are proportional to the box air-mass factors



Use of TROPOMI NO_2 product

Depending on the application different datasets should be extracted from the L2_NO2 file

	user application	*data sets needed*
# 1	Tropospheric chemistry / air quality model evaluation and data assimilation Validation with tropospheric NO_2 profile measurements (aircraft, balloon, MAX-DOAS)	N_v^{trop}, $\Delta N_v^{trop,kernel}$ M^{trop}, M, $\mathbf{A}$ † A_l^{TM5}, B_l^{TM5}, l_{tp}^{TM5}, p_s
# 2	Tropospheric column comparisons, e.g. with other NO_2 column retrievals	N_v^{trop}, ΔN_v^{trop}
# 3	Stratospheric chemistry model evaluation and data assimilation Validation with stratospheric NO_2 profile measurements (limb/occultation satellite observations)	N_v^{strat}, ΔN_v^{strat} M^{strat}, M, $\mathbf{A}$ ‡ A_l^{TM5}, B_l^{TM5}, l_{tp}^{TM5}, p_s
# 4	Stratospheric column comparisons, e.g. with ground-based remote sensors	N_v^{strat}, ΔN_v^{strat}
# 5	Whole atmosphere (troposphere + stratosphere) data assimilation systems	N_v, ΔN_v^{kernel} § $\mathbf{A}$ A_l^{TM5}, B_l^{TM5}, l_{tp}^{TM5}, p_s
# 6	Whole atmosphere (troposphere + stratosphere) comparisons with ground-based remote sensing (e.g. Pandora)	N_v^{sum}, ΔN_v^{sum} §
# 7	Visualisation of the NO_2 product	N_v^{trop}, N_v^{strat}, N_v^{sum} §

† The tropospheric kernel $\mathbf{A}^{trop}$ is derived from the total kernel $\mathbf{A}$ and the air-mass factors M and M^{trop}.
‡ The stratospheric kernel $\mathbf{A}^{strat}$ is derived from the total kernel $\mathbf{A}$ and the air-mass factors M and M^{strat}.
§ Note that the total NO_2 vertical column $N_v \equiv N_s/M$ is *not* the same as the sum $N_v^{sum} \equiv N_v^{trop} + N_v^{strat}$

John Douros (KNMI)

Application of the averaging kernels

The file contains the averaging kernel for the total column.

The tropospheric column $\mathbf{A}^{\text{trop}}$ is obtained in the following way

$$\mathbf{A}^{\text{trop}} = \frac{M}{M^{\text{trop}}}\mathbf{A} \quad , l <= l_{\text{tp}}^{\text{TM5}}$$
$$\mathbf{A}^{\text{trop}} = 0 \quad , l > l_{\text{tp}}^{\text{TM5}}$$

A model simulated satellite tropospheric NO2 column is obtained by multiplying the model partial column profile $x_{m,l}$ with the averaging kernel, or

$$N_{\text{v}}^{\text{trop,model}} = \sum_{l} A_{l}^{\text{trop}} x_{m,l}$$

Replacing the a-priori using the averaging kernels

The TROPOMI NO_2 tropospheric column may be re-computed using the profile $x_{m,l}$ from an alternative model (high-resolution regional air-quality model). Needed are the tropospheric averaging kernel and AMF, and the following equations:

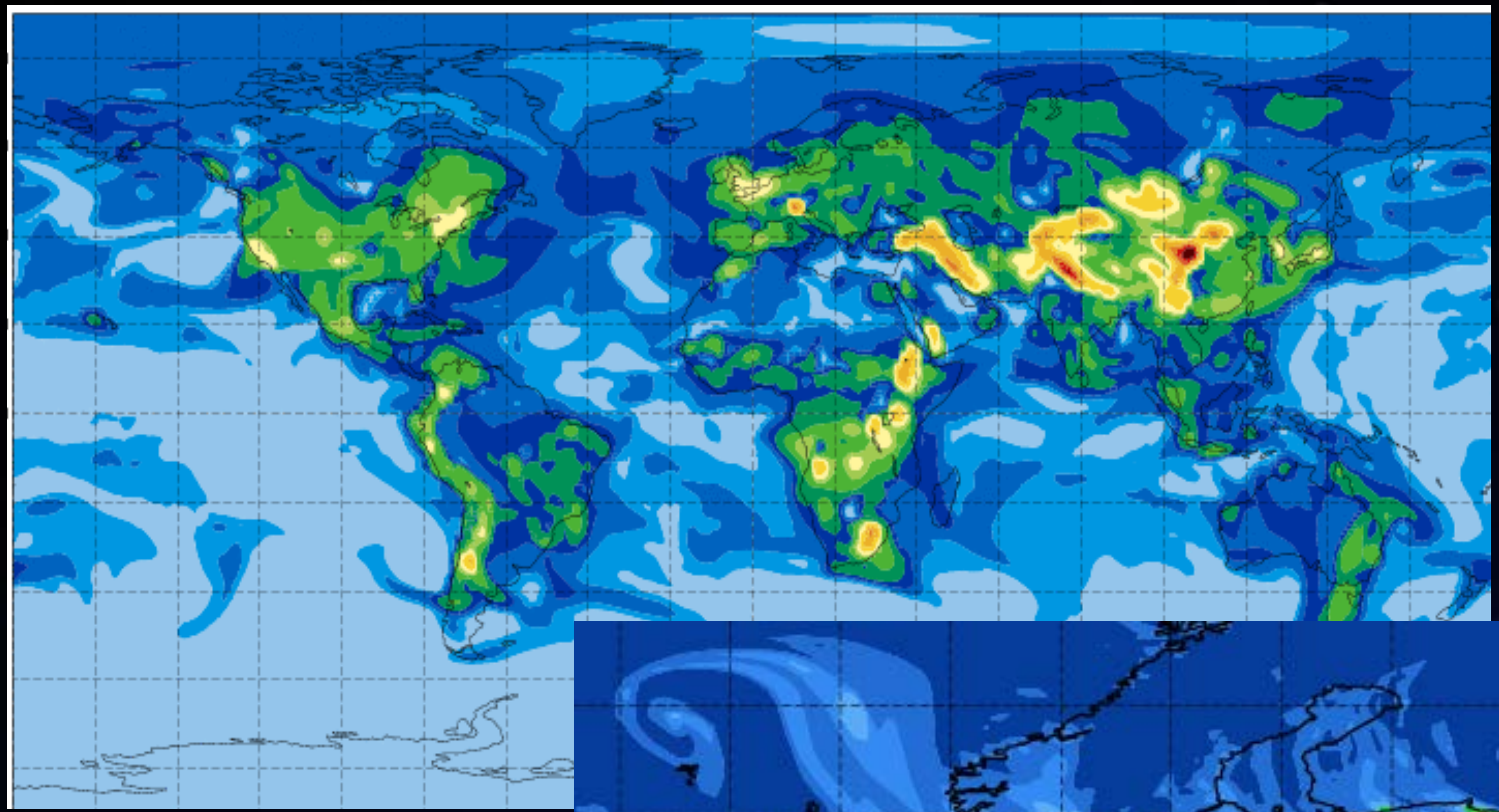
$$N_{\mathrm{v}}^{\mathrm{trop}'} = \frac{M^{\mathrm{trop}}}{M^{\mathrm{trop}'}} N_{\mathrm{v}}^{\mathrm{trop}}$$

$$\mathbf{A}^{\mathrm{trop}'} = \frac{M^{\mathrm{trop}}}{M^{\mathrm{trop}'}} \mathbf{A}^{\mathrm{trop}}$$

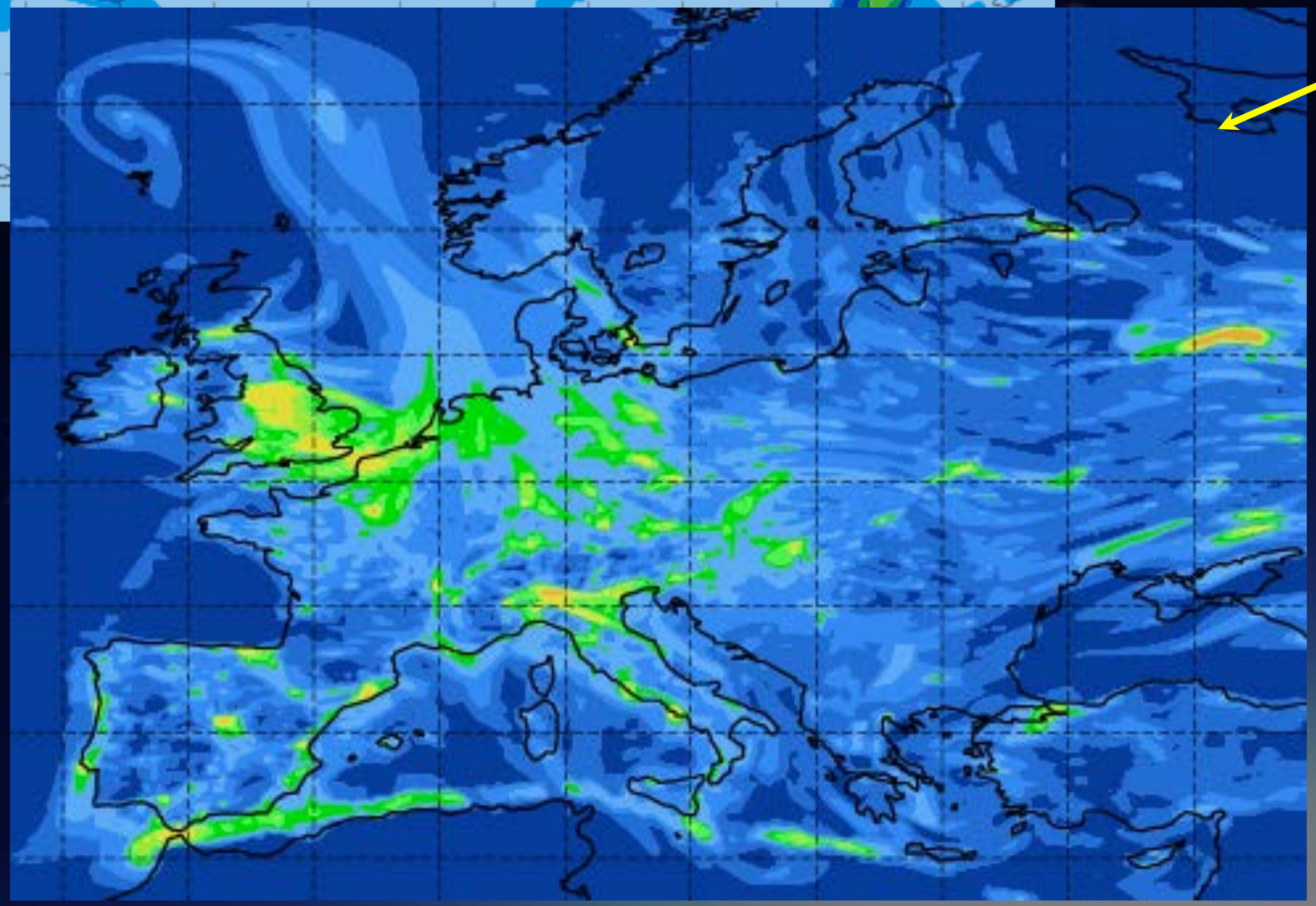
$$M^{\mathrm{trop}'} = M^{\mathrm{trop}} \sum_l A_l^{\mathrm{trop}} x'_{m,l} \Big/ \sum_l x'_{m,l}$$

All quantities on the left with a prime ′ are recomputed using the model NO_2 partial-column profiles $x'_{m,l}$. Other quantities are taken from the S5P_L2_NO2 file.

CAMS as main user of the Copernicus Sentinel 5P, 4, 5 composition observations

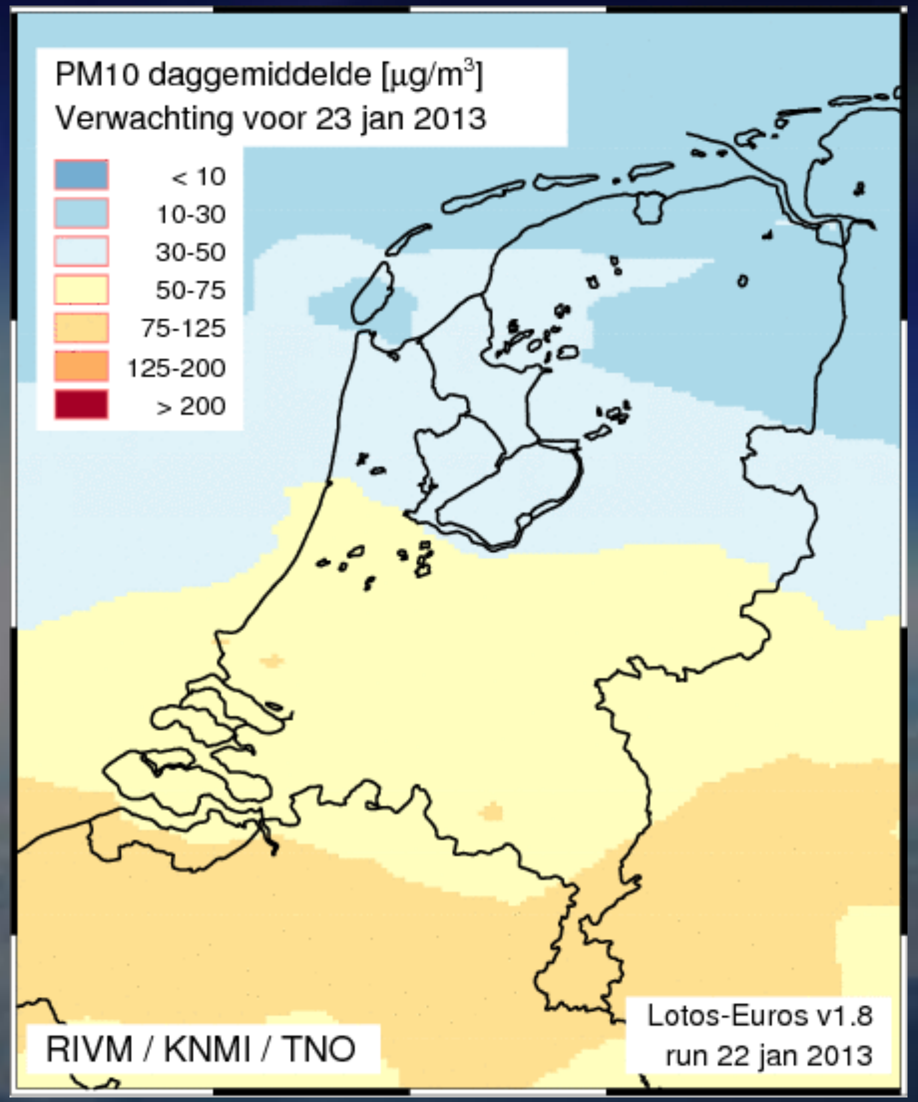


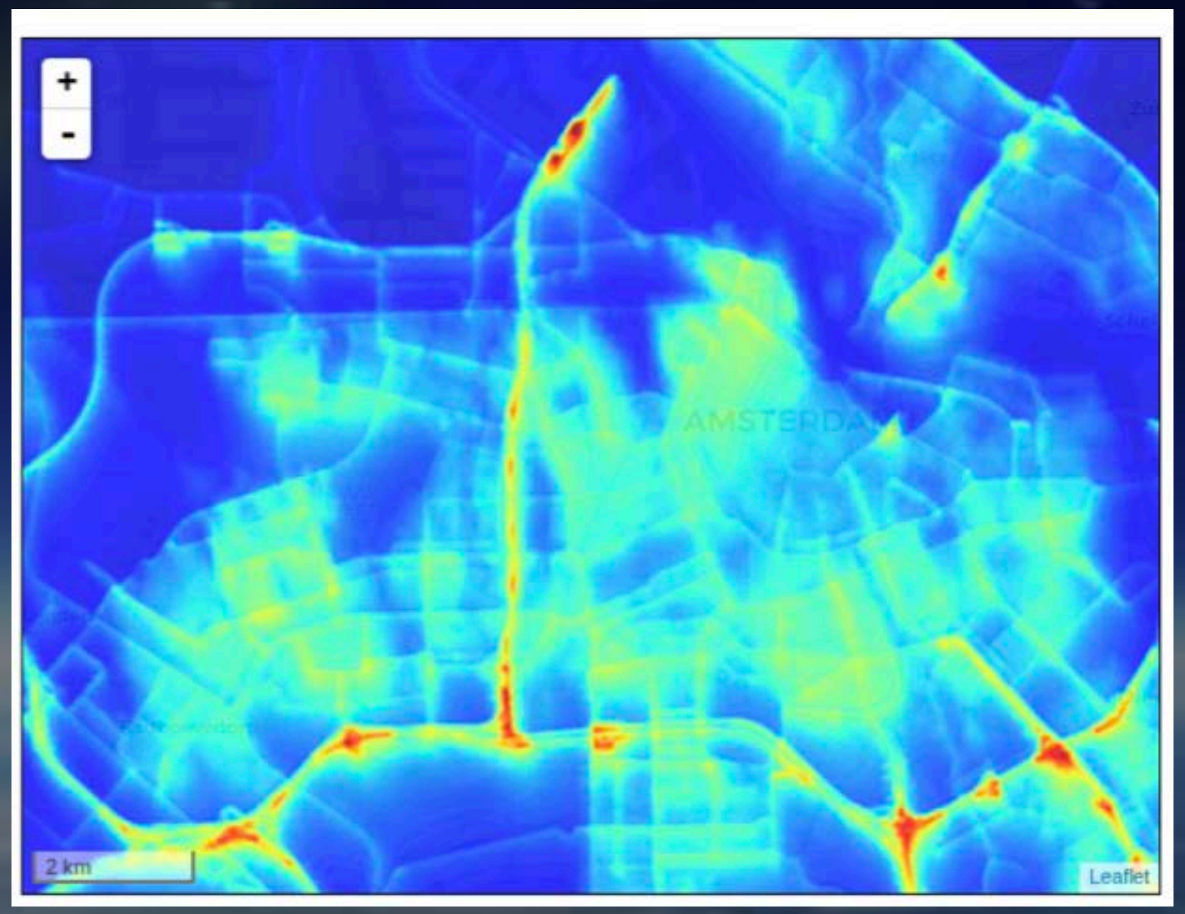
Assimilation
TROPOMI
observations



CAMS-Europe as boundary condition for
countries and city regions

Amsterdam





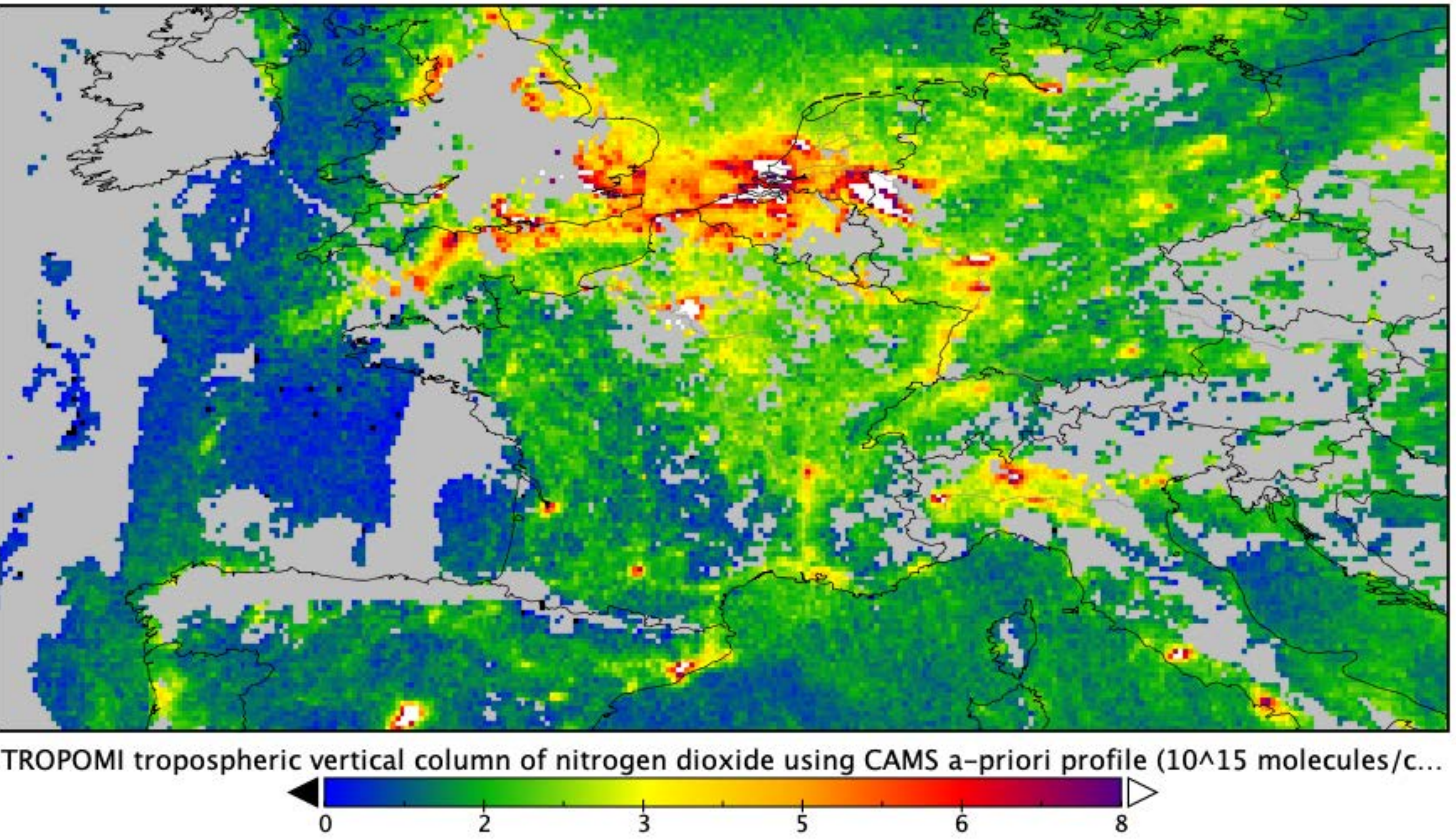
Analyses of CAMS-global as
boundary condition for CAMS-Europe

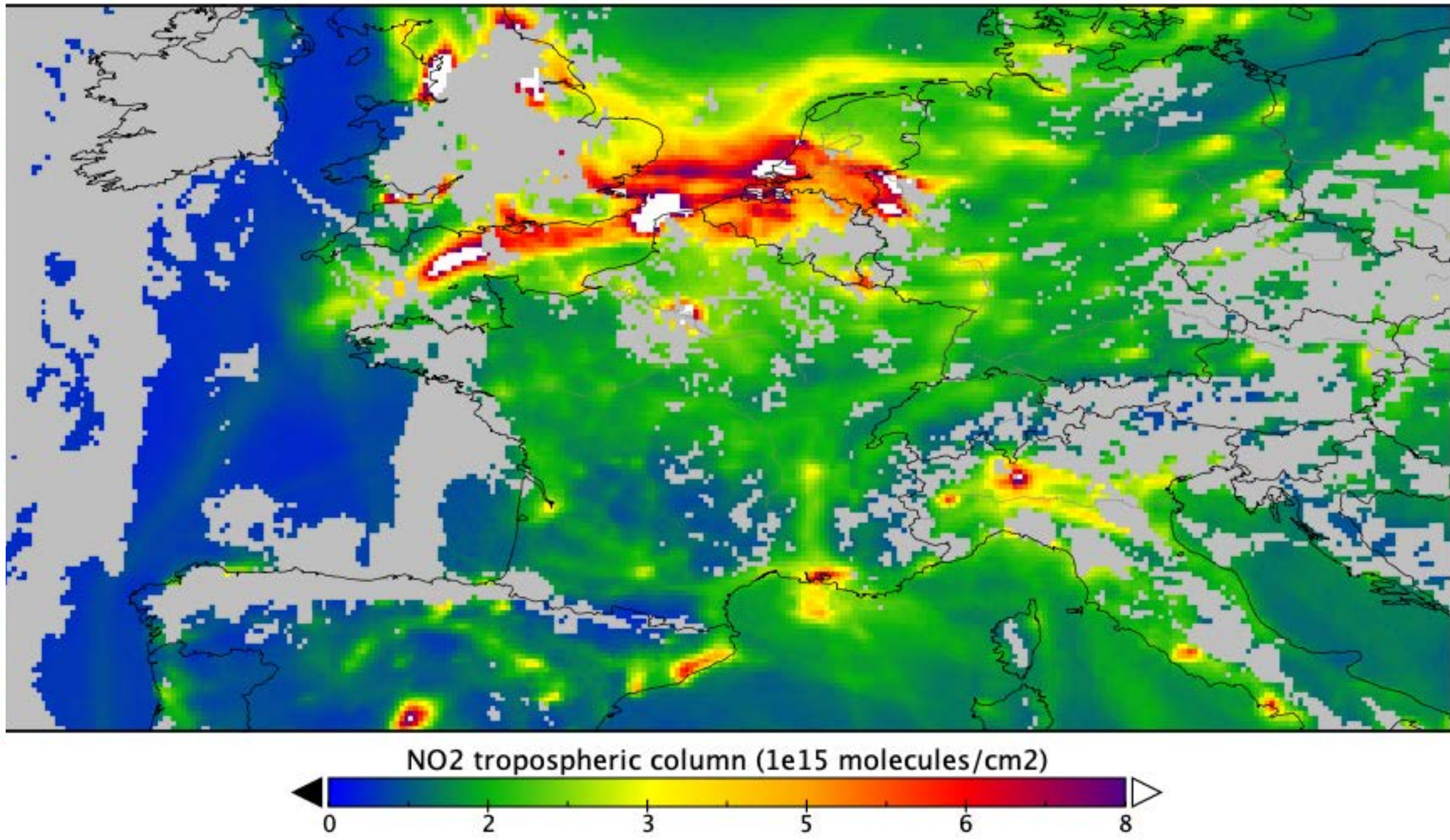
atmosphere.copernicus.eu

Using a-priori profiles from CAMS-regional AQ forecasts for Europe

TROPOMI NO2 based on CAMS-regional a-priori

CAMS-regional vertical column NO2

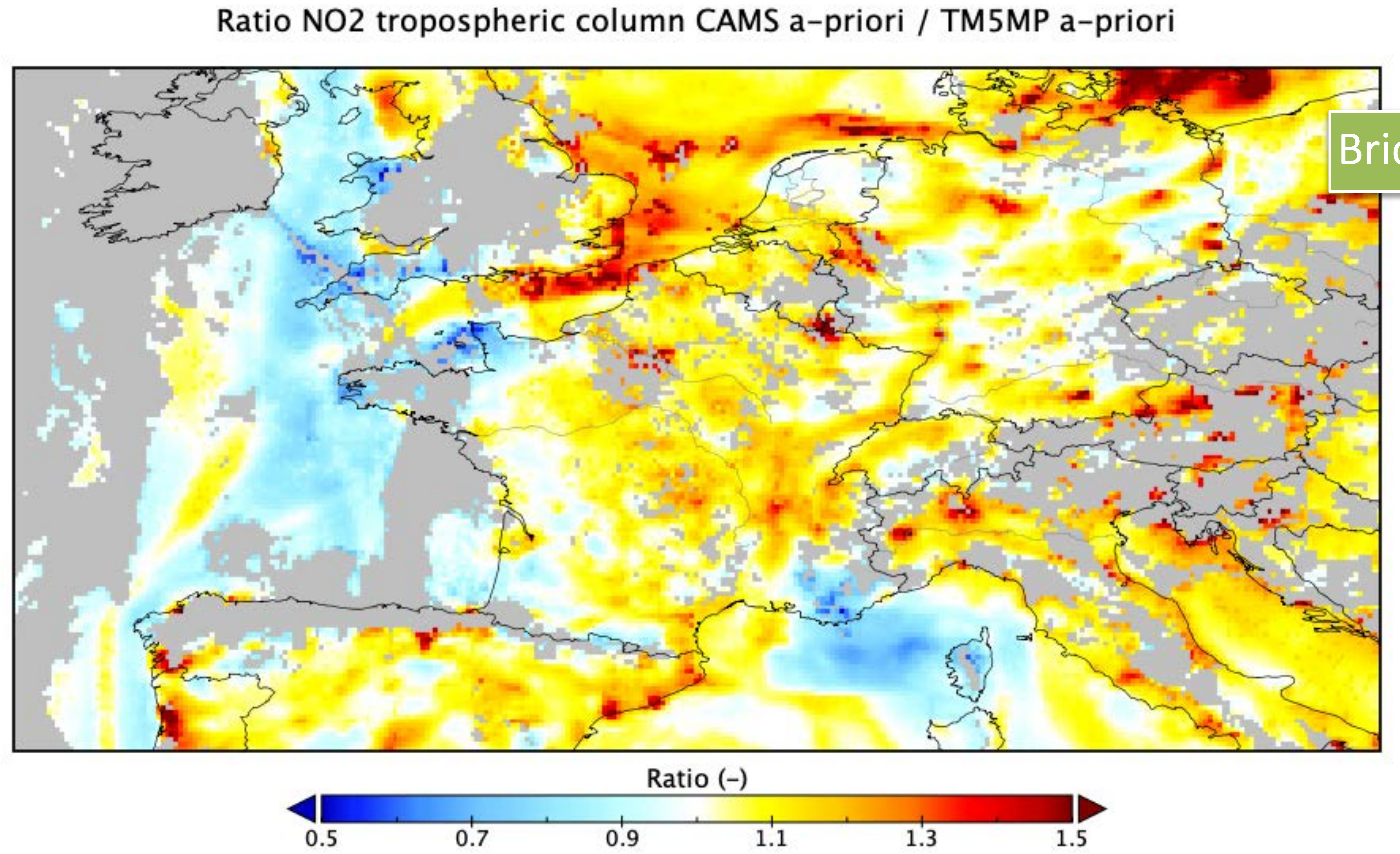




Single overpass, 26 July 2018

John Douros, KNMI

Using a-priori profiles from CAMS-regional AQ forecasts for Europe



Bridge the gap with MAXDOAS

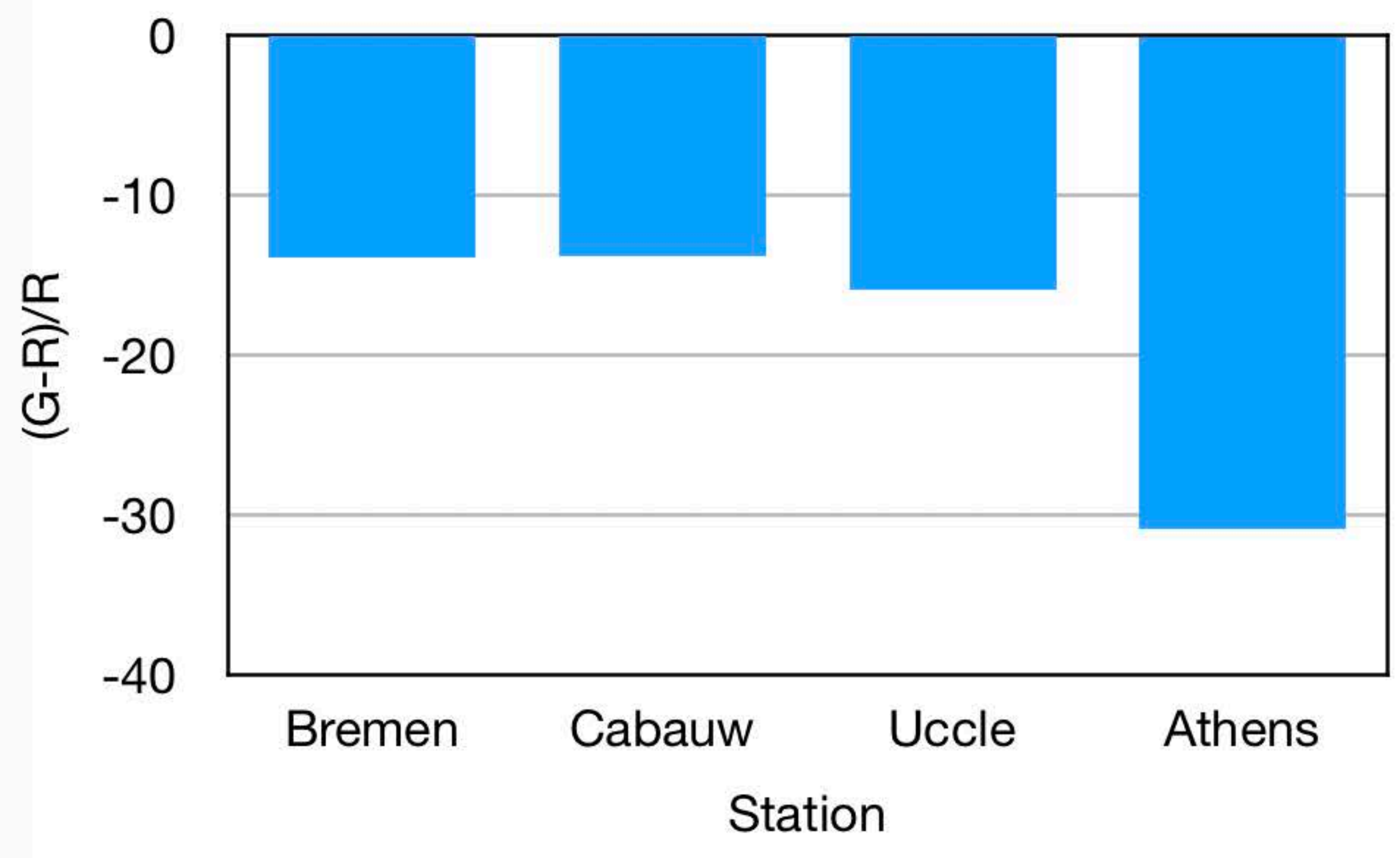
Tropospheric column increases by 10-50% over hotspots when using high-resolution regional model a-priori profiles
1x1 degree -> 0.1x0.1 degree

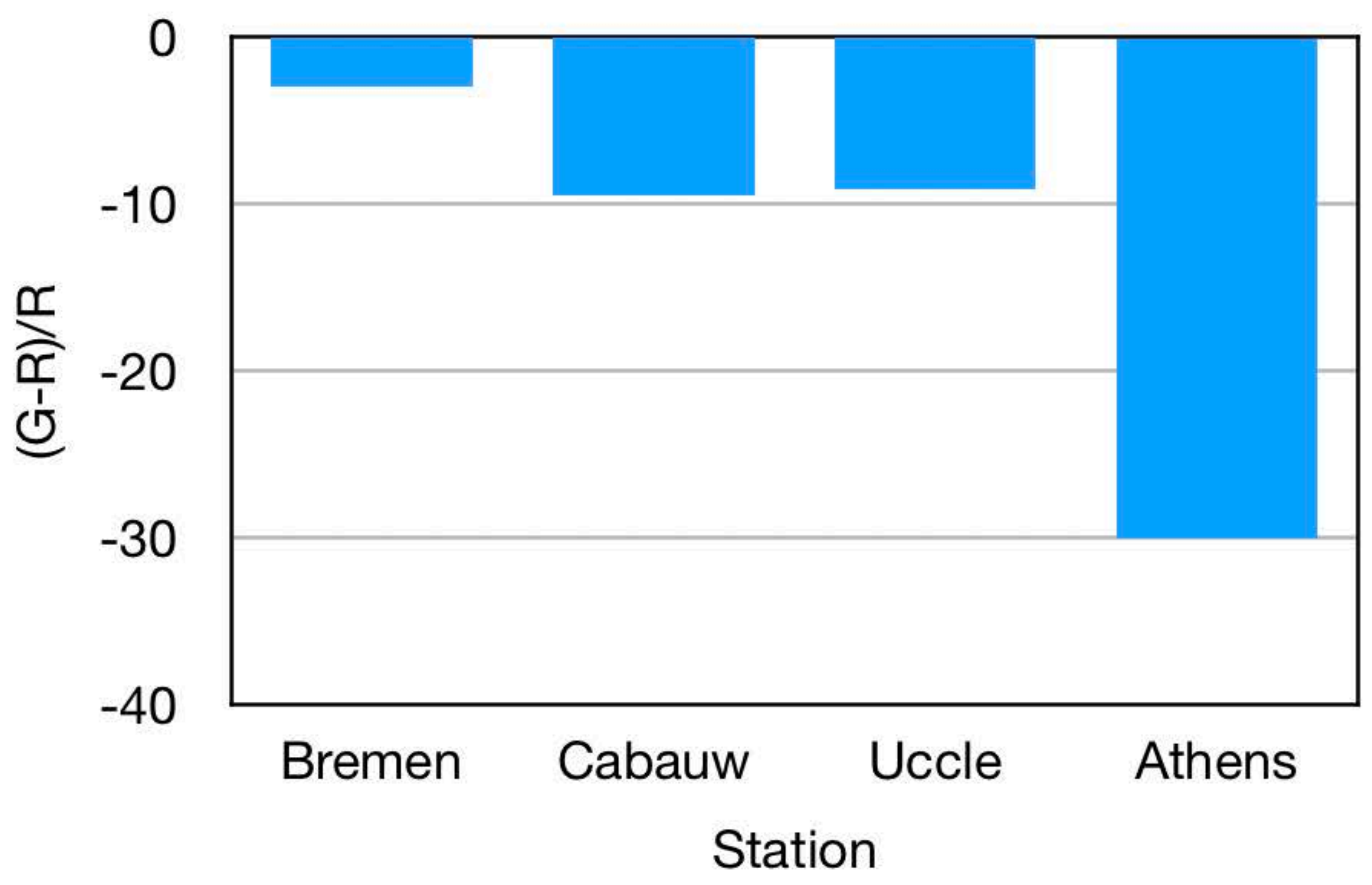
John Douros (KNMI)

Using a-priori profiles from CAMS-regional AQ forecasts for Europe

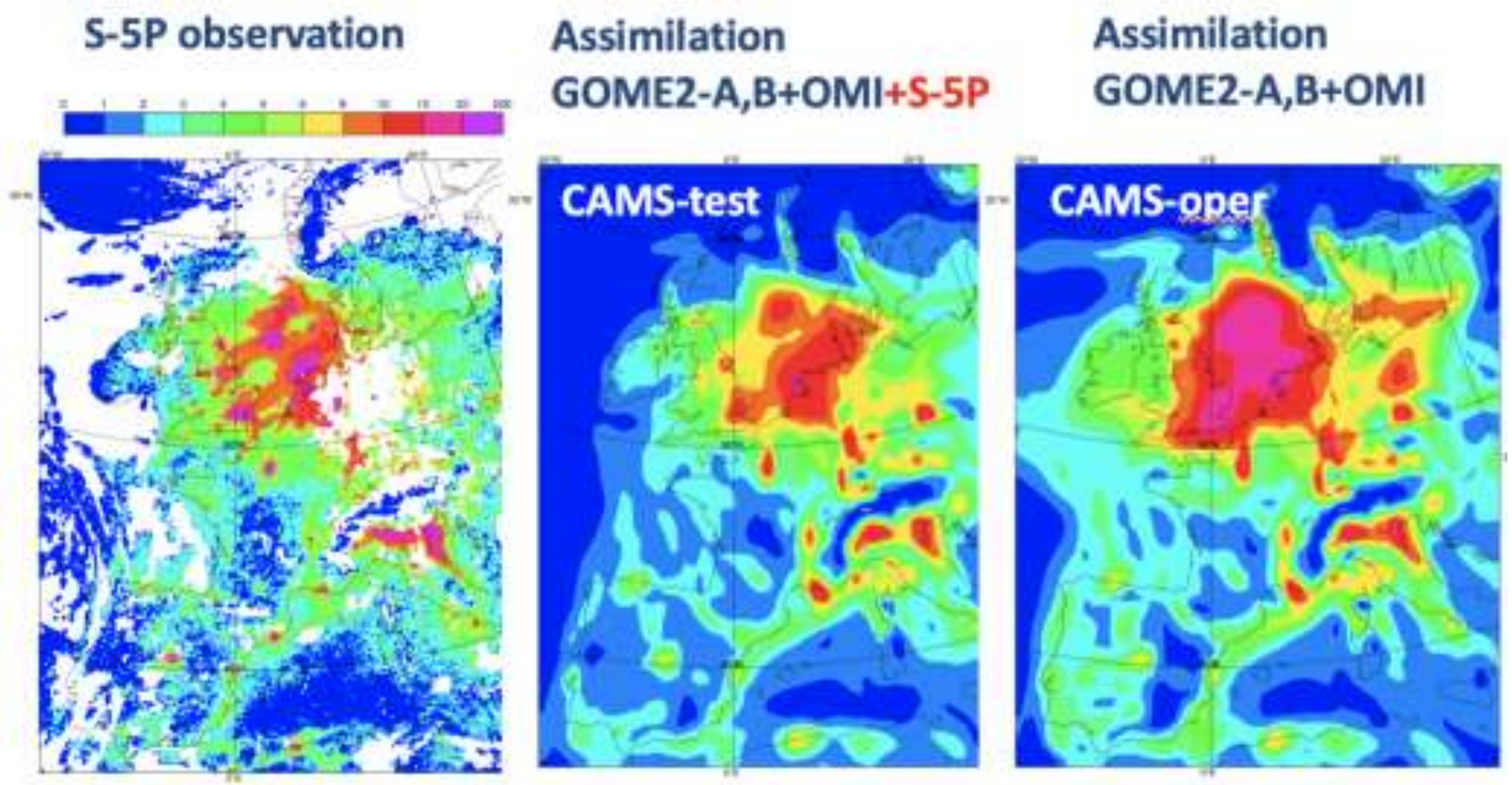
Ratio of retrievals @ MAX-DOAS stations, performed with:

- TM5-MP at a resolution of about 100x100 km
- CAMS-regional (European domain), resolution 10x10 km





Assimilation of TROPOMI NO2 with CAMS - example



CAMS global based on ECMWF-IFS: assimilation of TROPOMI NO2 (27/02/2019)

A. Inness, ECMWF

TROPOMI Conclusions

www.tropomi.eu

www.temis.nl

sentinels.copernicus.eu

#tropomi, @tropomi

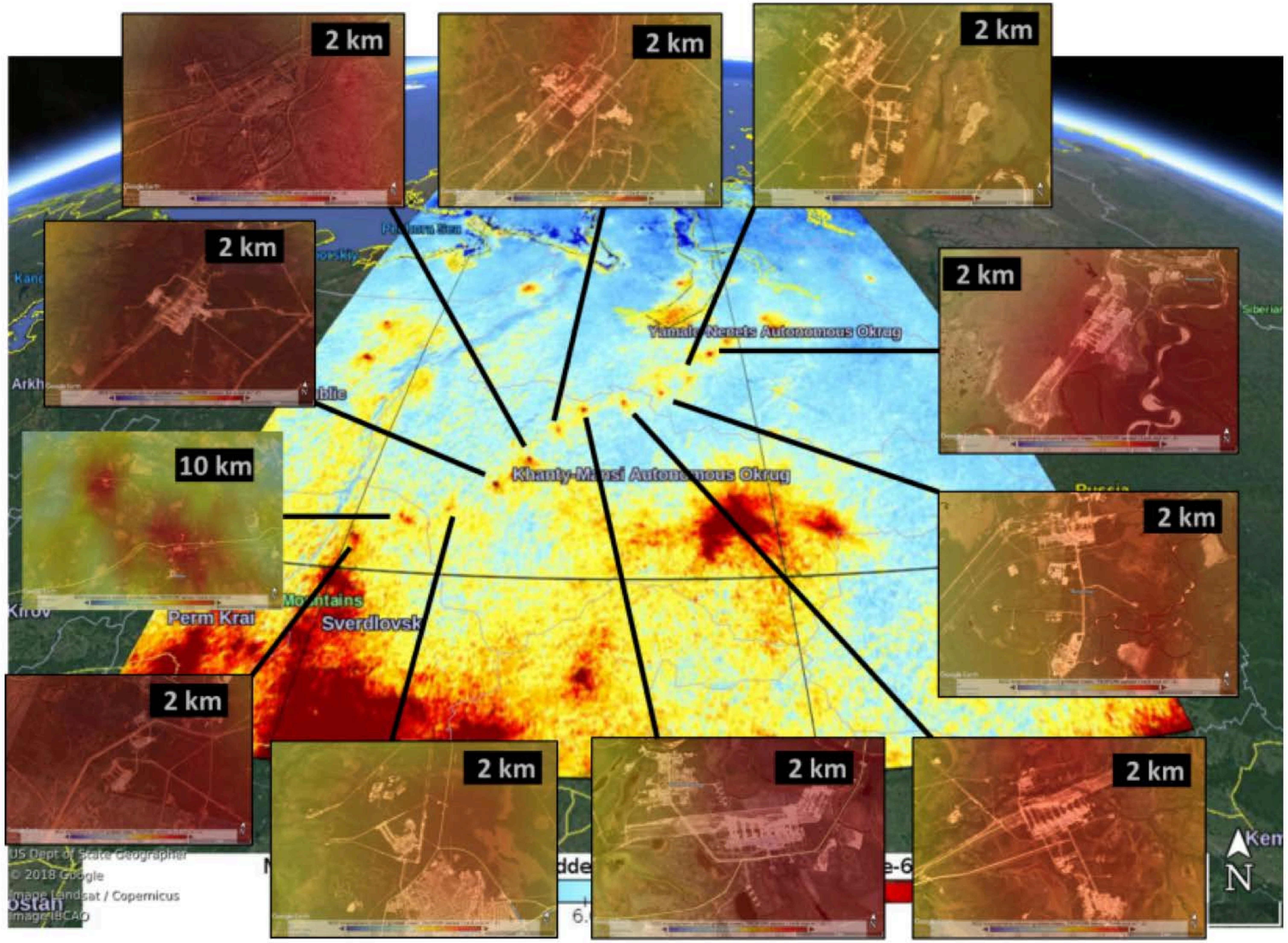
- A game changer in spatial resolution and signal-to-noise!
- NO_2 reprocessing (RPRO) for 30 April - October 2018 (v1.2) available together with v1.2/v1.3/v1.4 OFFL (1.5 year of data)
- Data product includes inputs and intermediate results, provides full traceability
- August 2019: Move to smaller pixels (5.5 x 3.5 km nadir)
- Troposphere: MAX-DOAS indicates NO_2 low bias of about 30%
  -> Resolution of the a-priori main source of uncertainty:
  need for high-resolution regional AQ model profiles
  -> Sensitivity to cloud pressure (ongoing research)
- **Keep tuned for new TROPOMI updates with new version of NO2 and Level 1 data mid-to-end 2020**
- **TROPOMI data will be increasingly in CAMS global models**

EXTRA SLIDES

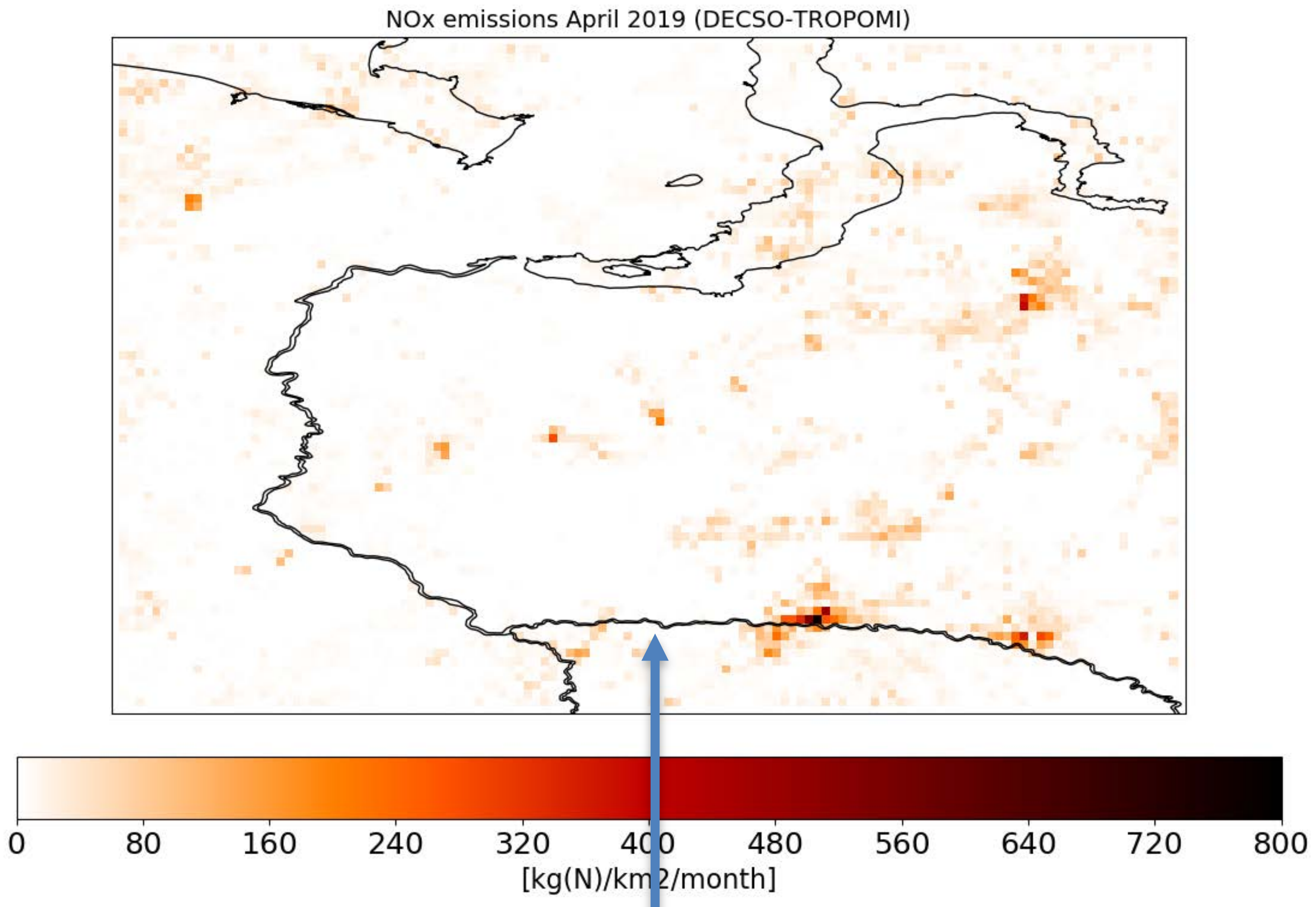
SENTINEL 5 PRECURSOR	
Launch	13 October 2017
Launcher	Rockot from Plesetsk Russia
Orbit	Polar Sun synchronous, altitude 824 km
Overpass time	13:30 local time
Mission duration	7 year
Satellite	Airbus Astrobus-M, height 3,55 m, 5,63 m diameter, mass 820 kg
Payload	Tropospheric Monitoring Instrument (TROPOMI)
Ground stations	Svalbard (Norway), Inuvik (Canada) and Kiruna (Sweden)
Data processing	DLR Oberpfaffenhofen (Germany) KNMI De Bilt, The Netherlands


NO2 tropospheric column (μmol/m^2)
5
20
35
50
65
80
95
TROPOMI NO2
Apr-Sep 2018
Cluj

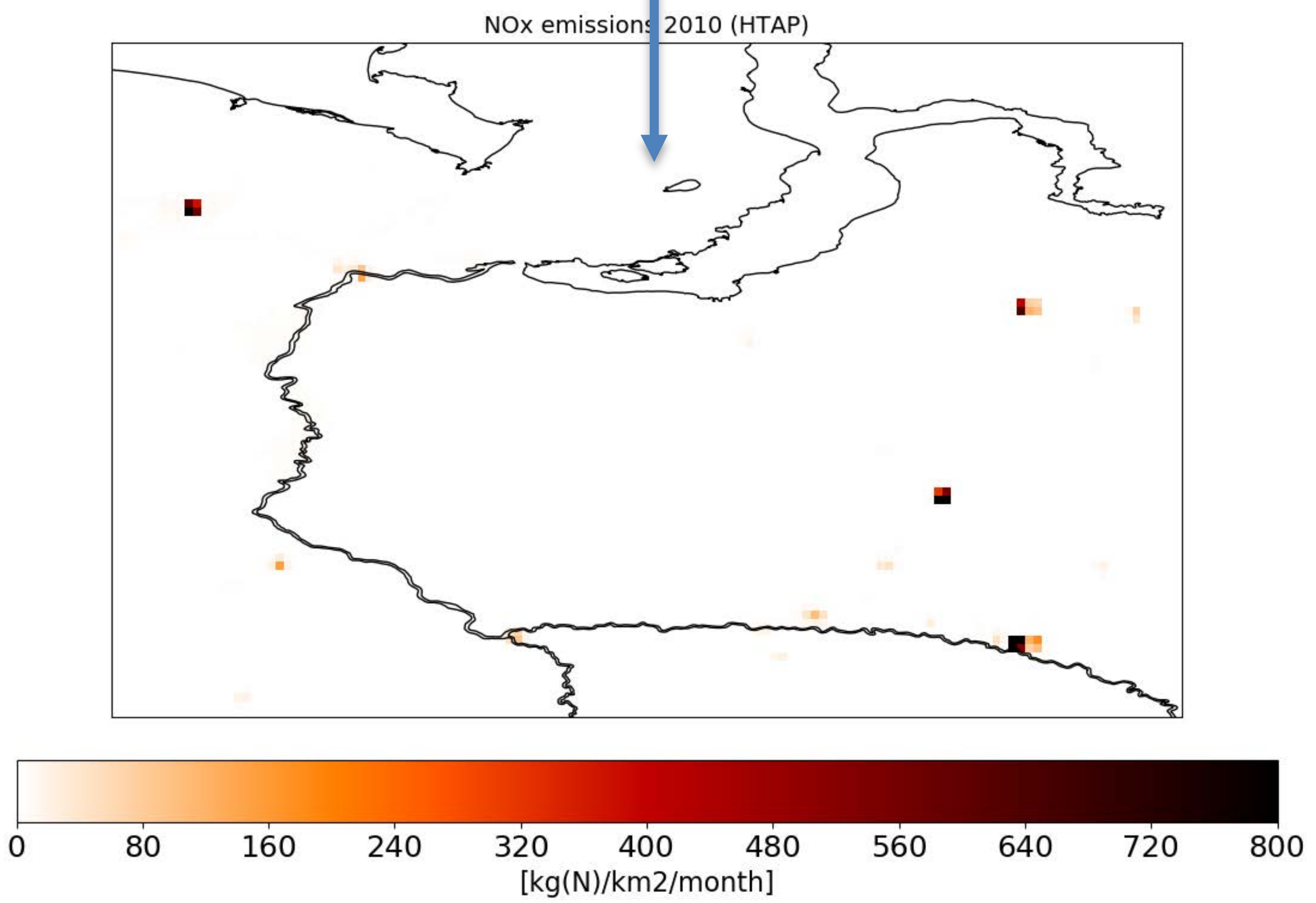

South America, August 2019



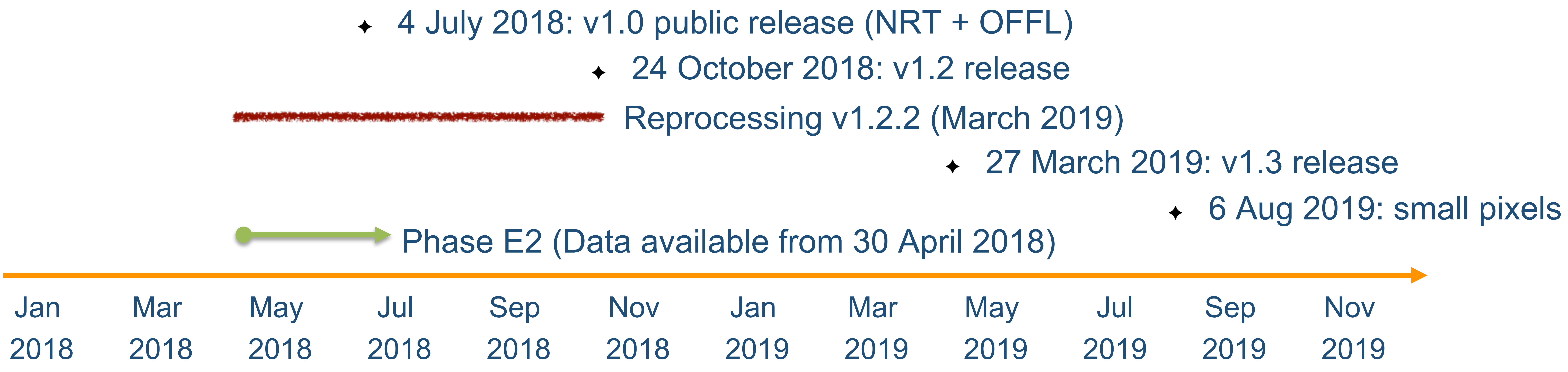
string of gas compressor stations along natural gas pipeline every ≈ 100 km



TROPOMI NO_2 emission inversion (DECSO) for April 2019 *compared with* bottom up emission inventory (HTAP/EDGAR)



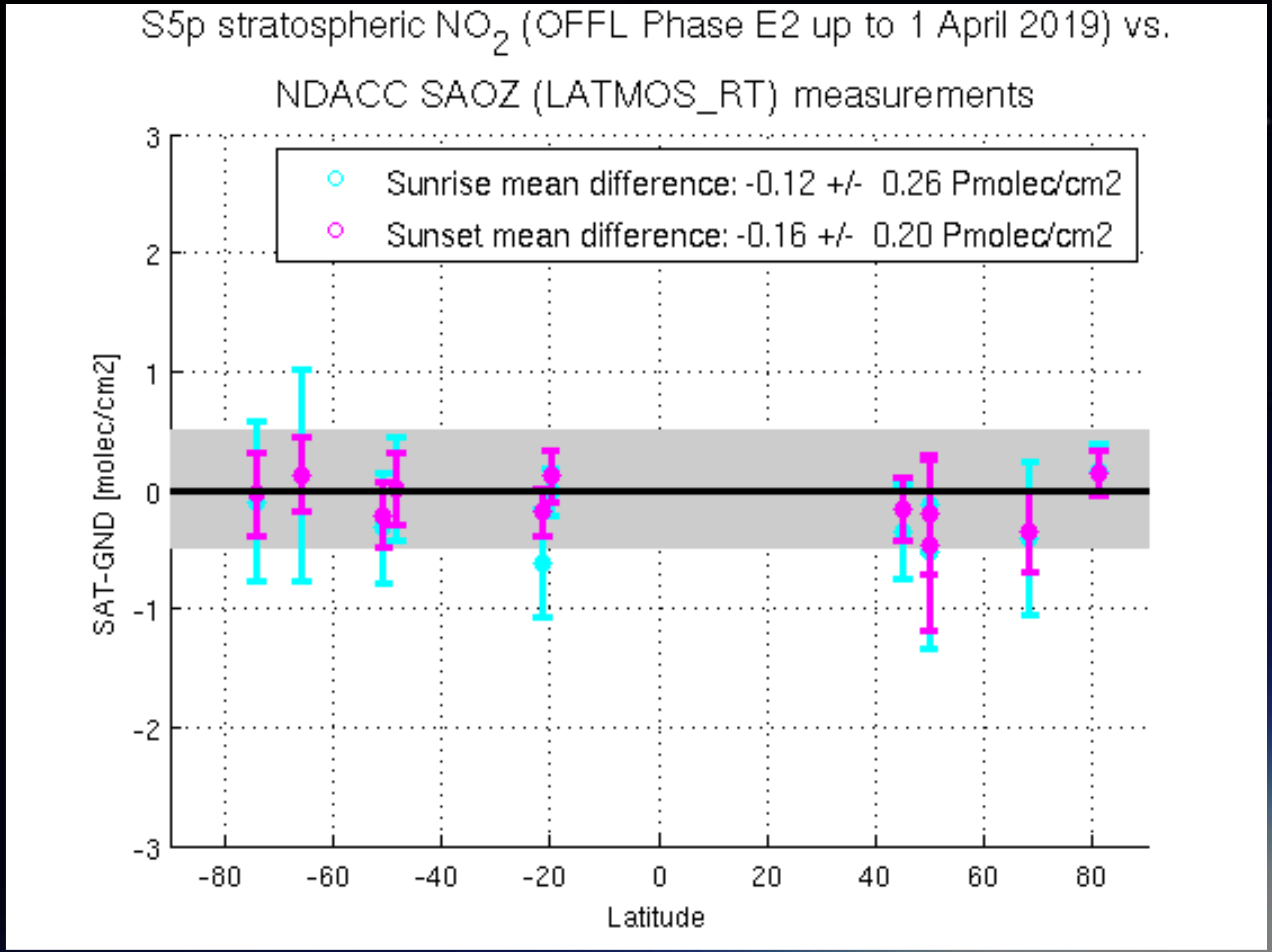
NO2: upgrades and reprocessing

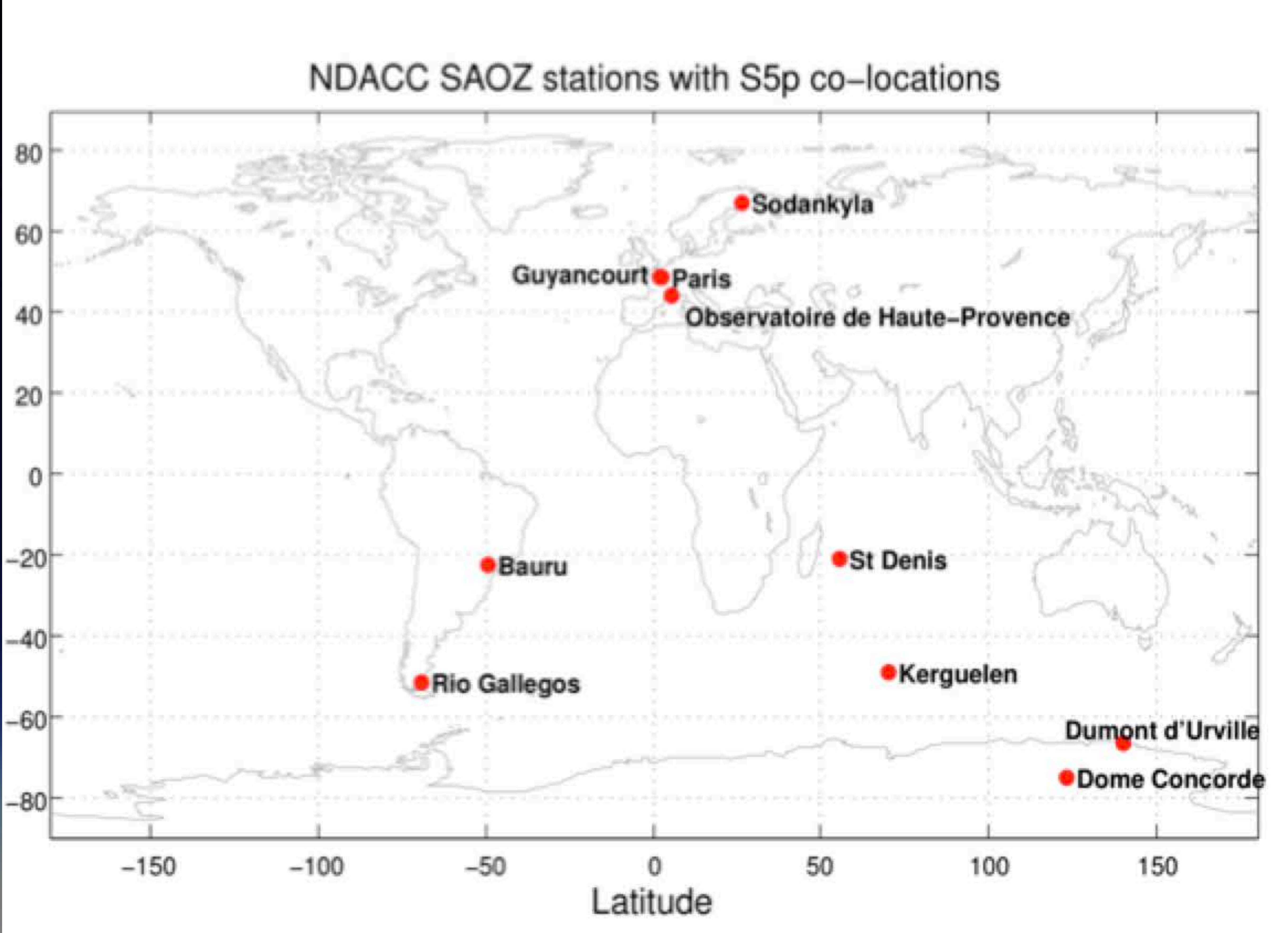


Each of these releases accompanied with documentation updates:

- **ReadMe (PRF)**
- **Product User Manual (PUM)**
- **Algorithm description (ATBD)**

S5P MPC: TROPOMI vs SAOZ





Steven Compernolle, Tijl Verhoelst, Gaia Pinardi, José Granville, Jean-Christopher Lambert (BIRA-IASB), Kai-Uwe Eichmann (IUP-B)