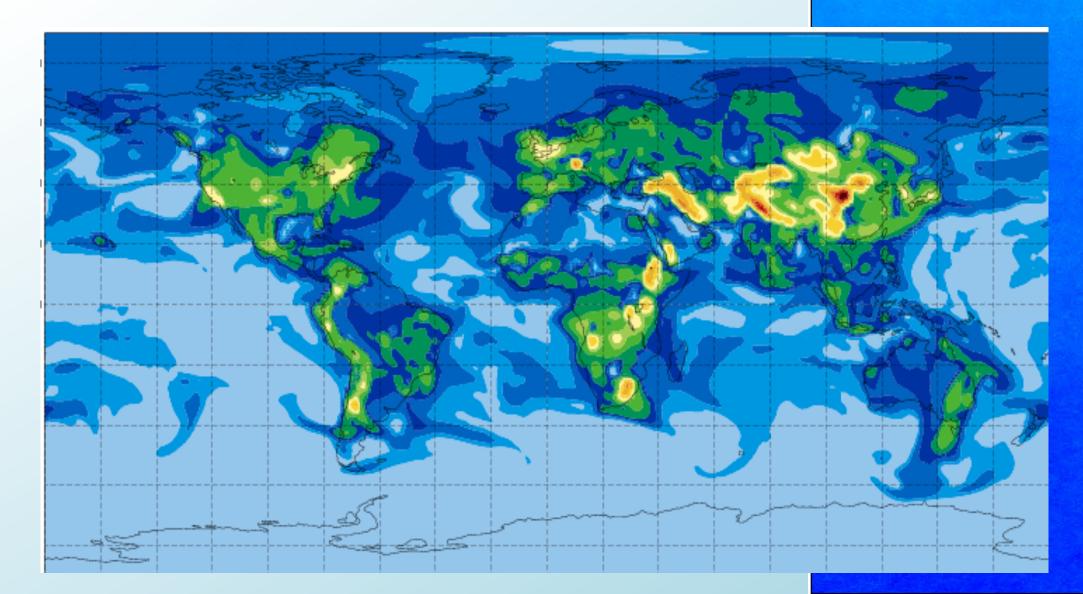


## Satellite observations from TROPOMI on Sentinel-5p: Measurements & Making the link to Models

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

### PAPILA summer school, 24 April 2020





	NO2 tropospheric column (µmol/r			
0	10	20	30	40

E/S



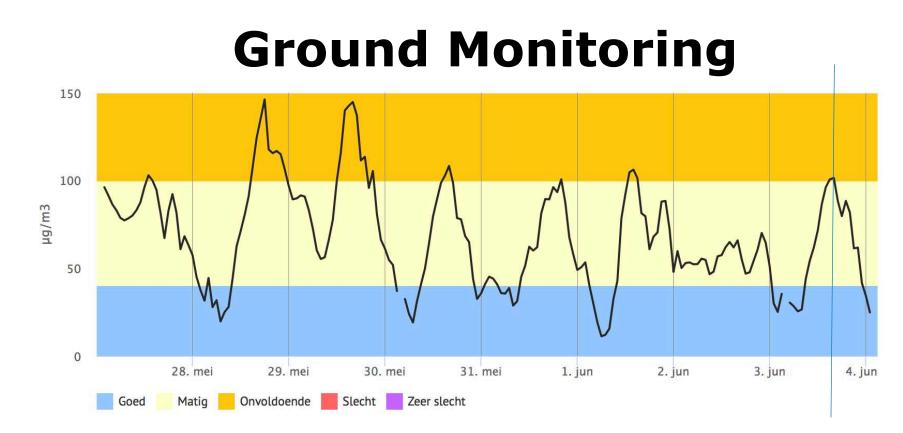
# How does satellite data fit in global air quality monitoring?





### **Vertical profile information**



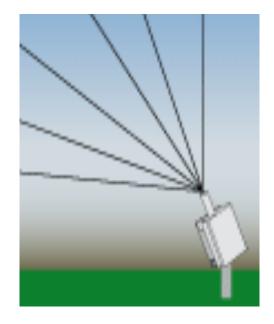


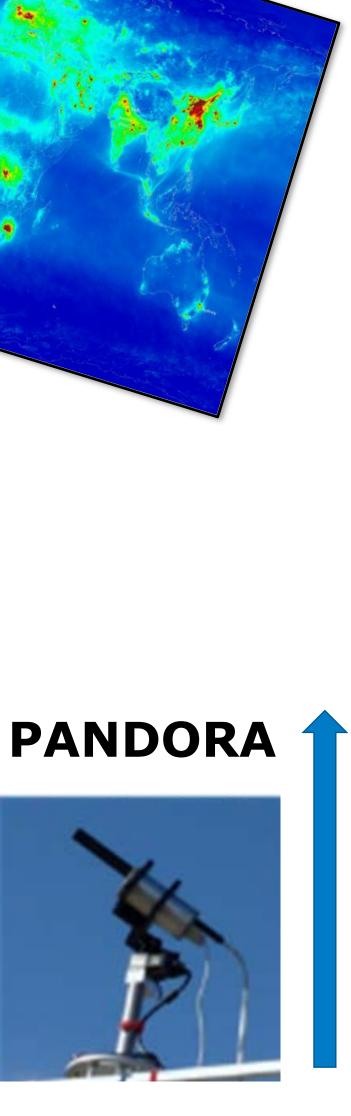




### Stratosphere

### MAX-DOAS, PANDORA





#### KNMI – Royal Netherlands Meteorological Institute -- R&D Satellite Observations Department Earth Science from Space **KNMI** is involved MSG

KNMI plays an important role in developing earth observation satellites and in processing and interpreting their data. Forecasts for weather and climate, air pollution and solar radiation are largely made with data from these satellites.

Geostationary satellites, such as MSG, orbit so as to maintain a fixed point above the Earth

– 36.000 km –

Polar satellites orbit at about 800 km from pole to pole, while the earth turns underneath

Northern lights

Thermosphere 85 km Meteorites

I.

0

S

0

Σ

Mesosphere 50 km

Weather balloon

Ozone layer, protects against UV radiation

Troposphere

In this layer of the atmosphere our weather takes place Important satellites with which KNMI works:

ΟΜΙ 2004

NASA/KNMI Measures ozone and air pollution MetOp 2006 ESA/EUMETSAT Ozone, wind and air pollution

What do our satellites measure?

**Ozone** layer Ozone is monitored using UV light

> Clouds Cameras take pictures of the earth

Wind Radar waves reflect from sea waves from which wind is calculated **Climate change** 

Greenhouse gases such as methane are measured using infrared light

**Air pollution** Small particles and gases,

such as nitrogen dioxide, particulate matter and volcanic ash, are measured using UV light



2002-2021 ESA/EUMETSAT Cloudiness, air pollution, sun and precipitation

in the entire process from inception to use of satellite data.

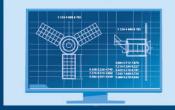


Formulating requirements





Design







#### Data processing



#### **Data interpretation**



To customers Univer-Aviation sities Government Meteoro-Citizens logists

ESA/KNMI Air pollution, ozone and climate change

TROPOMI

2017

Aeolus 2018 ESA/KNMI Wind profiles

EarthCARE 2019 -and climate change



Measuring air pollution is increasingly important. NO<sub>2</sub> measurements show that the air in Europe is not clean:

high high



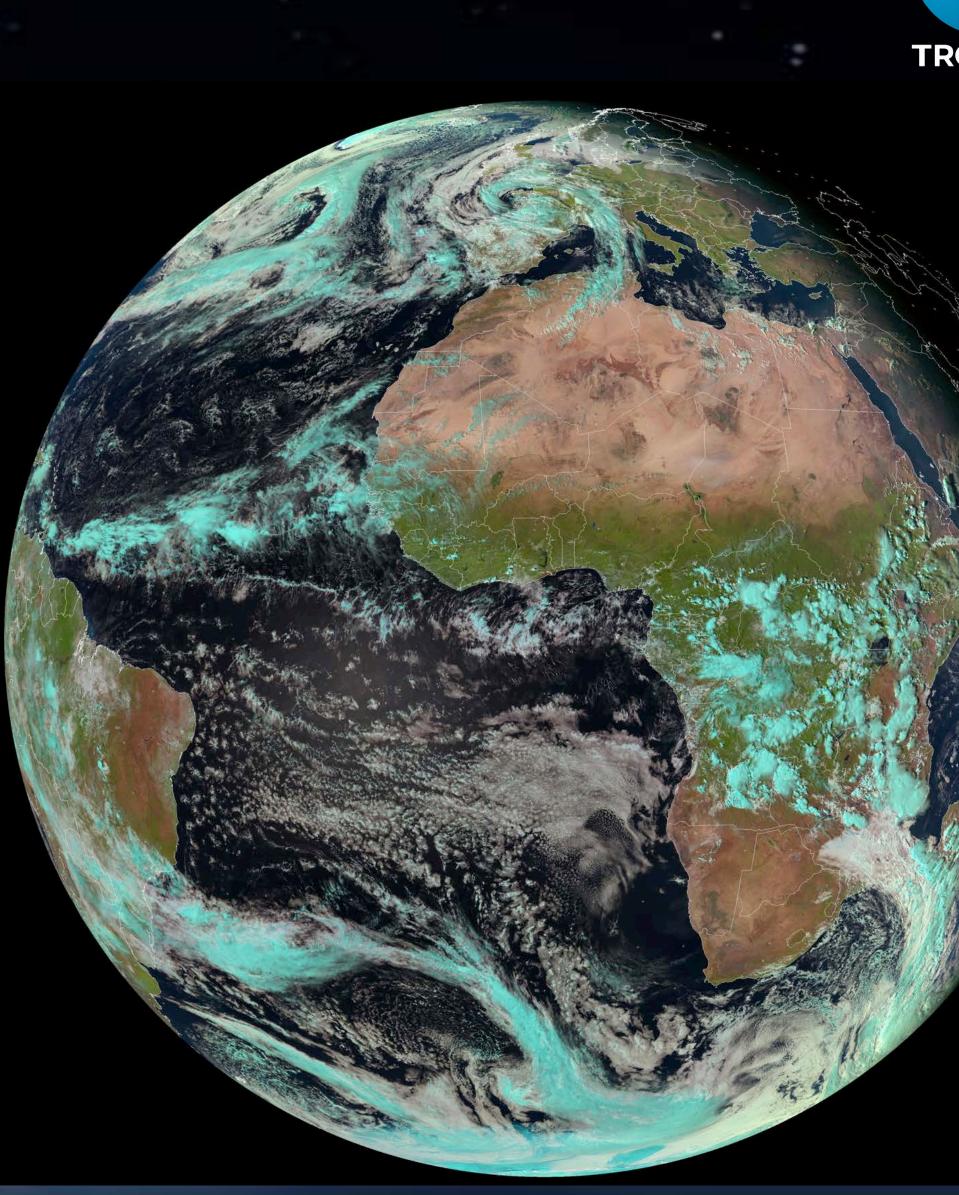
The biggest air pollutants are

- Nitrogen dioxide (NO2)
- Particulate matter (PM)
- Ozone (O3**)**

low

## 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

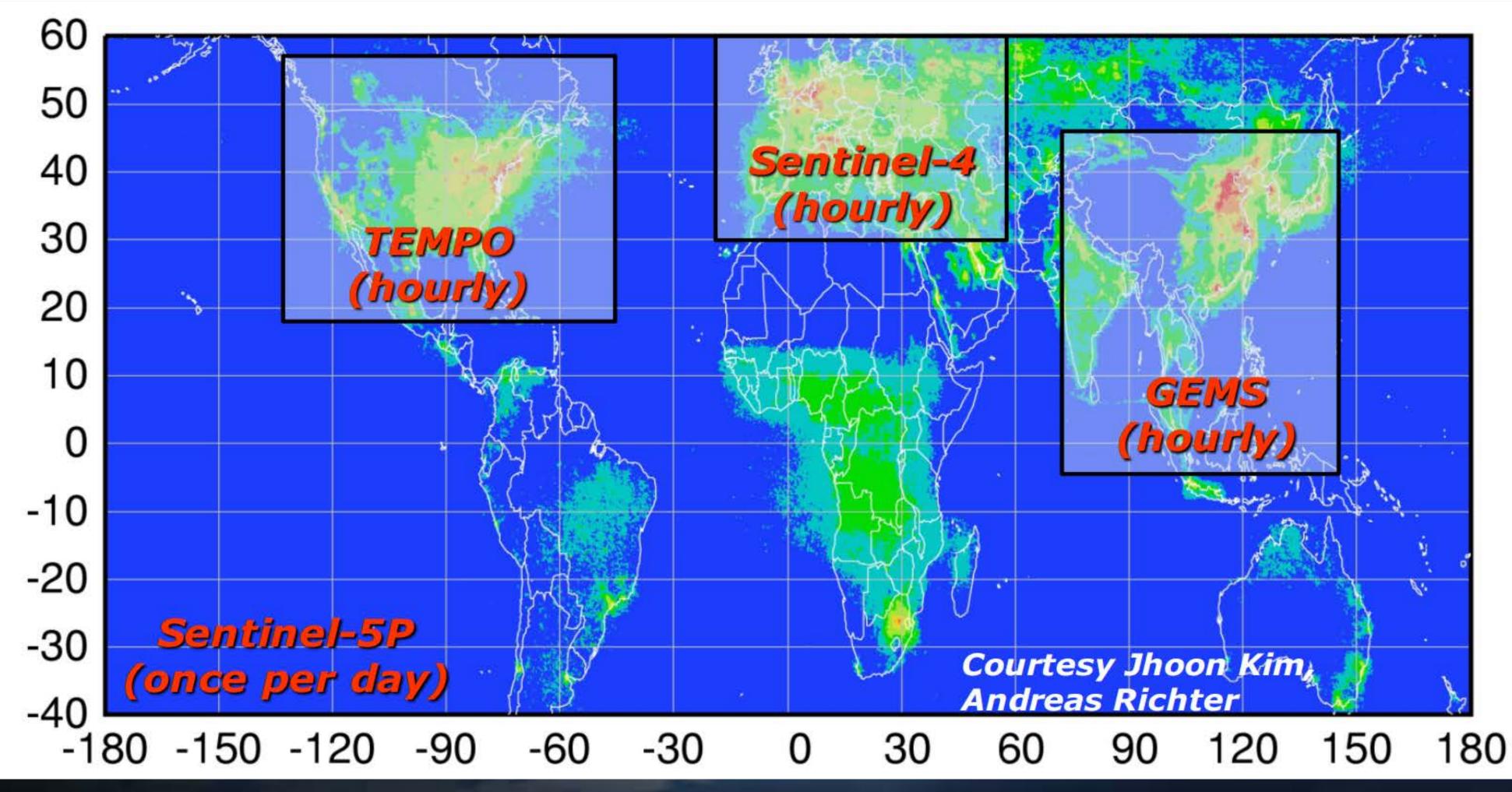






## GEO + LEO Observing Strategy

### Global pollution monitoring constellation: Tropospheric chemistry missions funded for launch 2016–2021





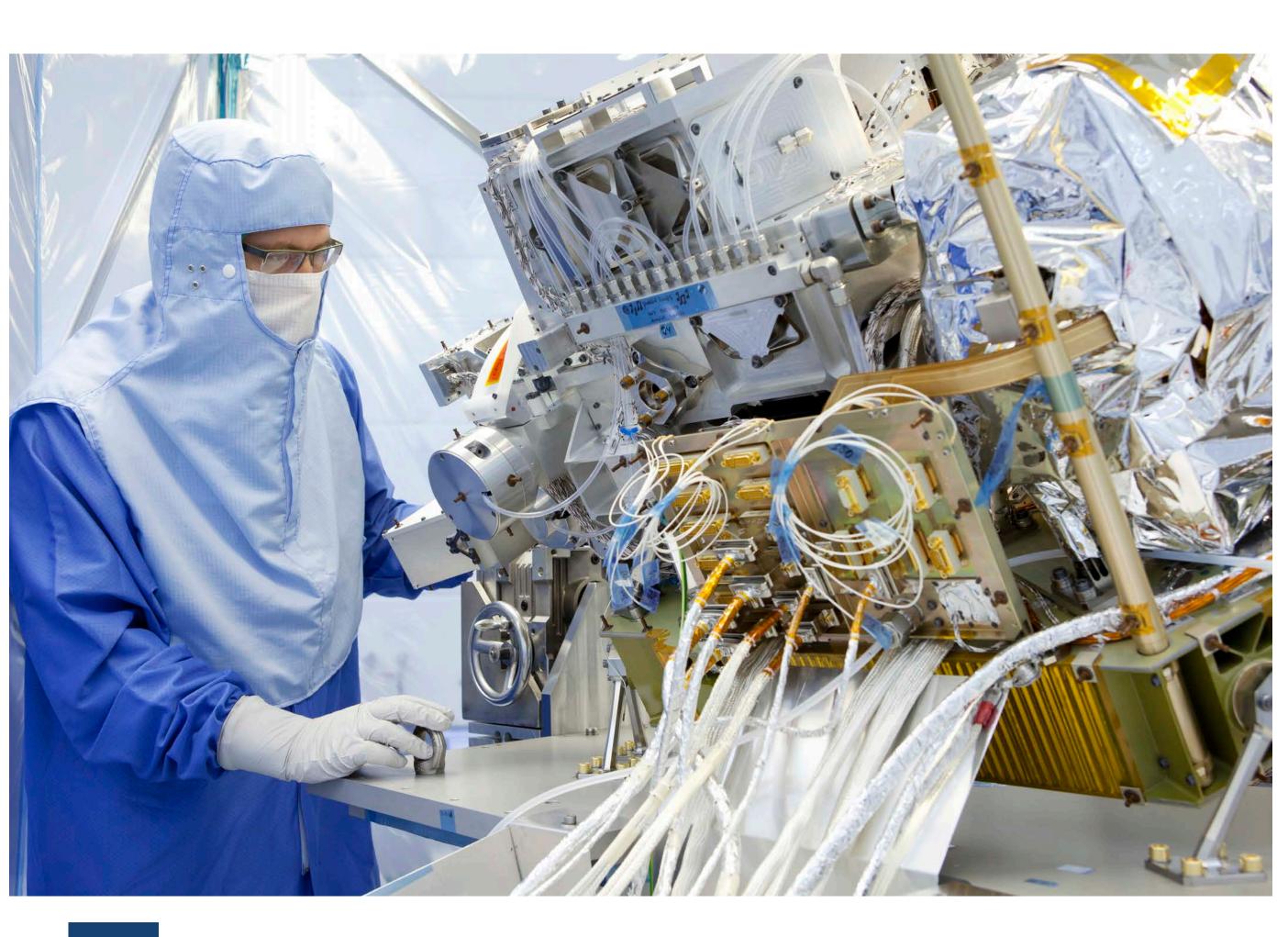


## Focus on TROPOMI: **TROPOspheric Monitoring Instrument** > Monitoring atmospheric composition, for:

- - 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
  - <u>www.tropomi.eu</u> &
  - https://scihub.copernicus.eu/



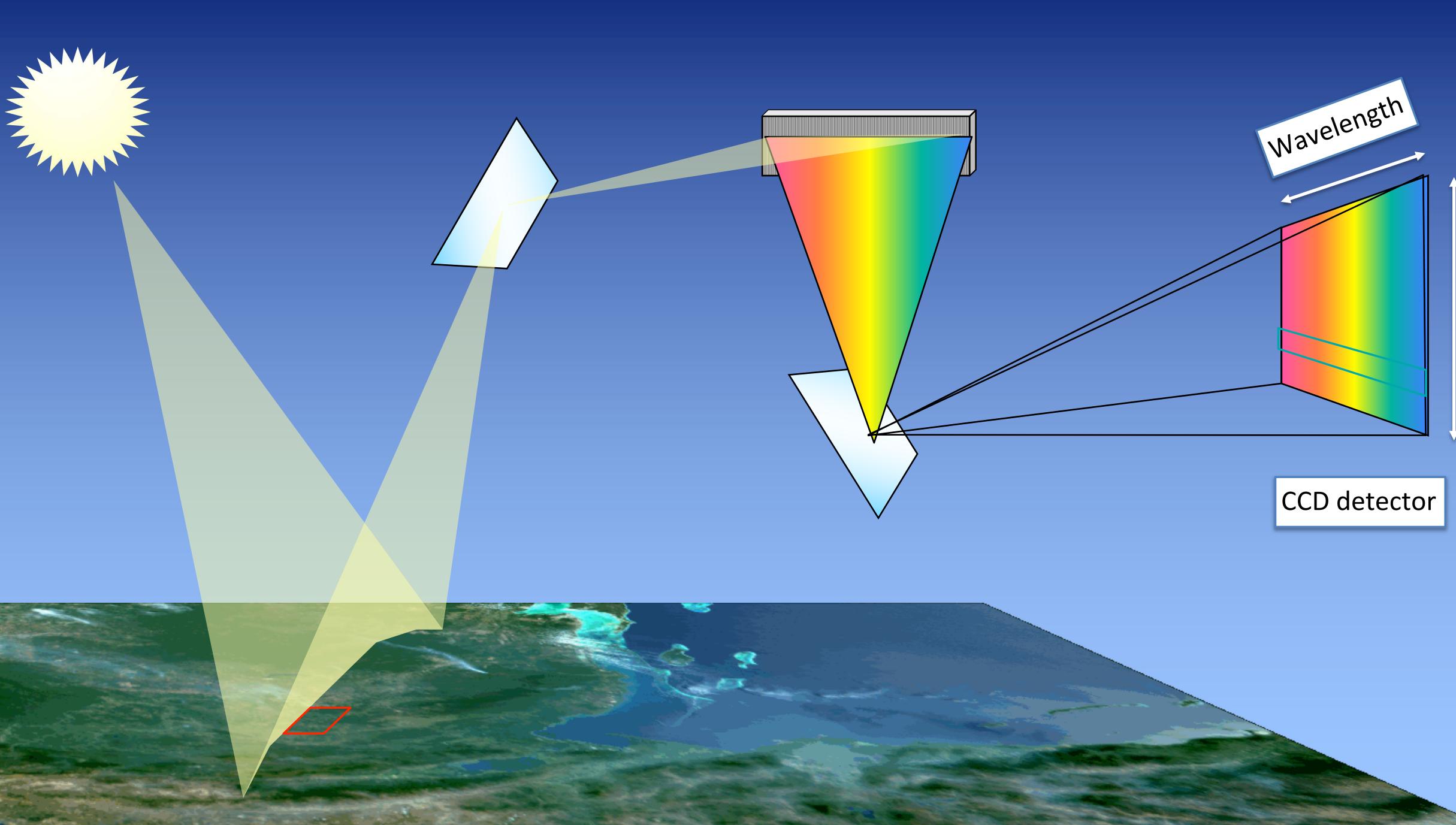








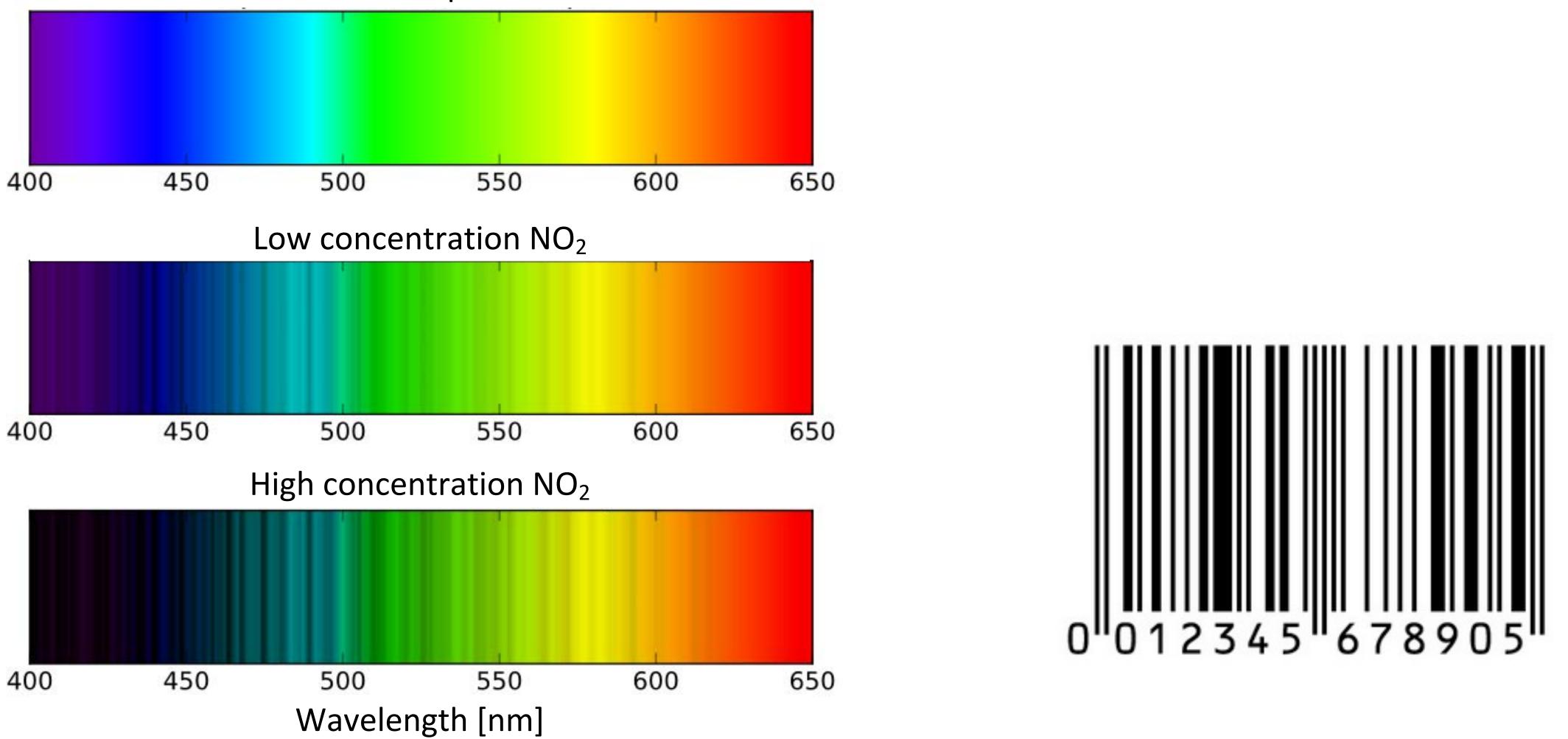


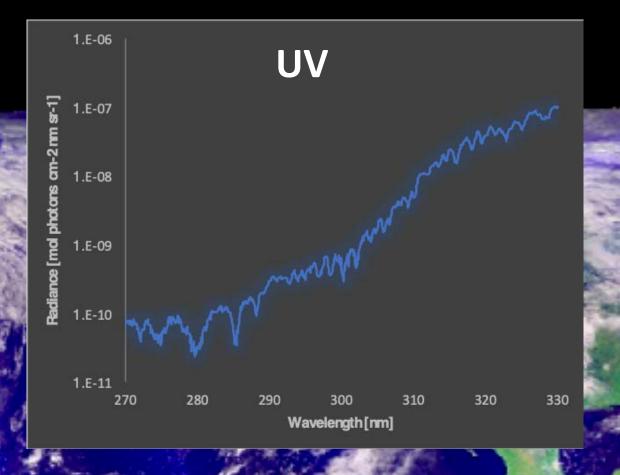




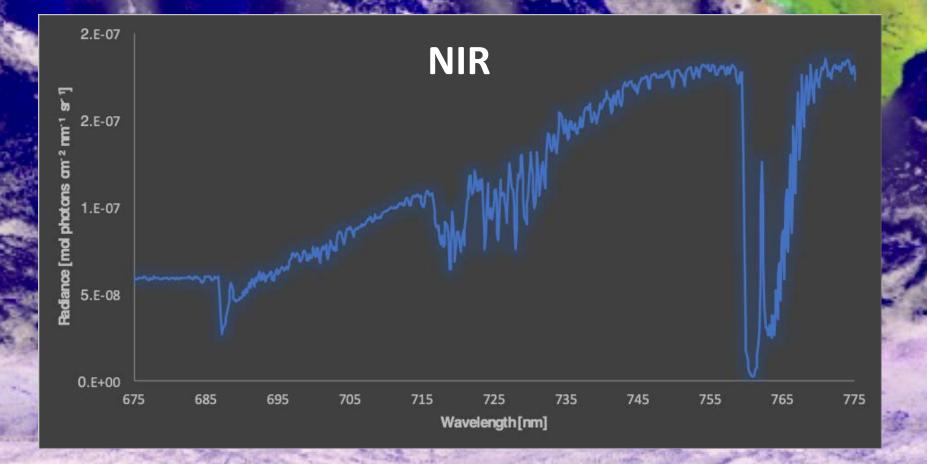
### From spectra to concentrations

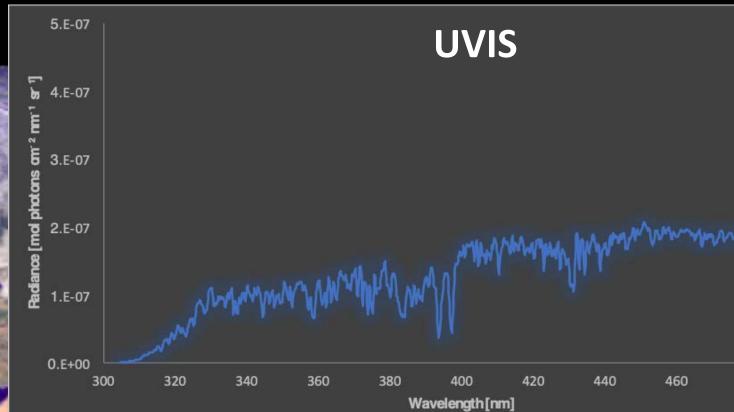
No absorption

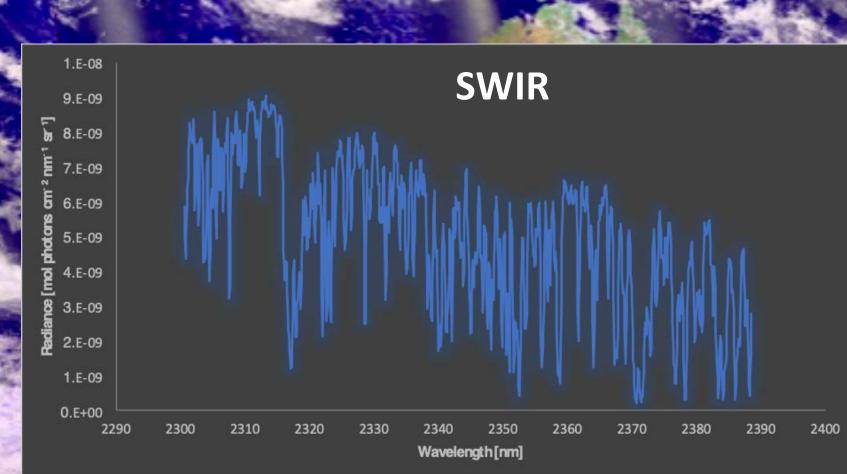


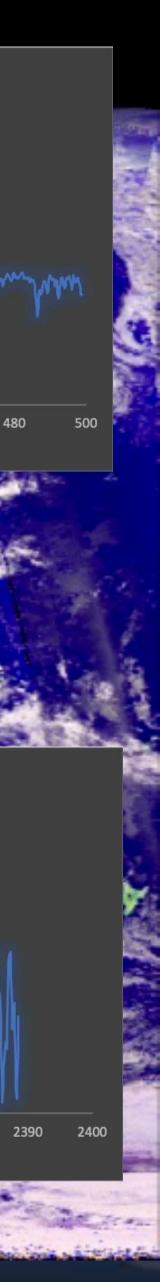


1 scanline per second 440 spectra per scanline **3000 scanlines per orbit** 15 orbits per day 20 million groundpixels per day 225 Gbyte raw data per day 1 Tbyte L1b data per day





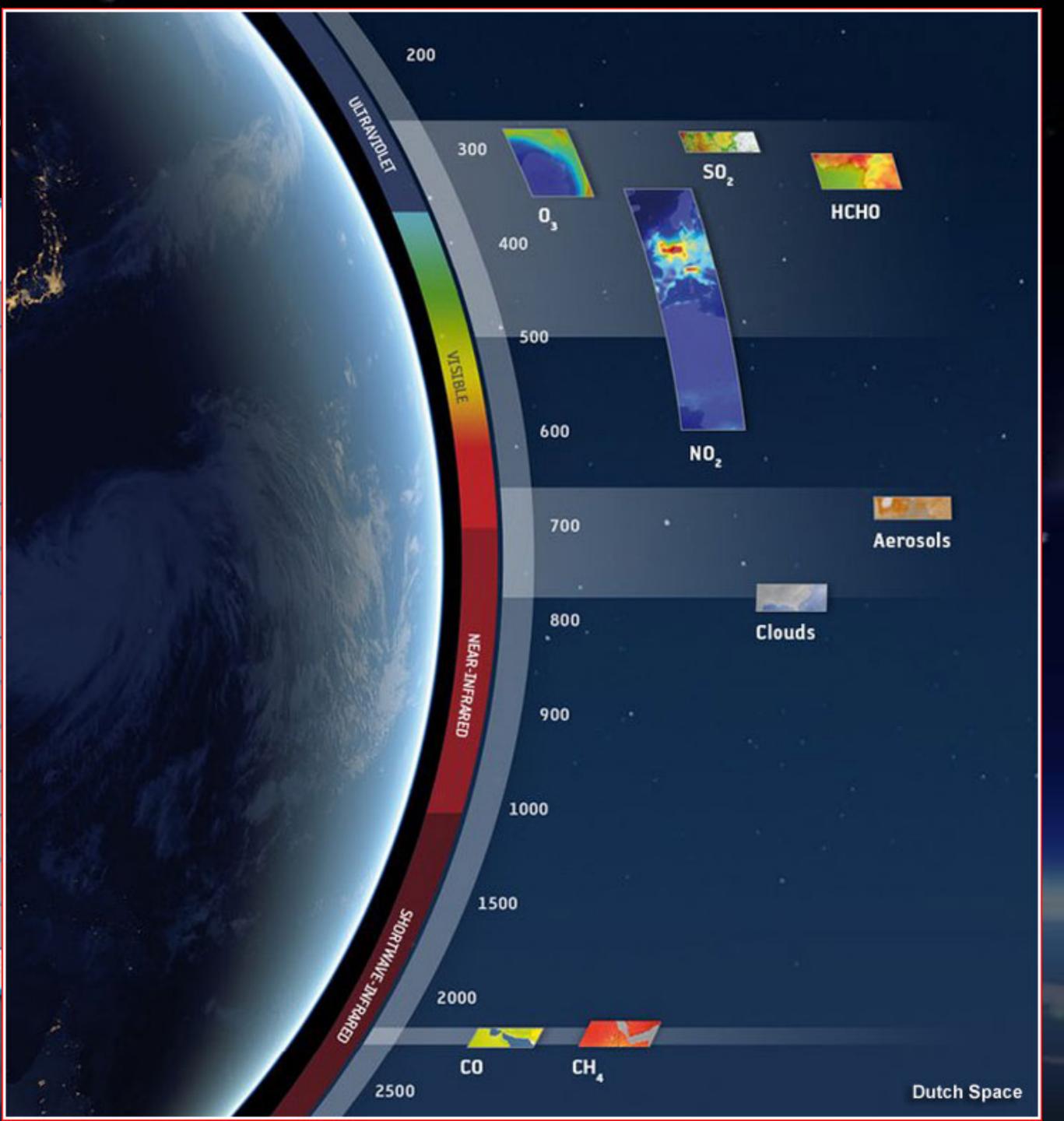




## TROPOMI Level 2 Data Pro

Parameter	Data Product	
	Ozone Profile	
Ozone	Total Ozone	
	Tropospheric Ozone	
	Stratospheric NO <sub>2</sub>	
NO <sub>2</sub>	Tropospheric NO <sub>2</sub>	
50.	SO <sub>2</sub> enhanced	
SO <sub>2</sub>	Total SO <sub>2</sub>	
Formaldehyde	Total HCHO	
CO 🔵	Total CO	
Methane 📂	Total CH <sub>4</sub>	
	Cloud Fraction	
Cloud	Albedo (Optical Thickness)	
	Cloud Height (Pressure)	
Aarocal	Aerosol Layer Height	
Aerosol	Aerosol Type	
Surface UV	Provided by FMI in frame of the	

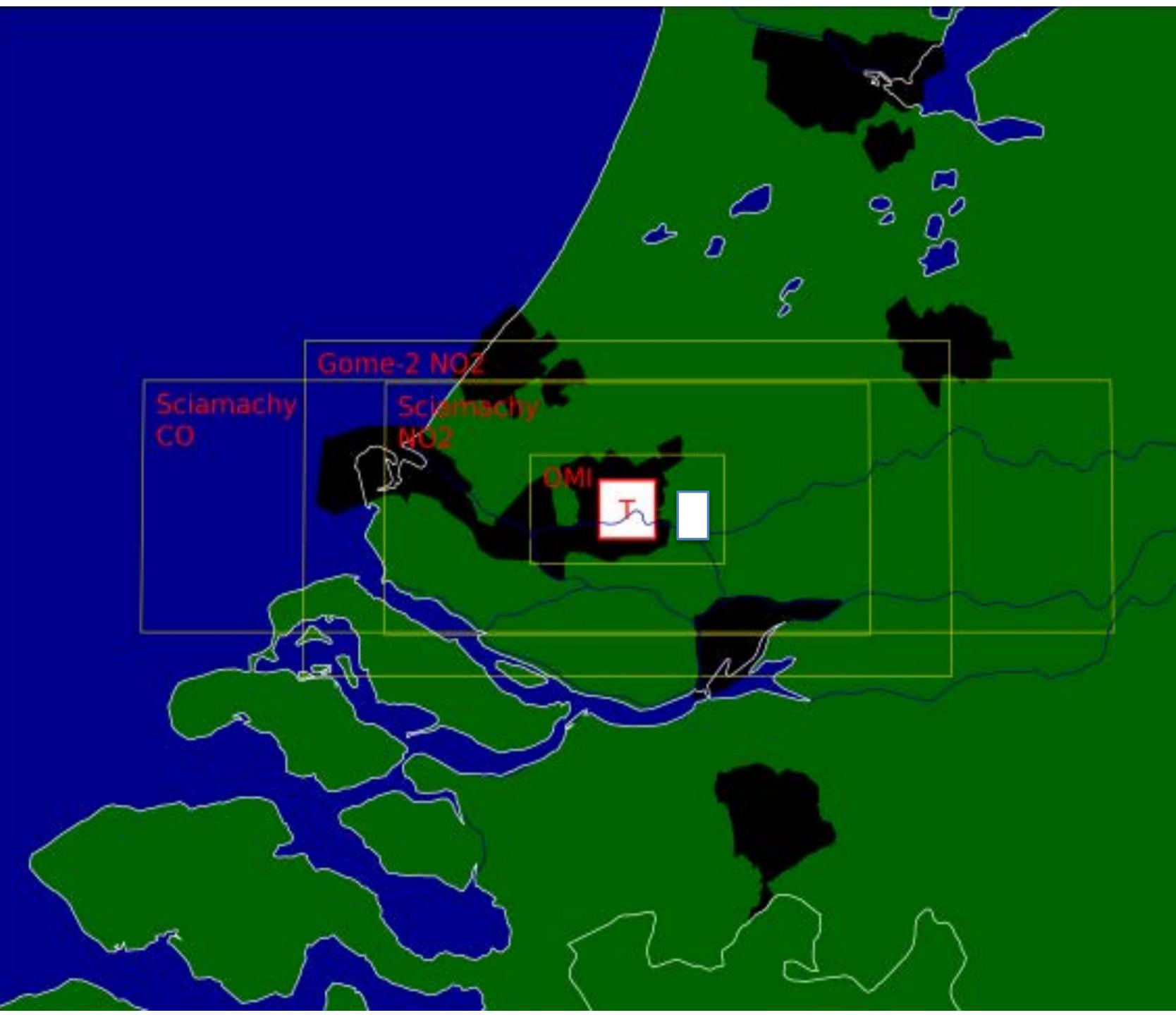
### KNMI | DLR | BIRA-IASB | SRO



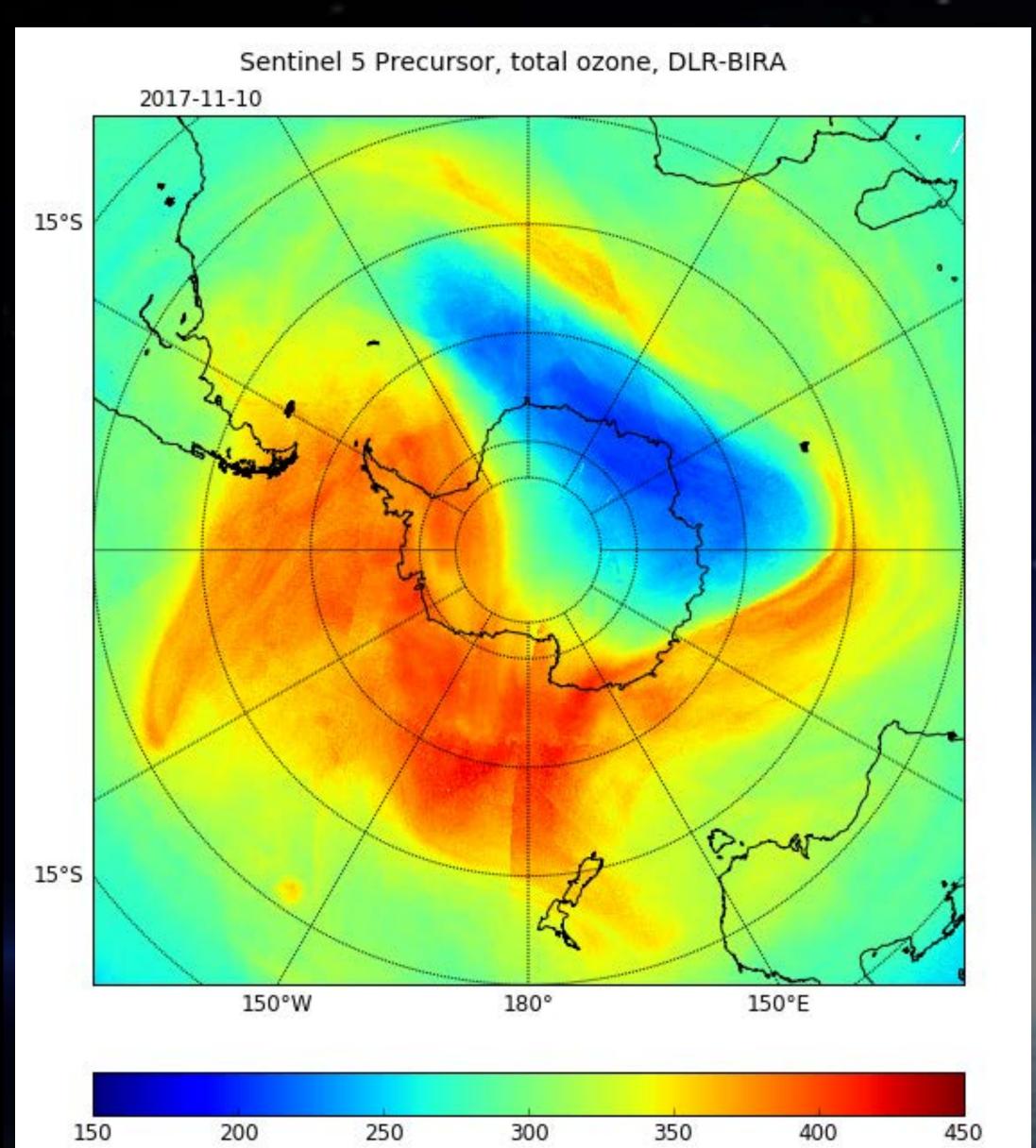
## Spatial Resolution:

Further decreased to 3.5 x 5.5 km in August 2019

Individual source Identification, Intra-city variability

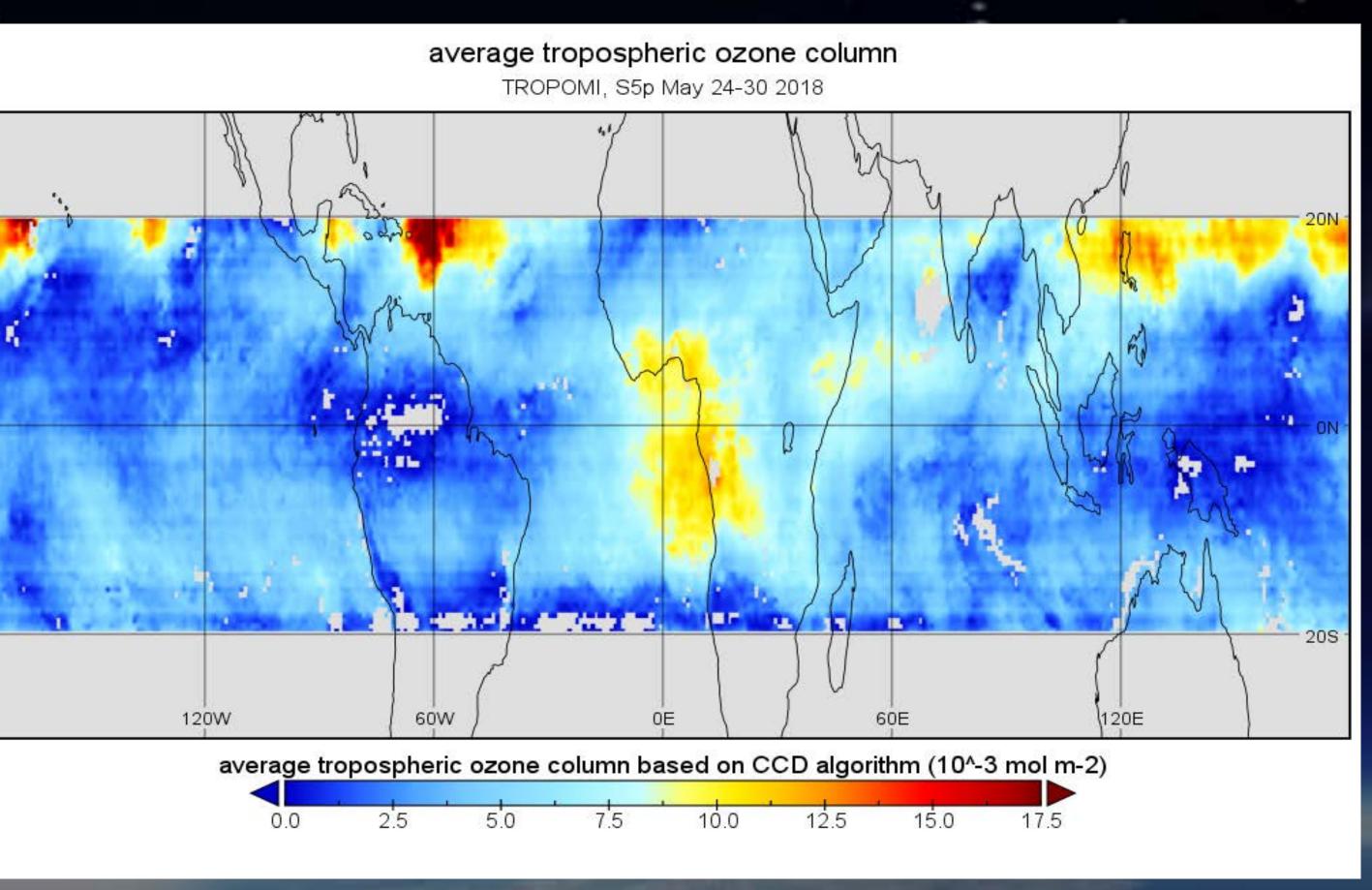


## TROPOMI Ozone data products: stratosphere & troposphere

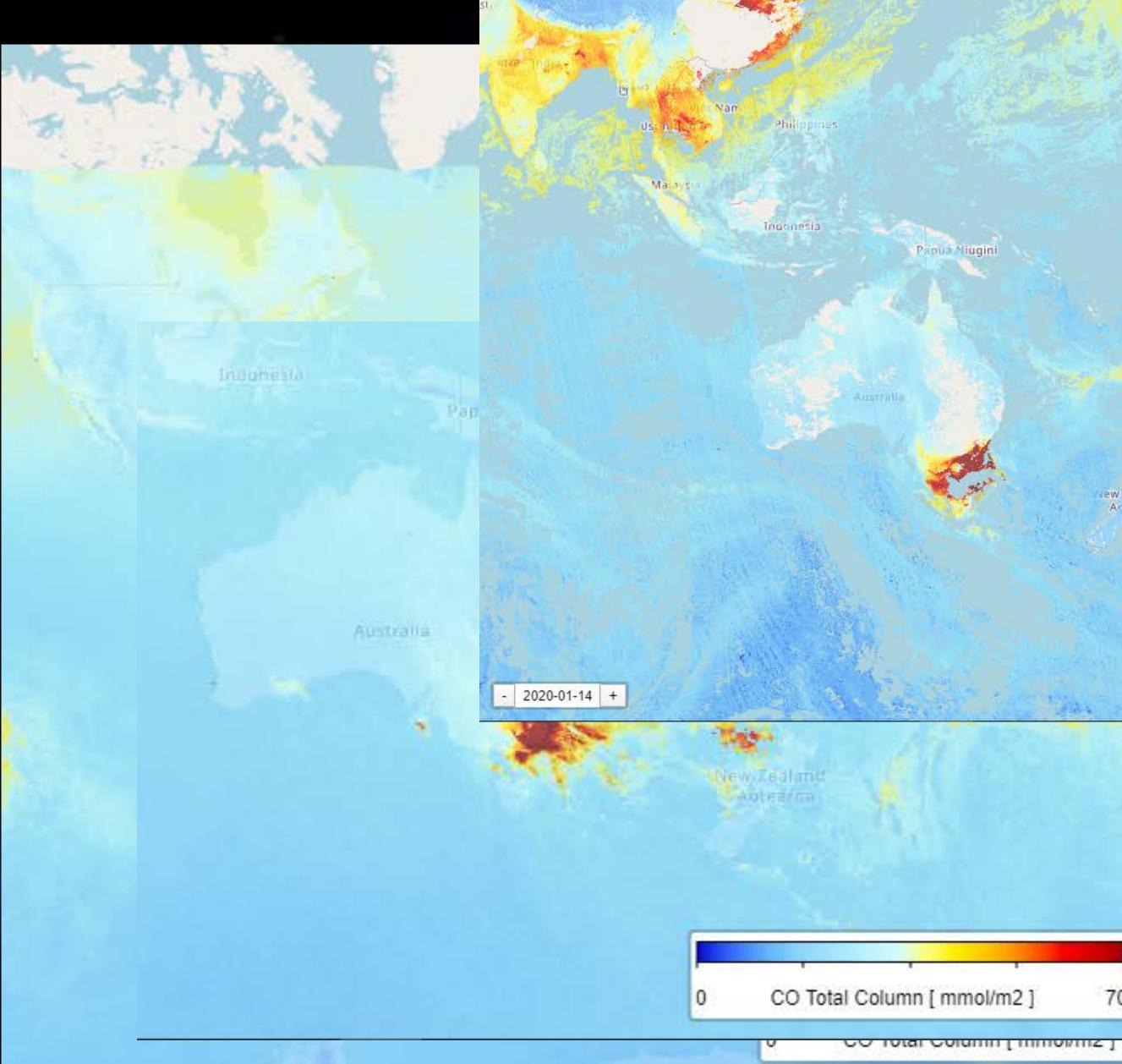


DU





## Carbon Monoxide



### 13 January 2020: Bushfire Smoke **Transport to South America**

hiled States

México

lew Zealand Antearoal

70

10

CO Total Column [ mmol/m2 ]

70

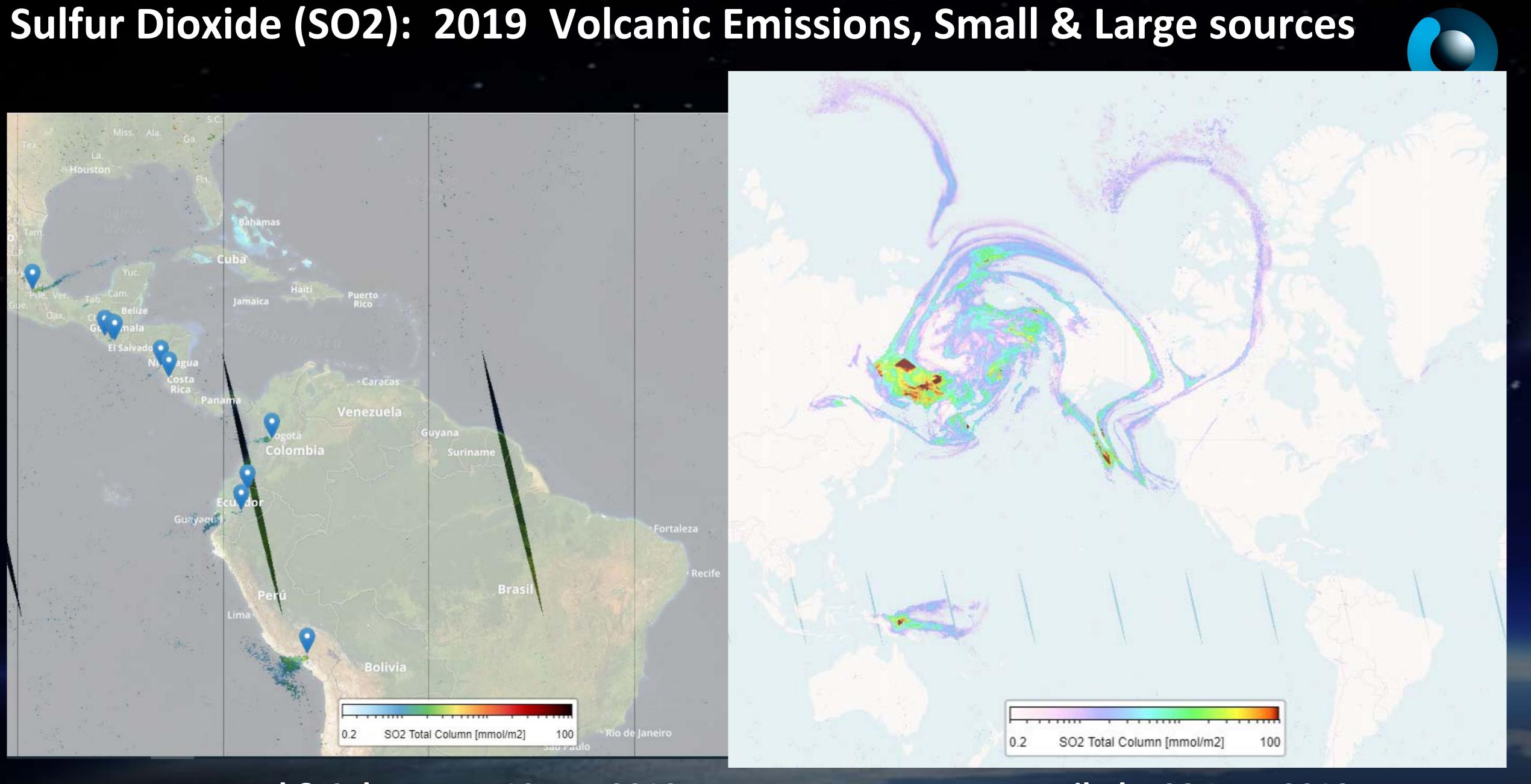
TROPOMI data @ KNMI/SRON/NSO/ESA, Map data @ OpenStreetMap

Amentina

TROPOMI data @ KNMI/SRON/NSO/ESA, Map data @ OpenStreetMap

TROPOMI data © KNMI/SRON/





Popocatepetl & Sabancava, 19 Dec 2019

### Raikoke 28 June 2019

## Raikoke Volcano SO<sub>2</sub> in the stratosphere observed by TROPOMI



Image Landsat // Copernious Image IBCAO Data Sio, NOAA, U.S. Navy, NGA, GEBCO Image U.S. Geological Survey

Datum van beeldmateriaal: 14-12-2015 breedte 77.400881° lengte 37.358031° verh 0 m ooghoogte 8457.84 km 💭



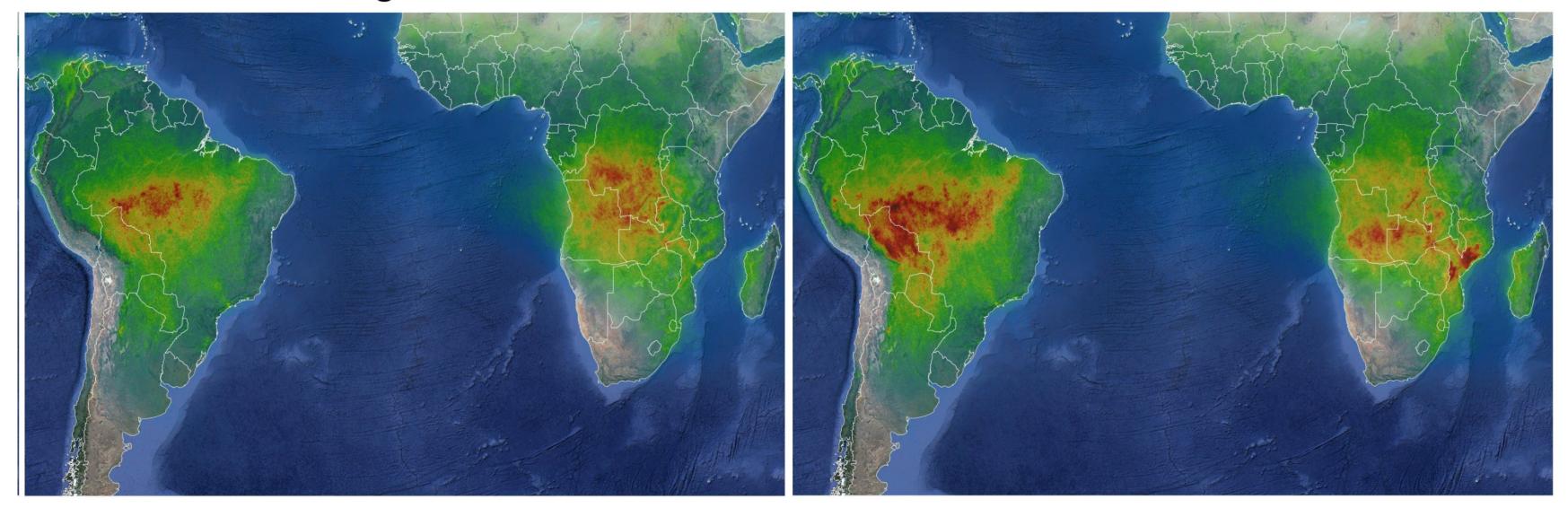
Aug.2018

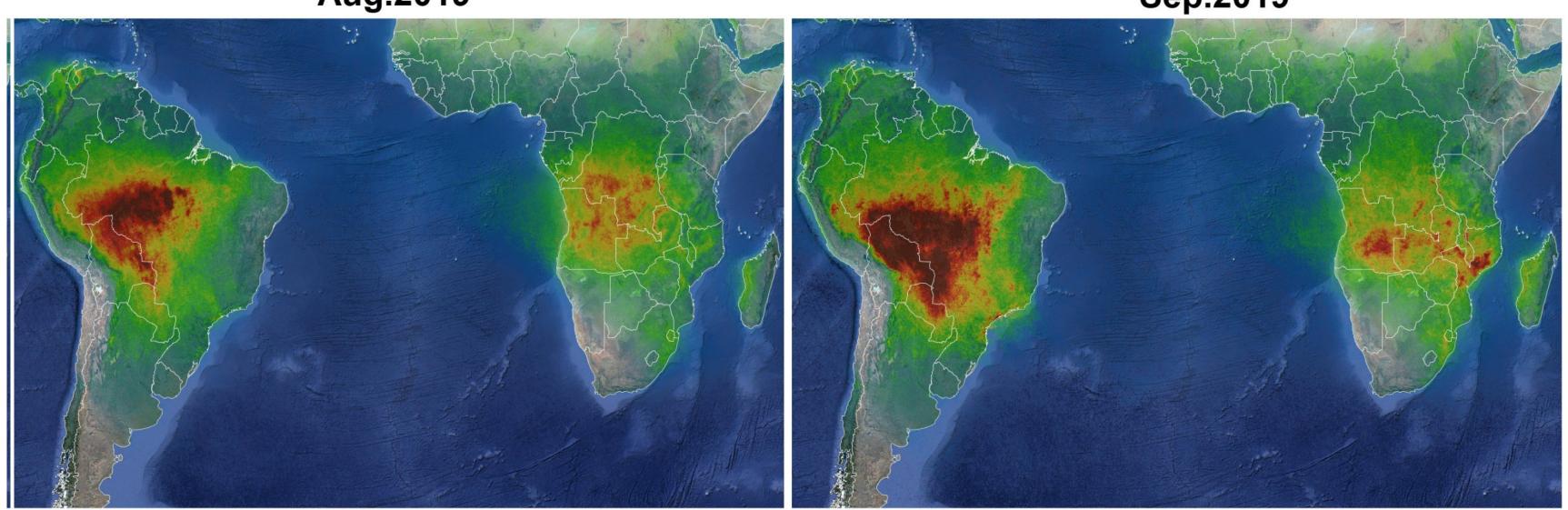
### Formaldehyde:

## Temperaturedependent emission

### Primarily Biogenic & Combustion sources

Isabelle De Smedt BIRA-IASB

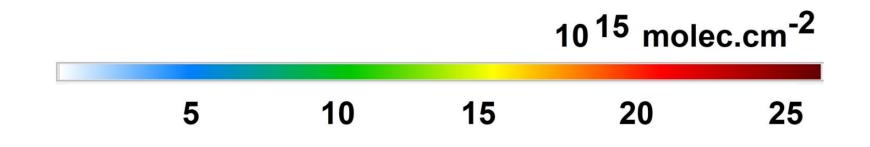




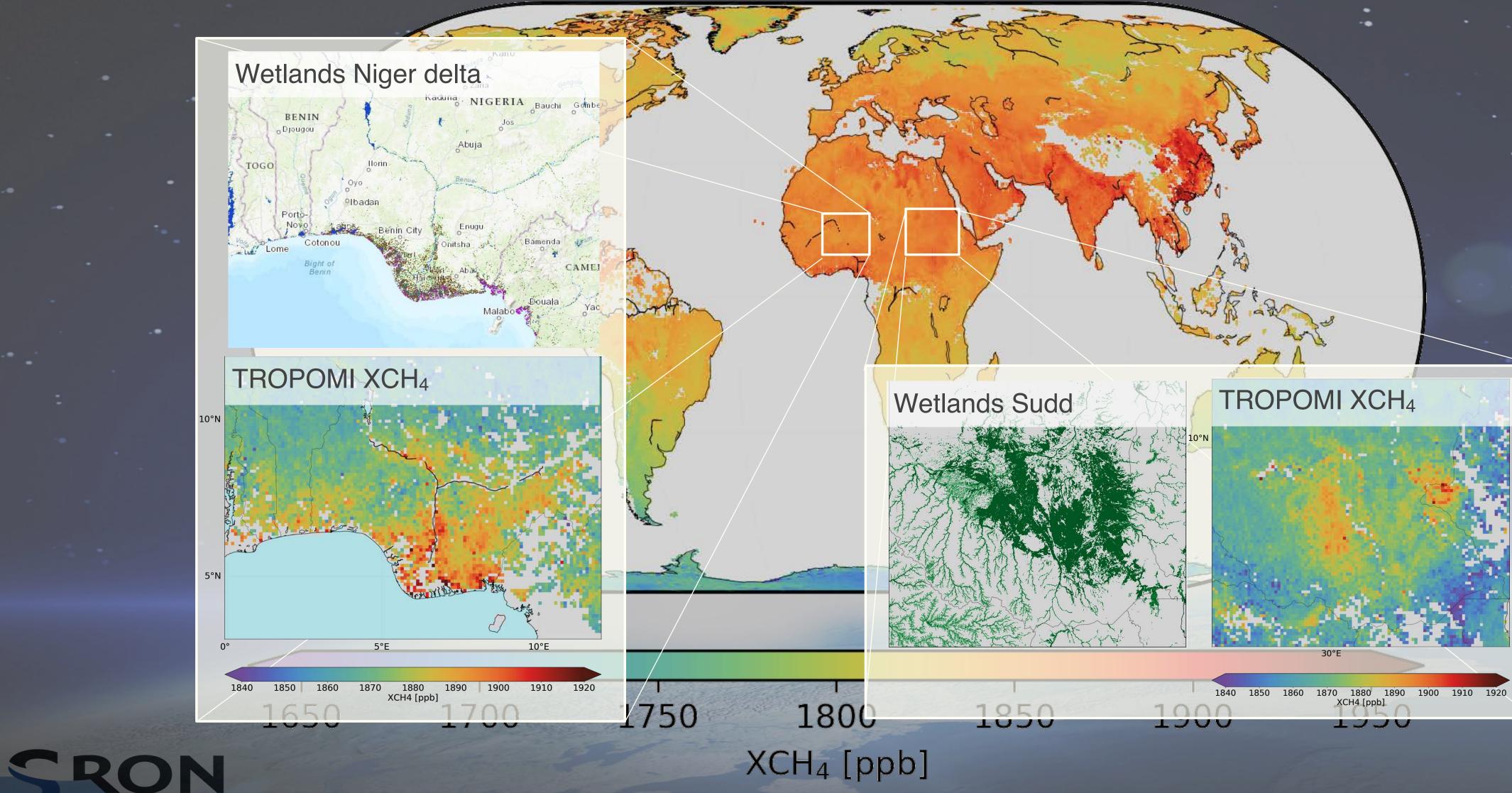
#### Sep.2018

Aug.2019

Sep.2019



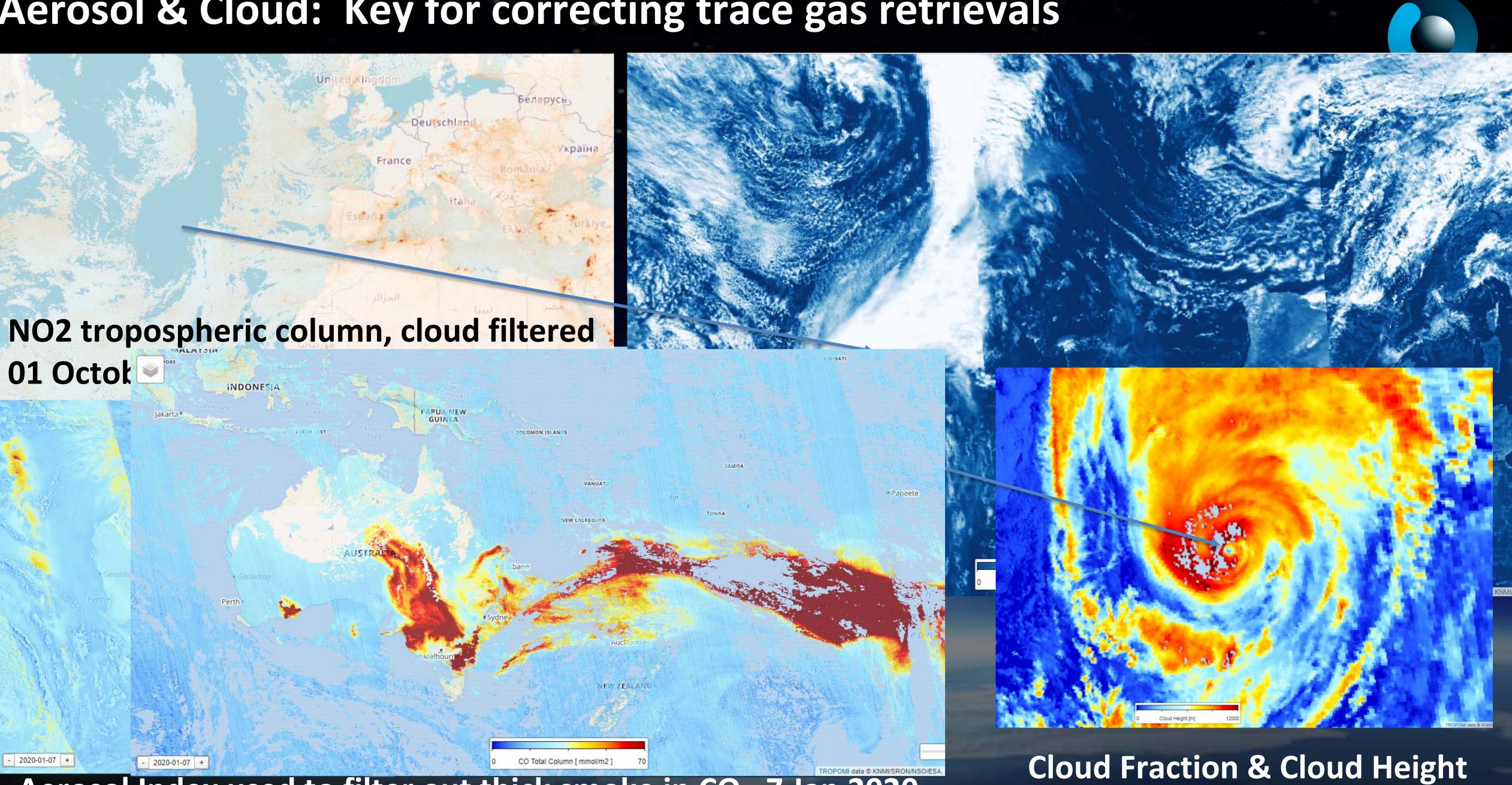
## Methane (CH4): Wetland emission seen by TROPOMI



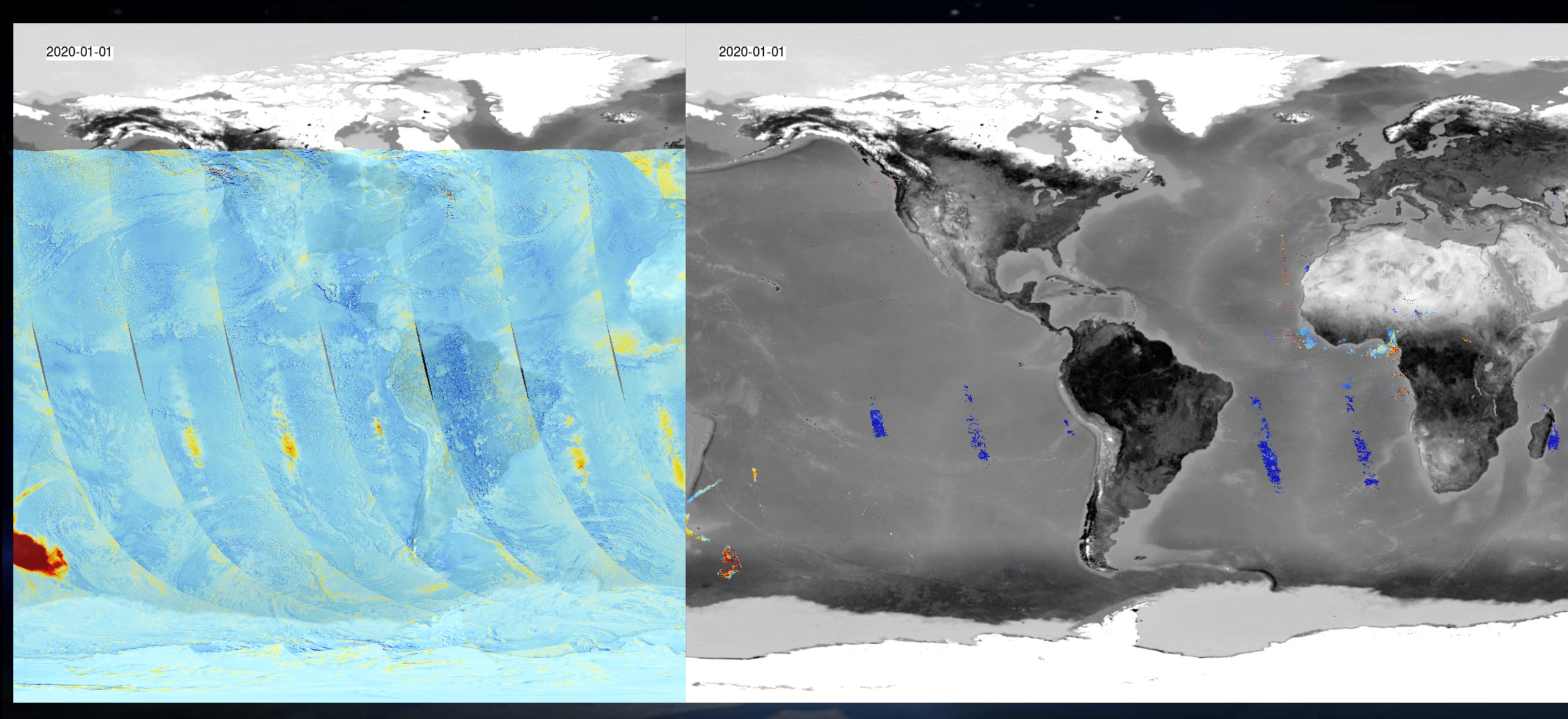
#### TROPOMI



### Aerosol & Cloud: Key for correcting trace gas retrievals

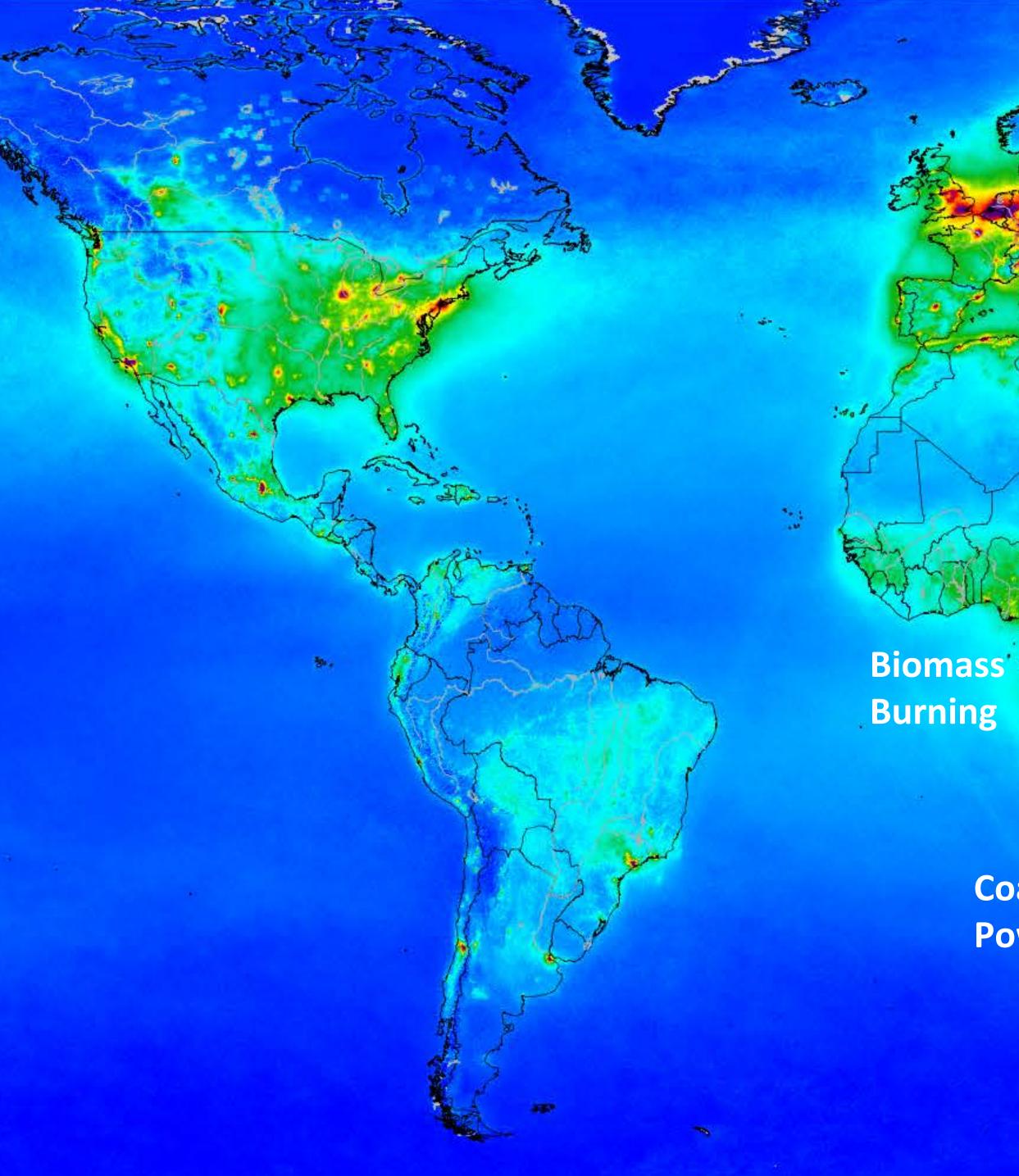


Aerosol Index used to filter out thick smoke in CO, 7 Jan 2020









Oil & Gas Activity

**Shipping Lanes** 

Coal-fired Power Plants

S5P NO2 April 2018 - Maart 2019



## Shipping Lanes

000

Ksar El Keb

Duezzane

TROPOMI

srém

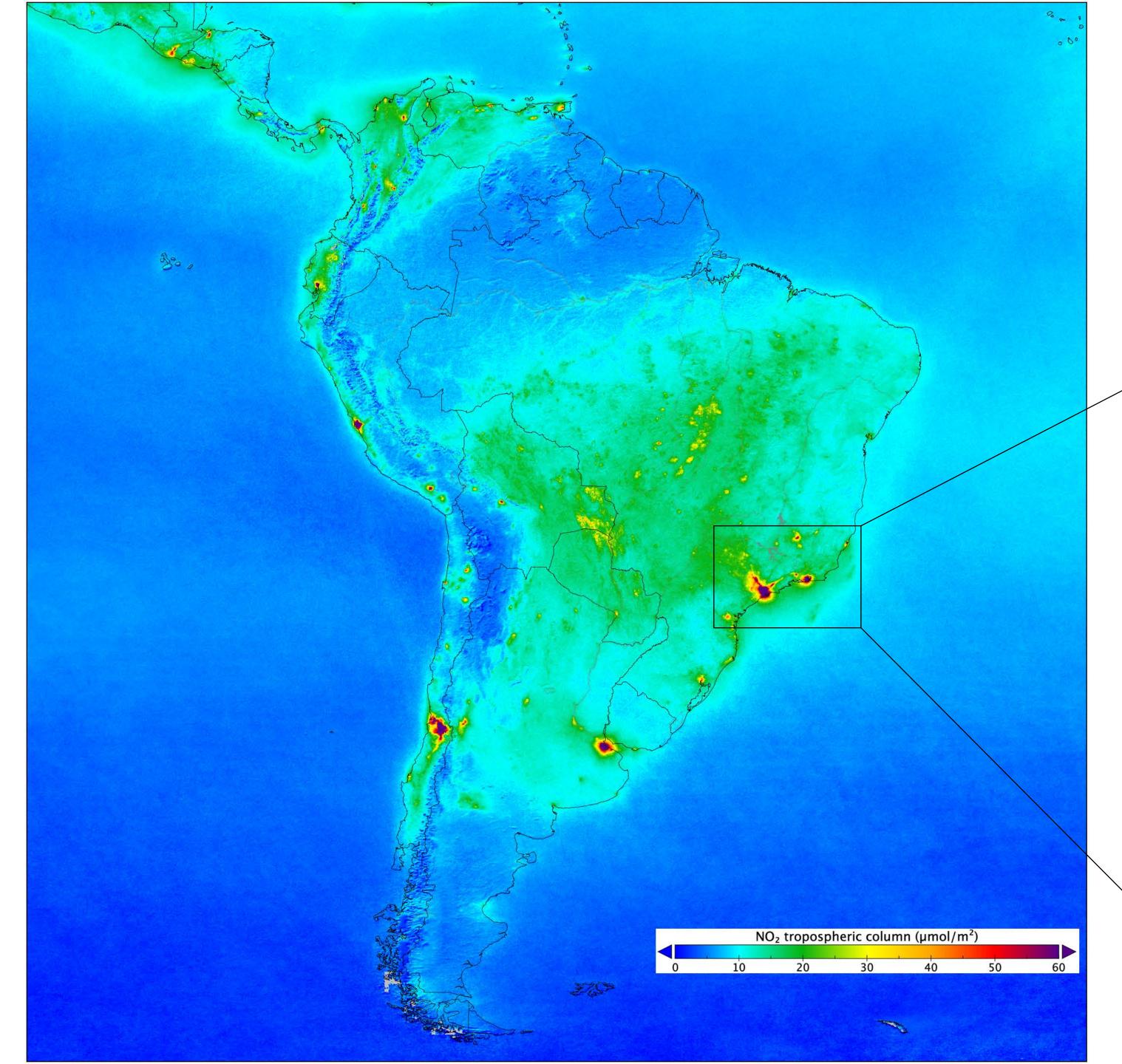
Evora

State Street

Portalegre

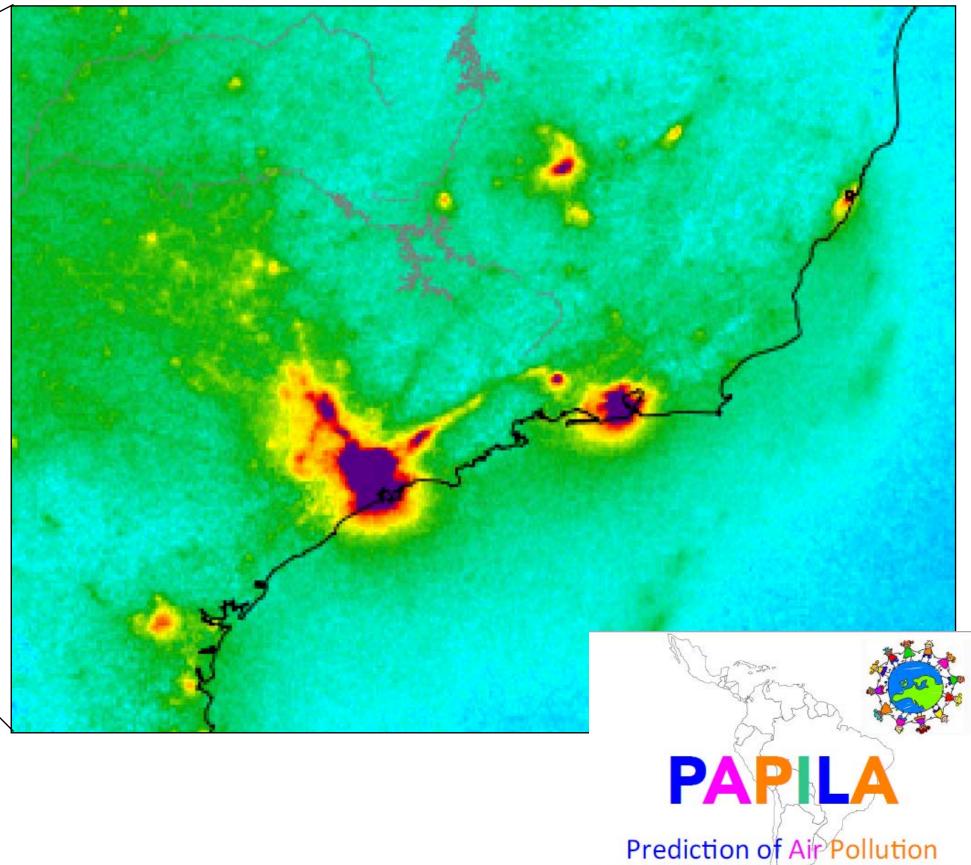
**Strait of Gibraltar, 20 February 2018** S5P TROPOMI NO<sub>2</sub> Symbols: AIS Ship Lengths



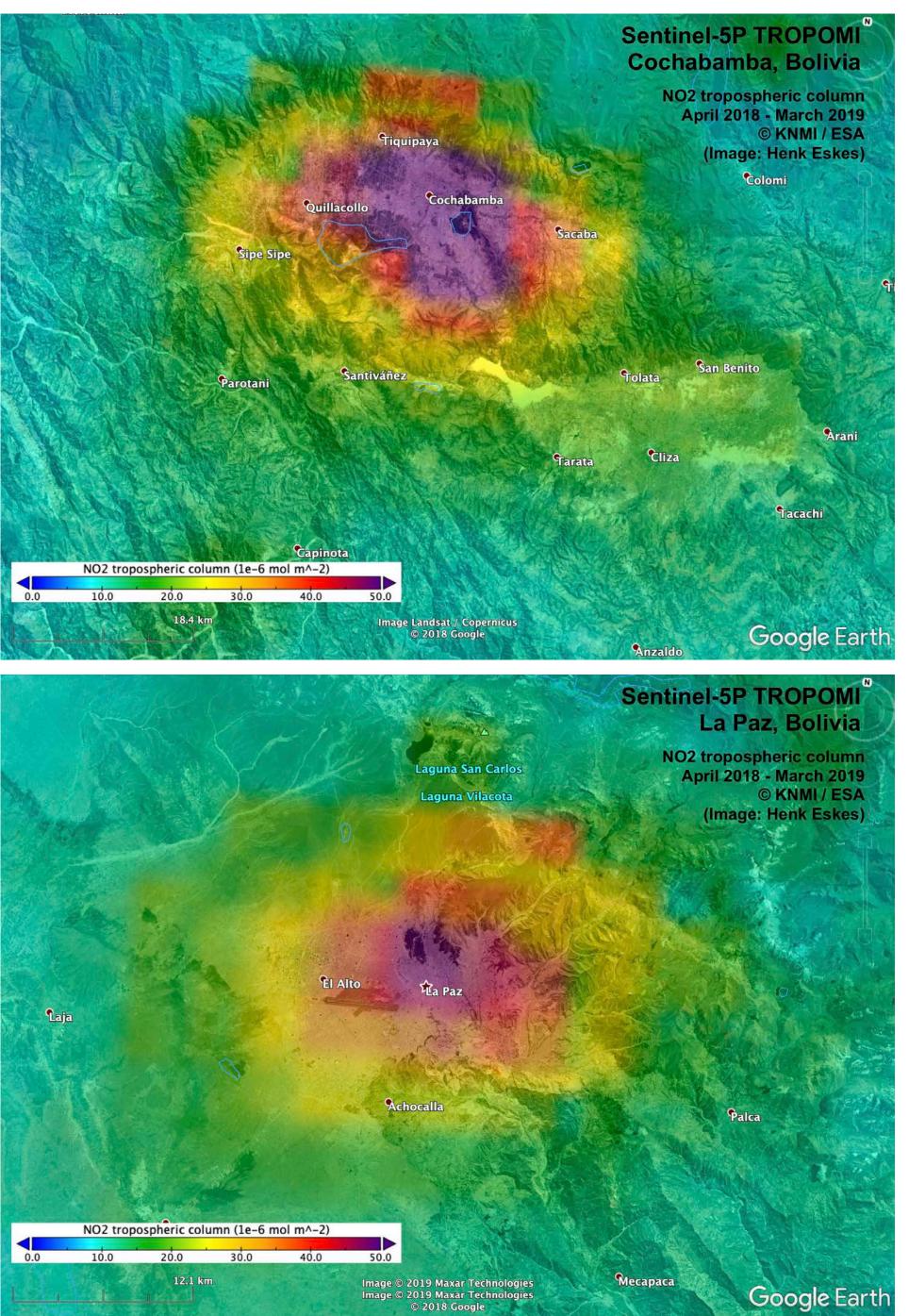


**Sentinel-5P TROPOMI** NO<sub>2</sub> tropospheric column

**Annual Average 2019** 





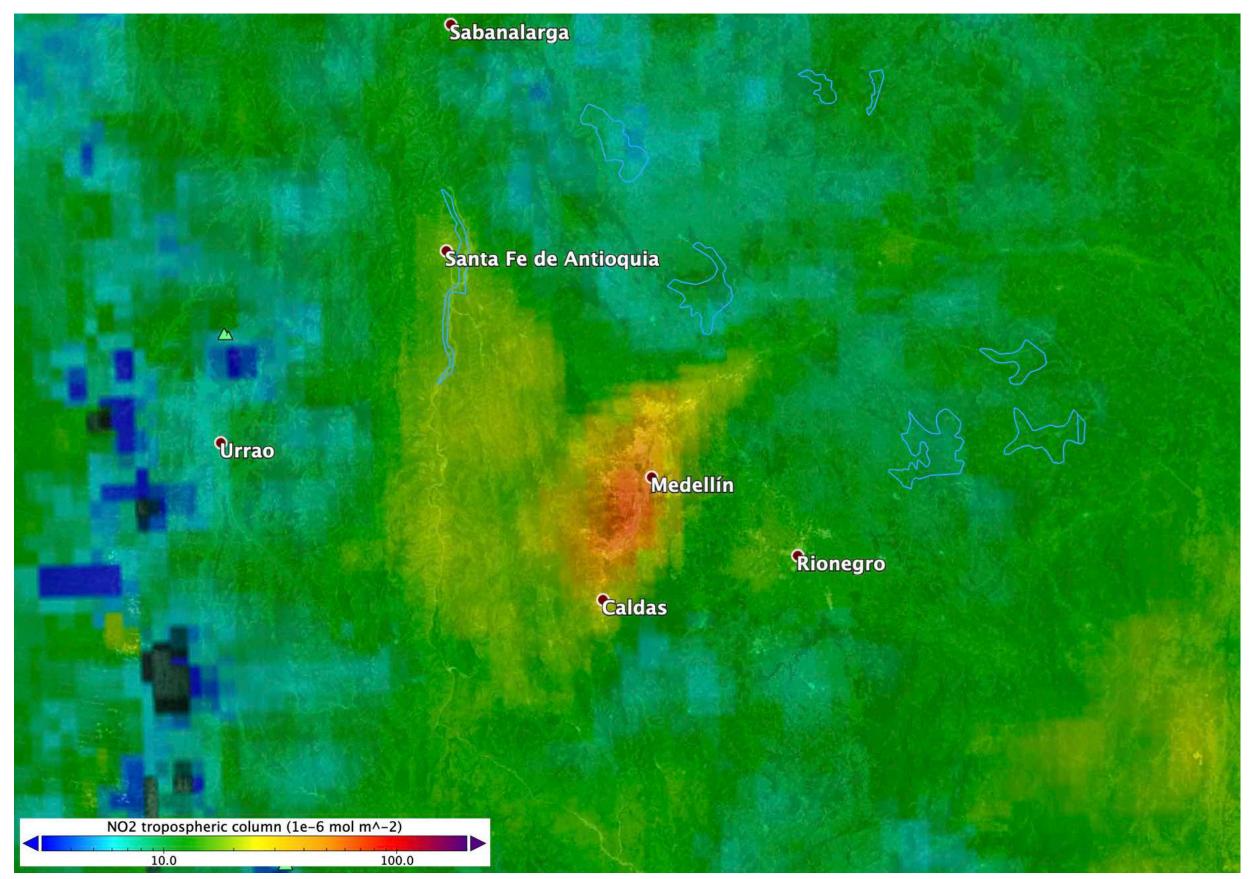


### Cochabamba, Bolivia

### La Paz, Bolivia

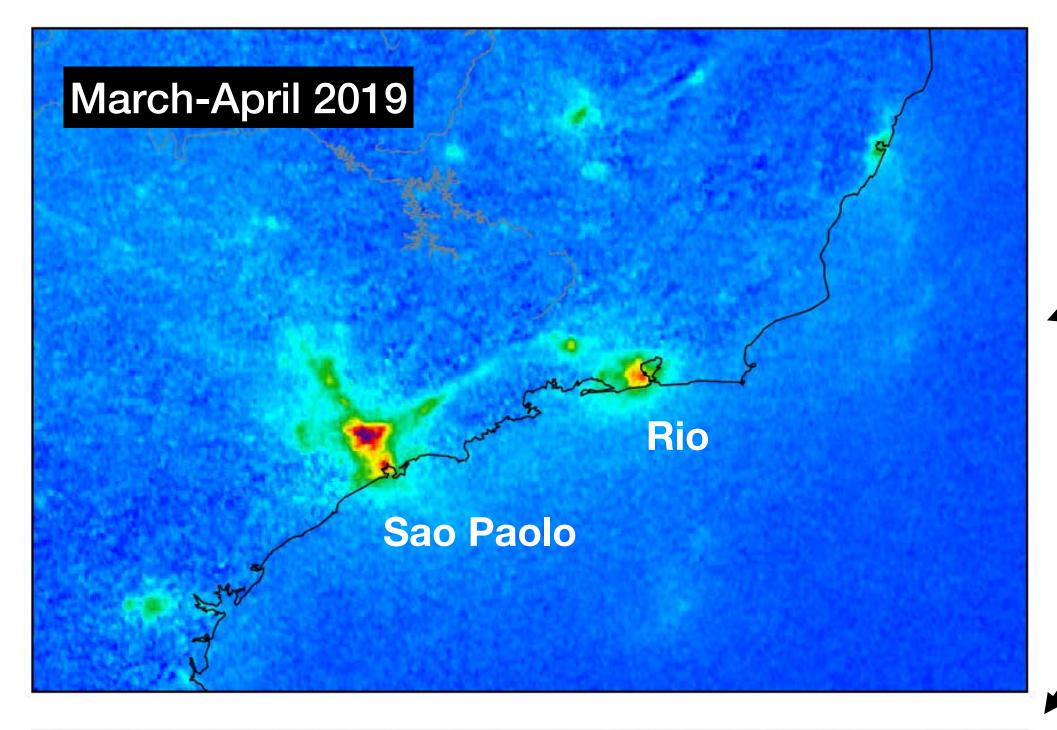
## Zoom images of NO<sub>2</sub>: City footprints, Annual average

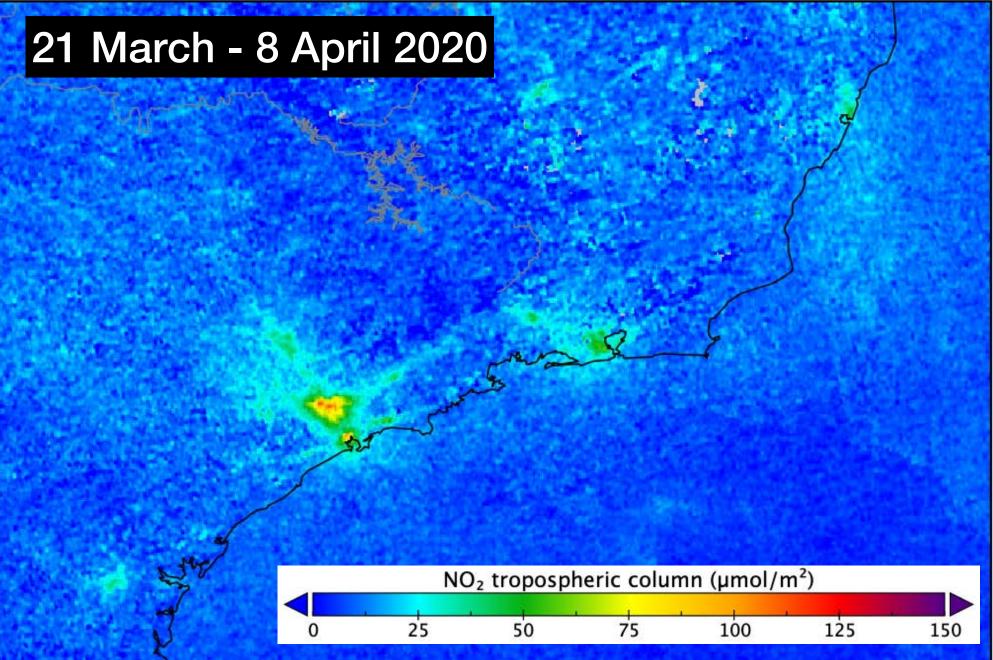
#### Medellin, Colombia









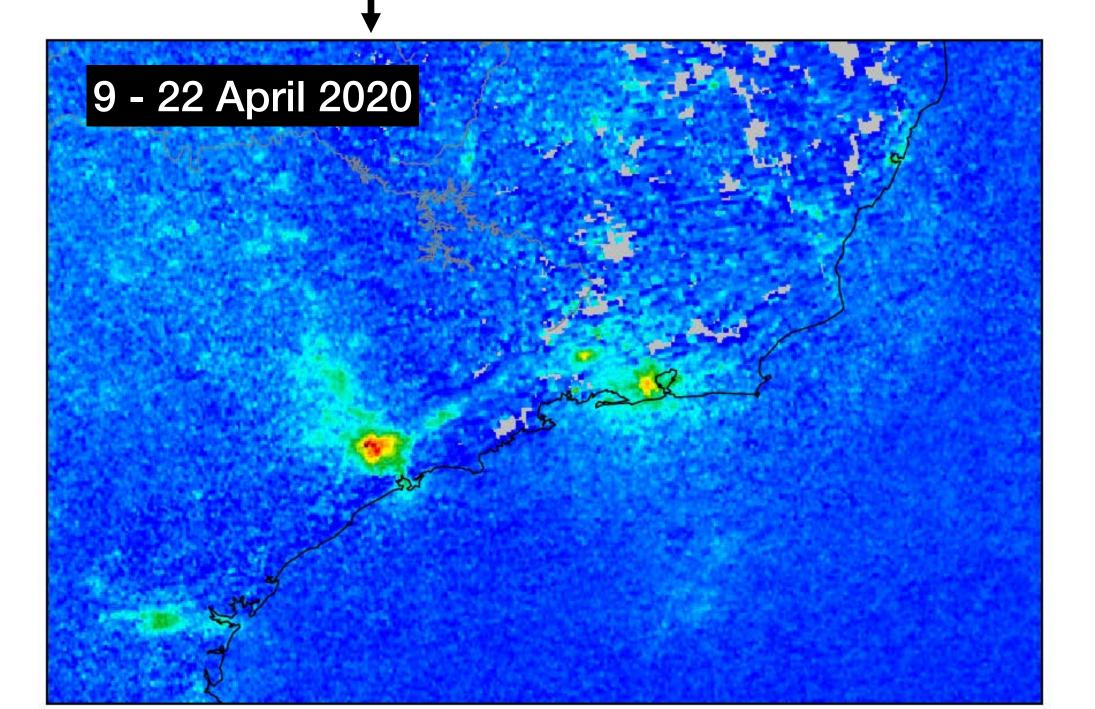


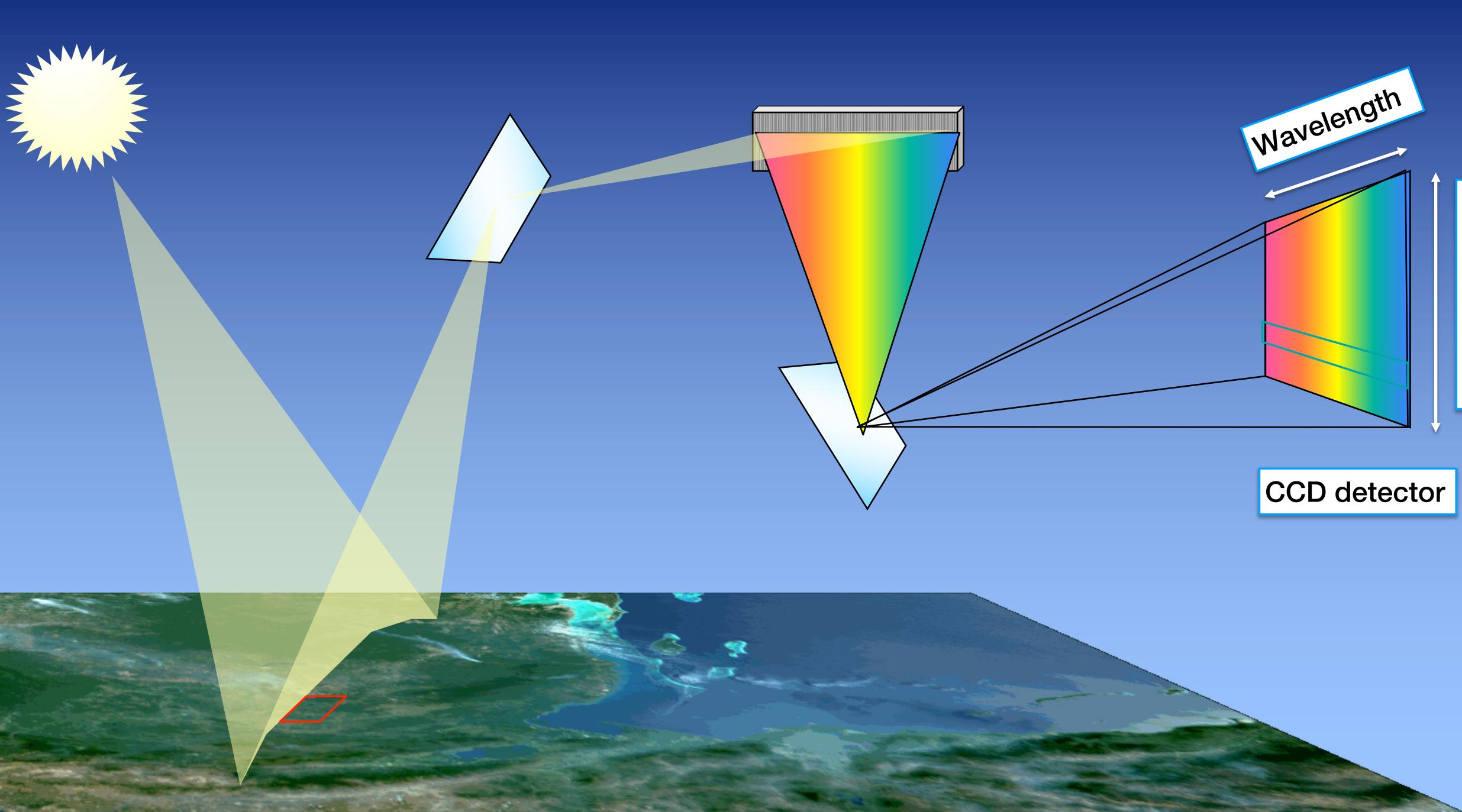
# Reduction in NO2 in Brazil related to Covid-19 measures

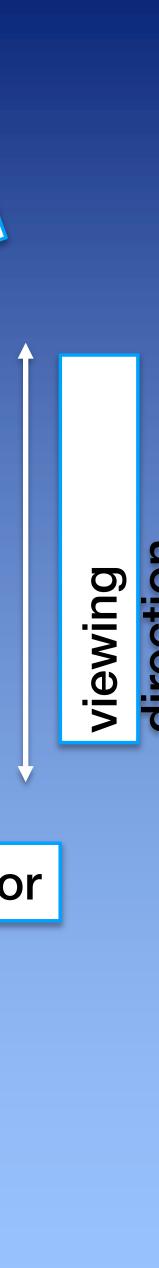
2019

First weeks after lockdown

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





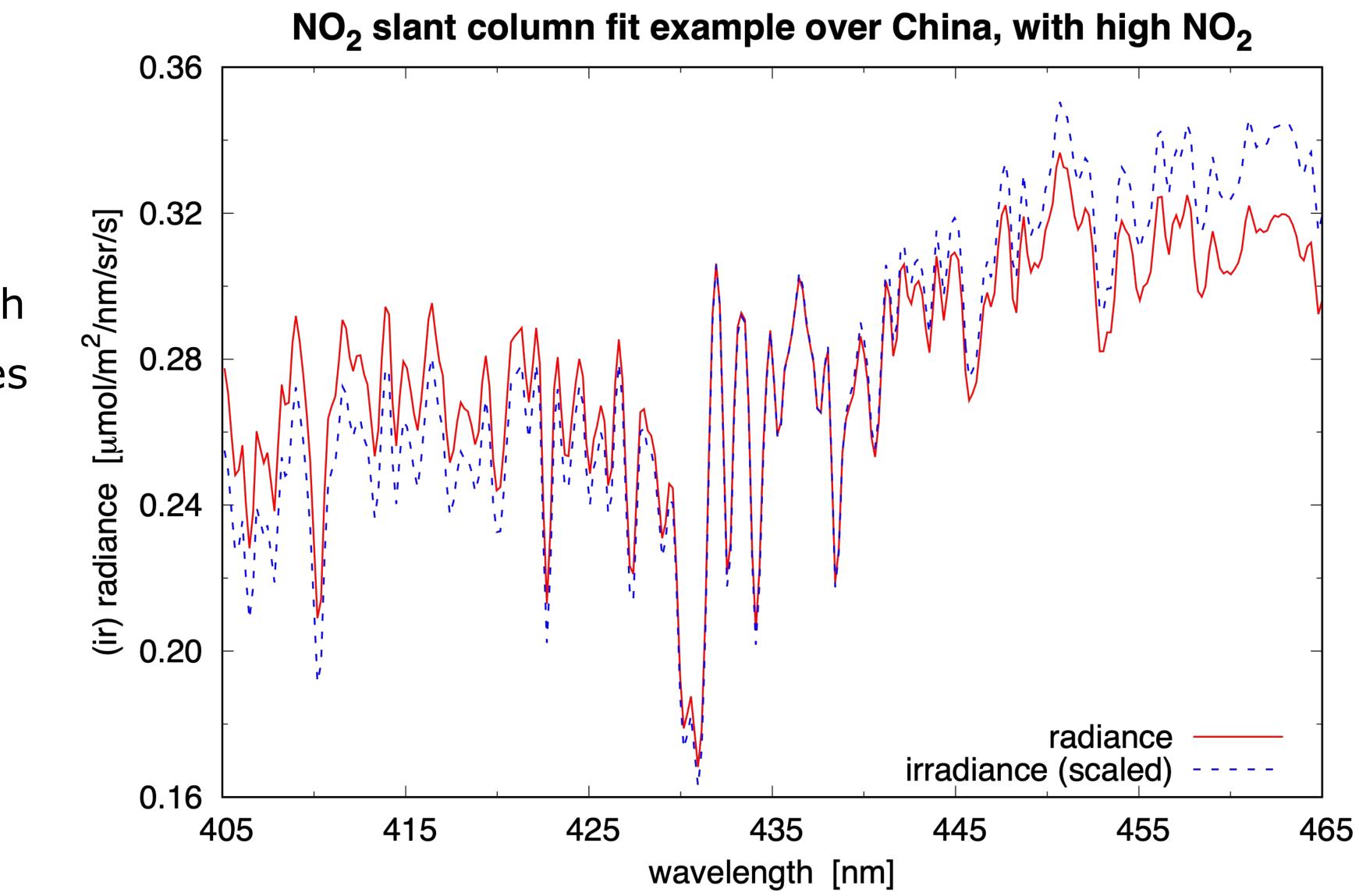


## **Spectral observations in the wavelength range for NO**<sub>2</sub>

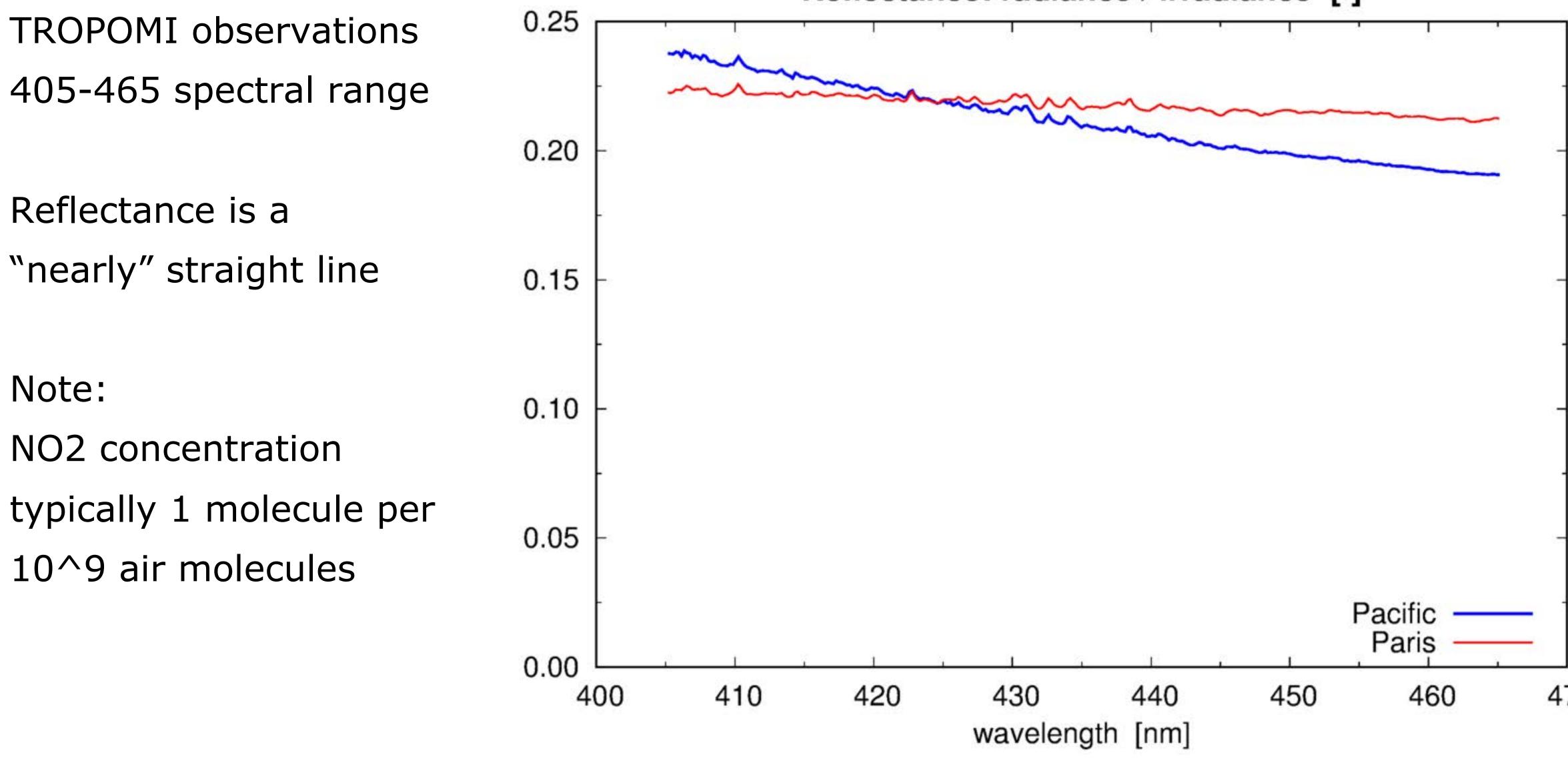
**TROPOMI** observations 405-465 spectral range

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**



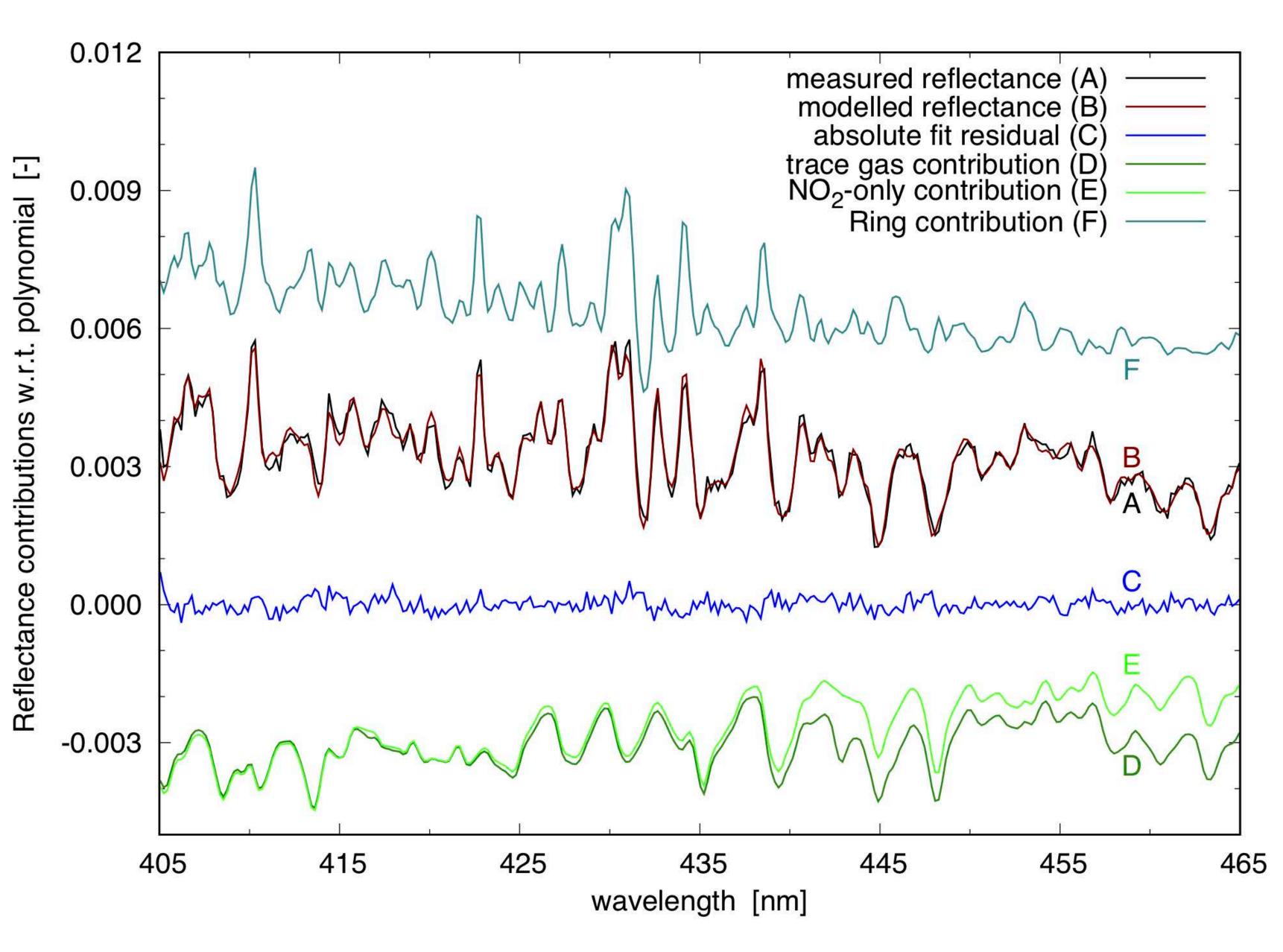
#### Reflectance: radiance / irradiance [-]



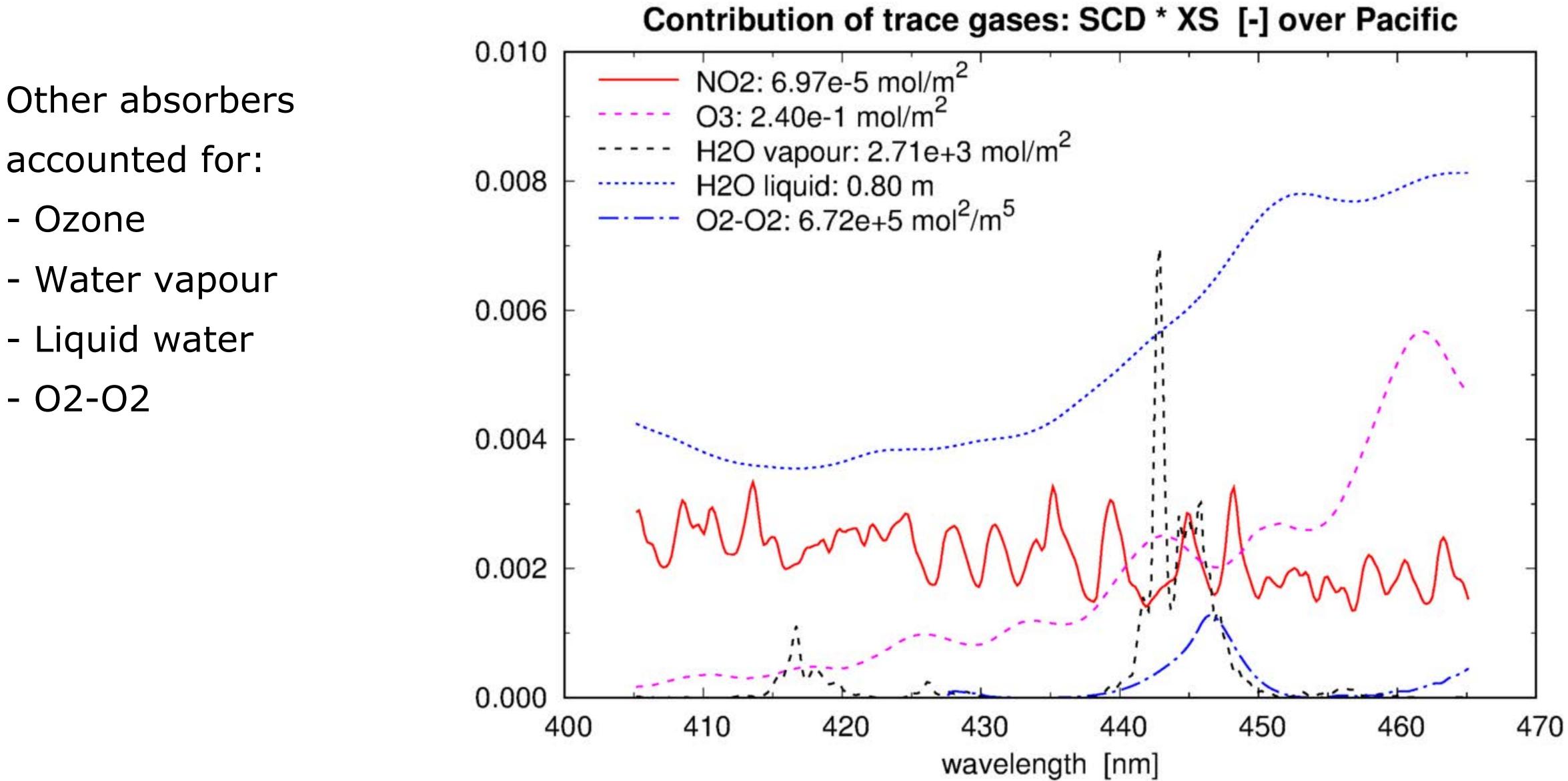
### **Reflectance:** Separating NO<sub>2</sub> contribution from other spectral features

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**



## 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  $\sim 1e-4$
- 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 NO2 along the path of the light through the atmosphere

What is still unknown?

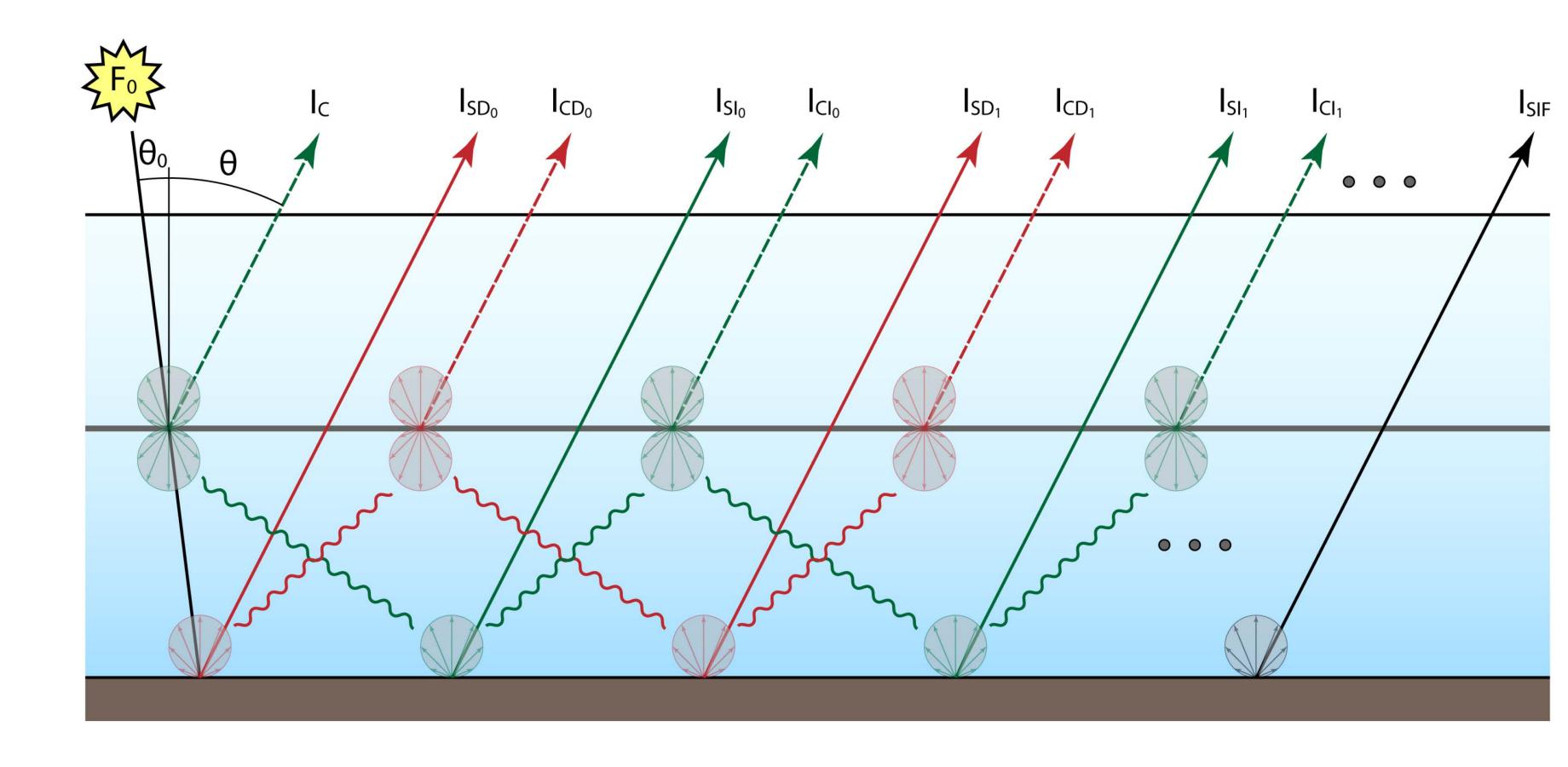
Where did the light go? Where is the NO2 located? (At what altitude? Vertical distribution?) Quantify both of these unknowns using an *air mass factor* 

## 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?

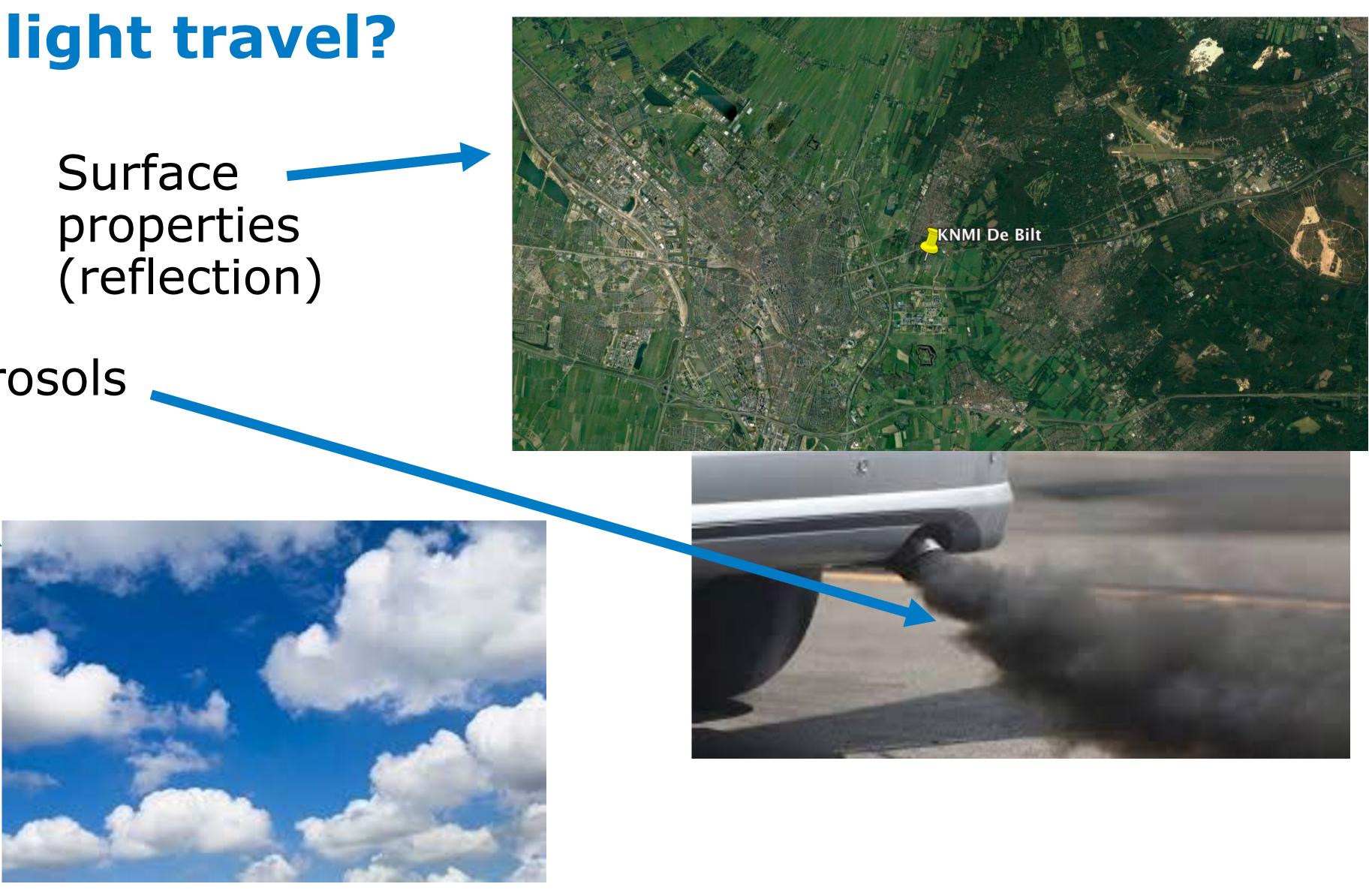
Aspects that influence the light path:

properties

Clouds

Aerosols

### **Air-mass factor**



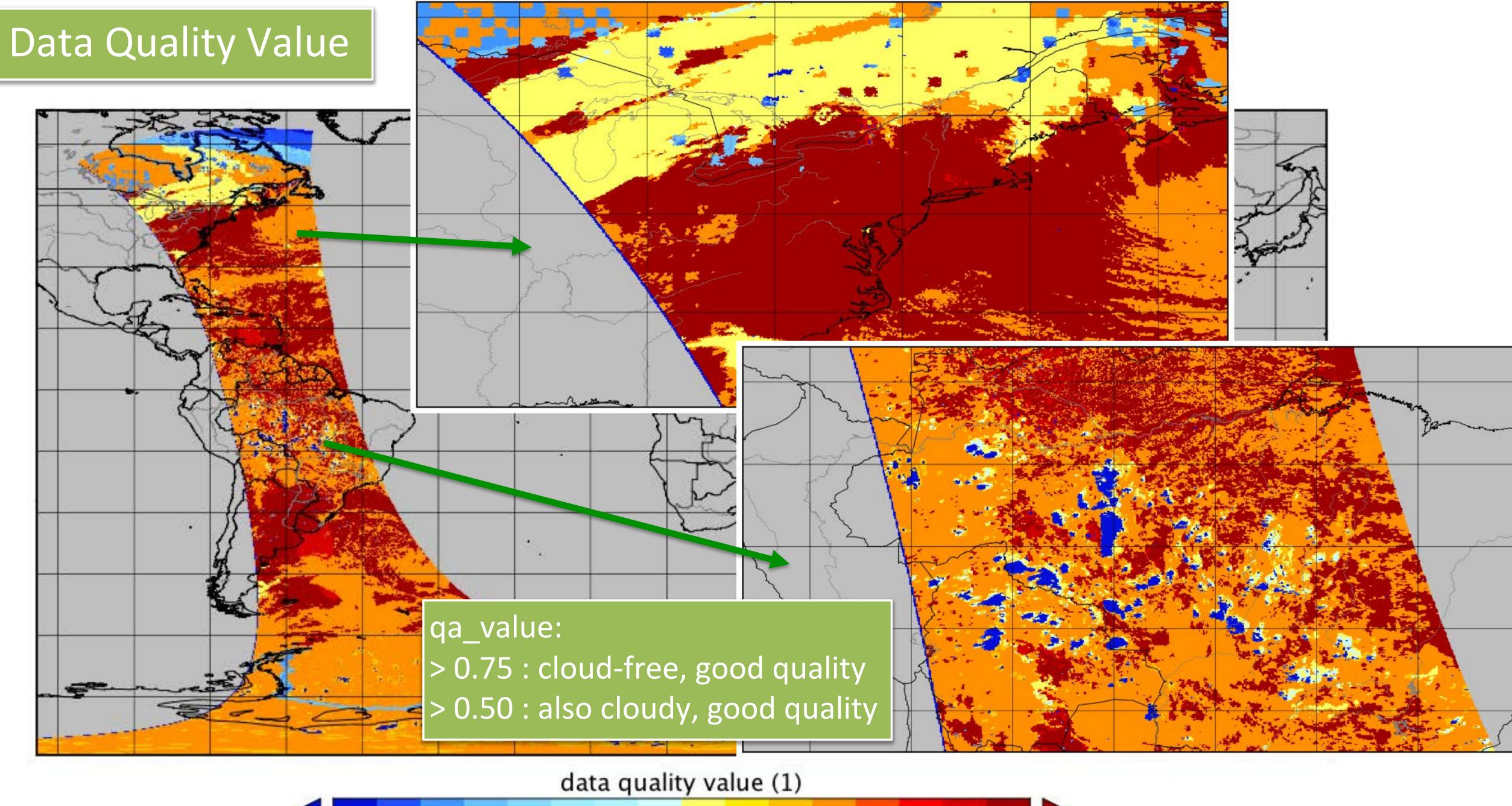
### Filtering to remove clouds: using the *qa\_value*

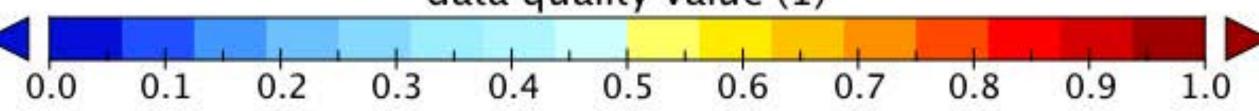
• qa\_value > 0.75

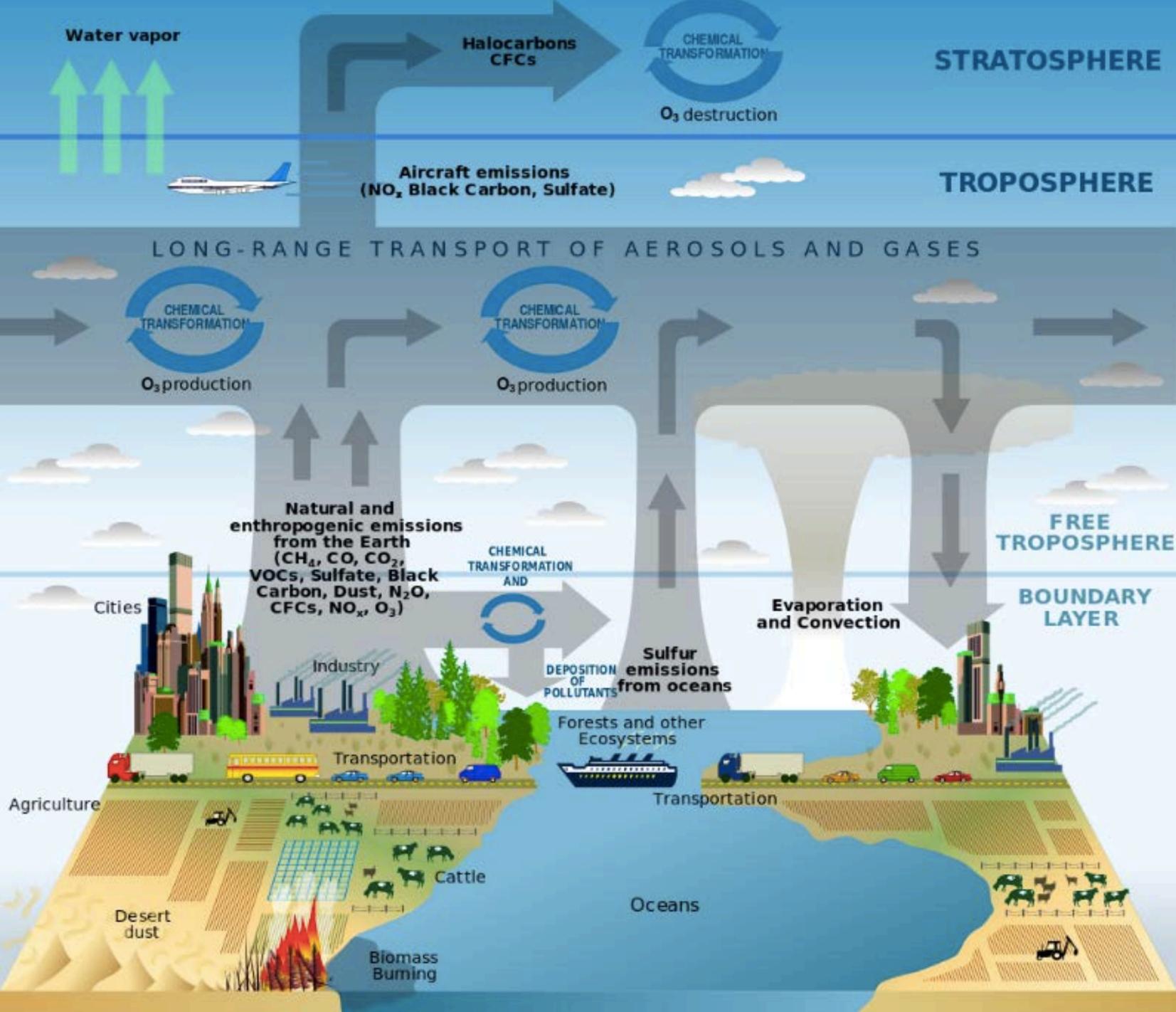
This is the recommended pixel filter. It removes cloud-covered scenes (cloud radiance fraction > 0.5), partially snow/ice covered scenes, errors, and problematic retrievals.

• 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.







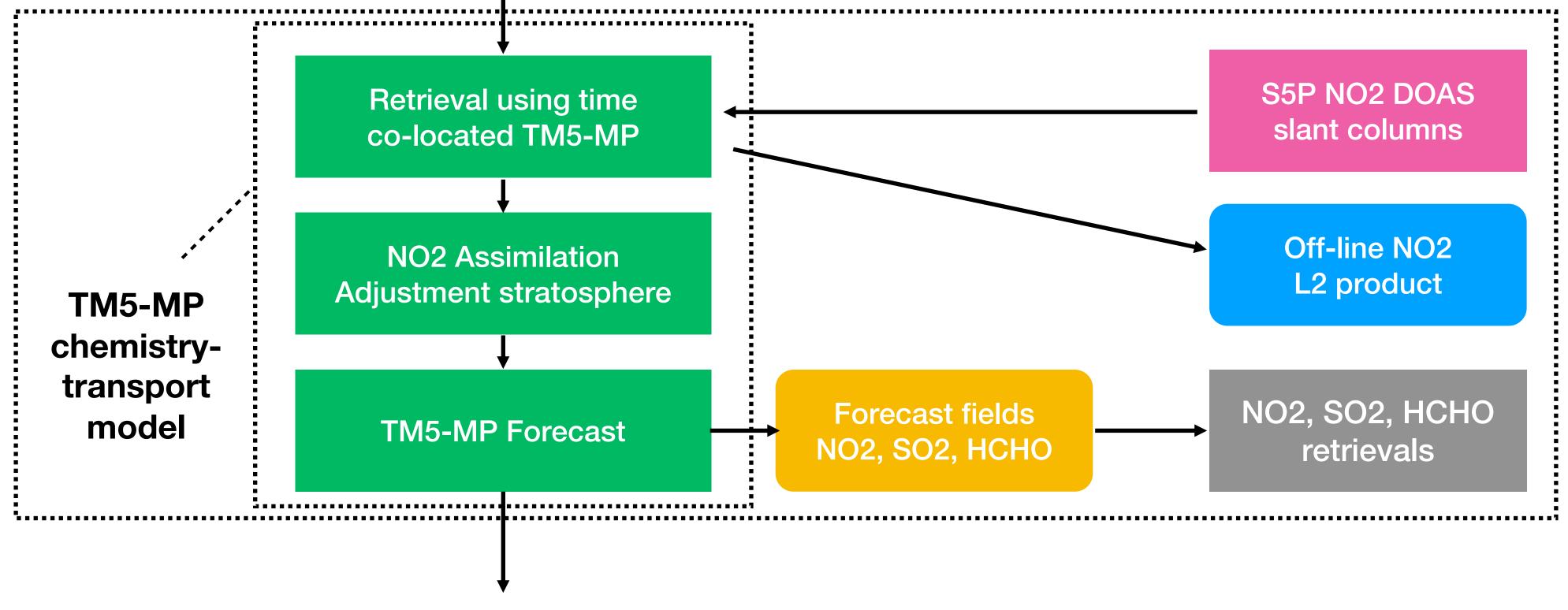
# Where is the NO<sub>2</sub>?



General circulation models including chemistry



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

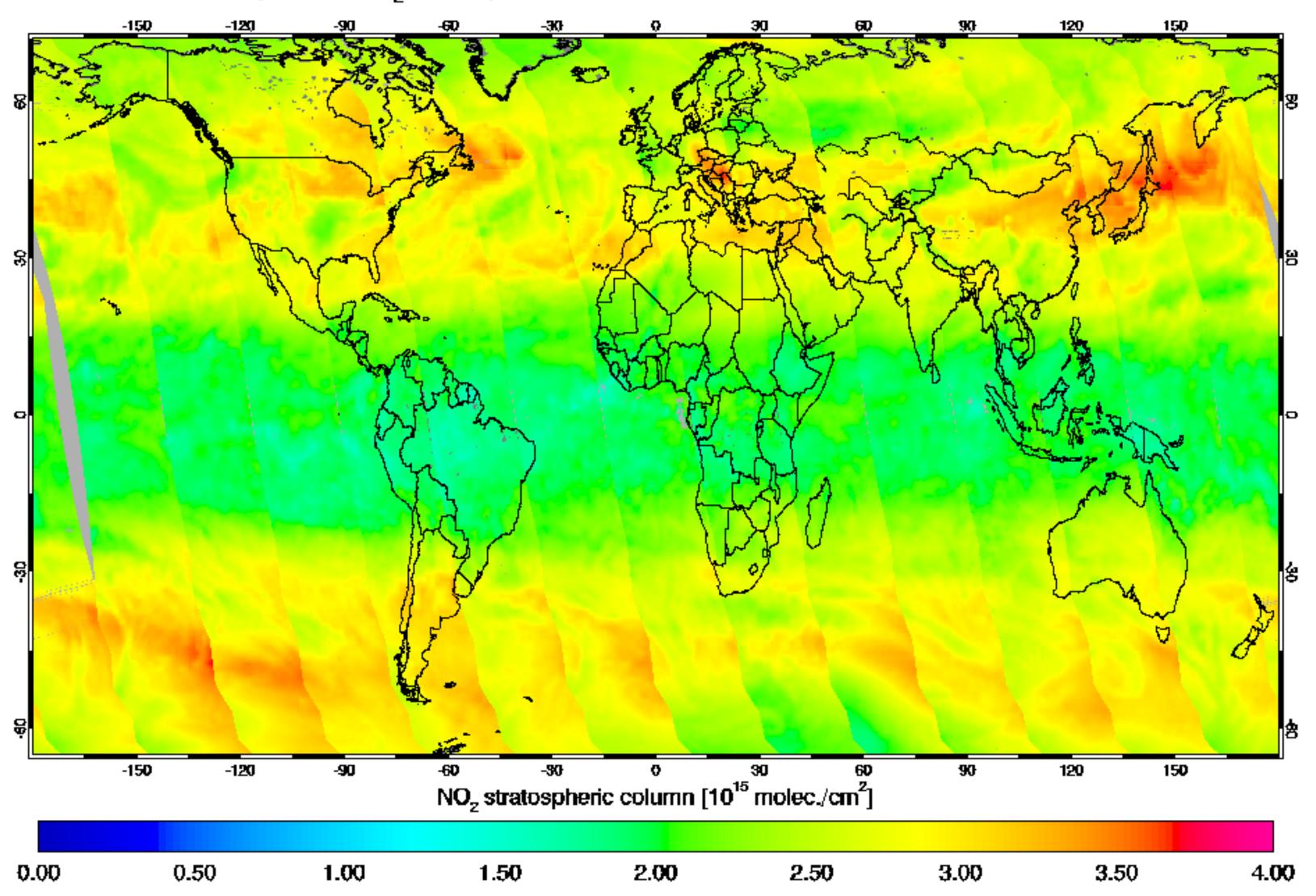


Next day

# The TM5 model provides a priori information about NO2 vertical profile

#### Stratosphere: from assimilation in TM5-MP

TROPOMI stratospheric NO<sub>2</sub> 01 Apr 2018



KNMI/ESA

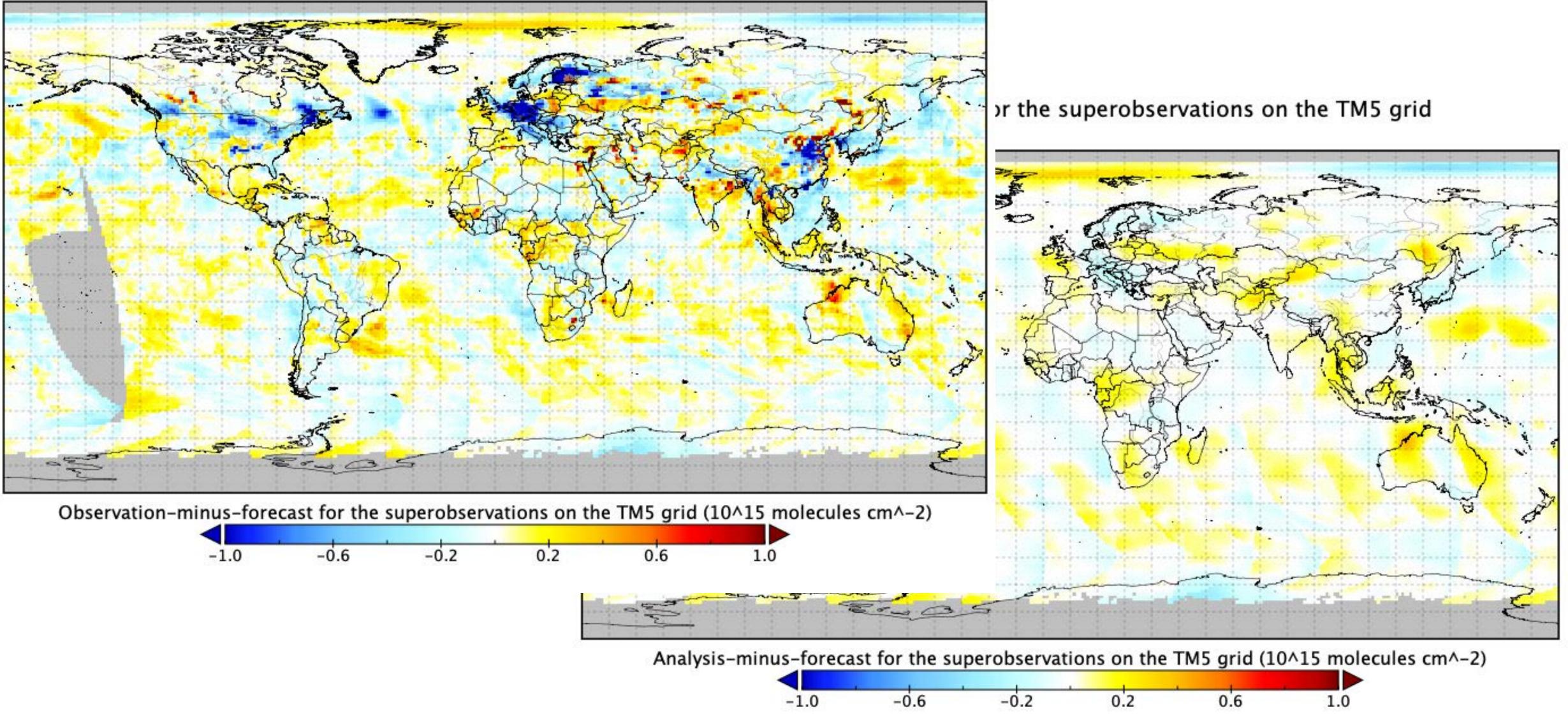
Tropospheric column = Total column minus stratospheric column

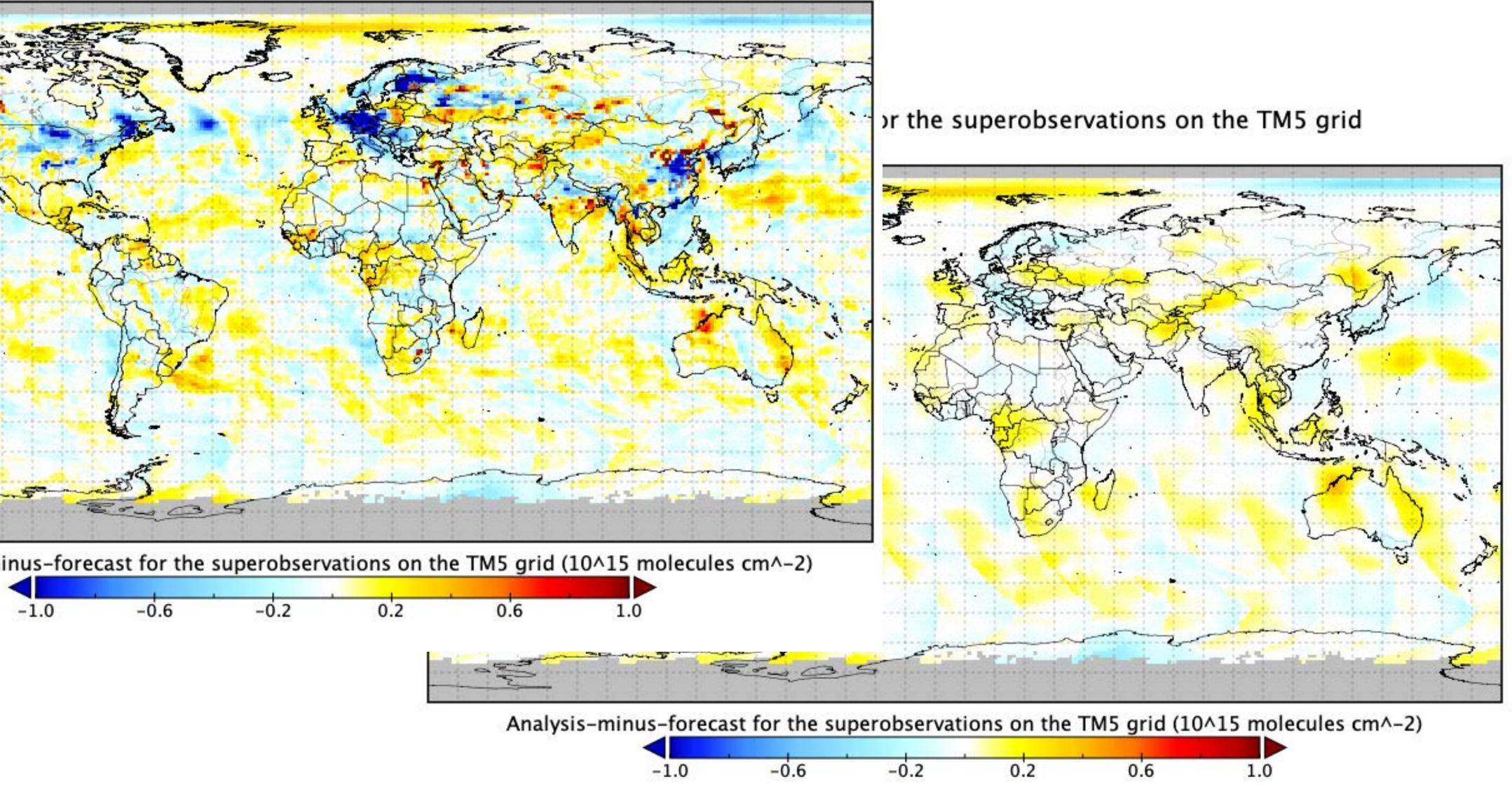
Stratospheric column determined by: -> Atmospheric dynamics -> Diurnal cycle (chemistry)



#### Stratosphere: from assimilation in TM5-MP

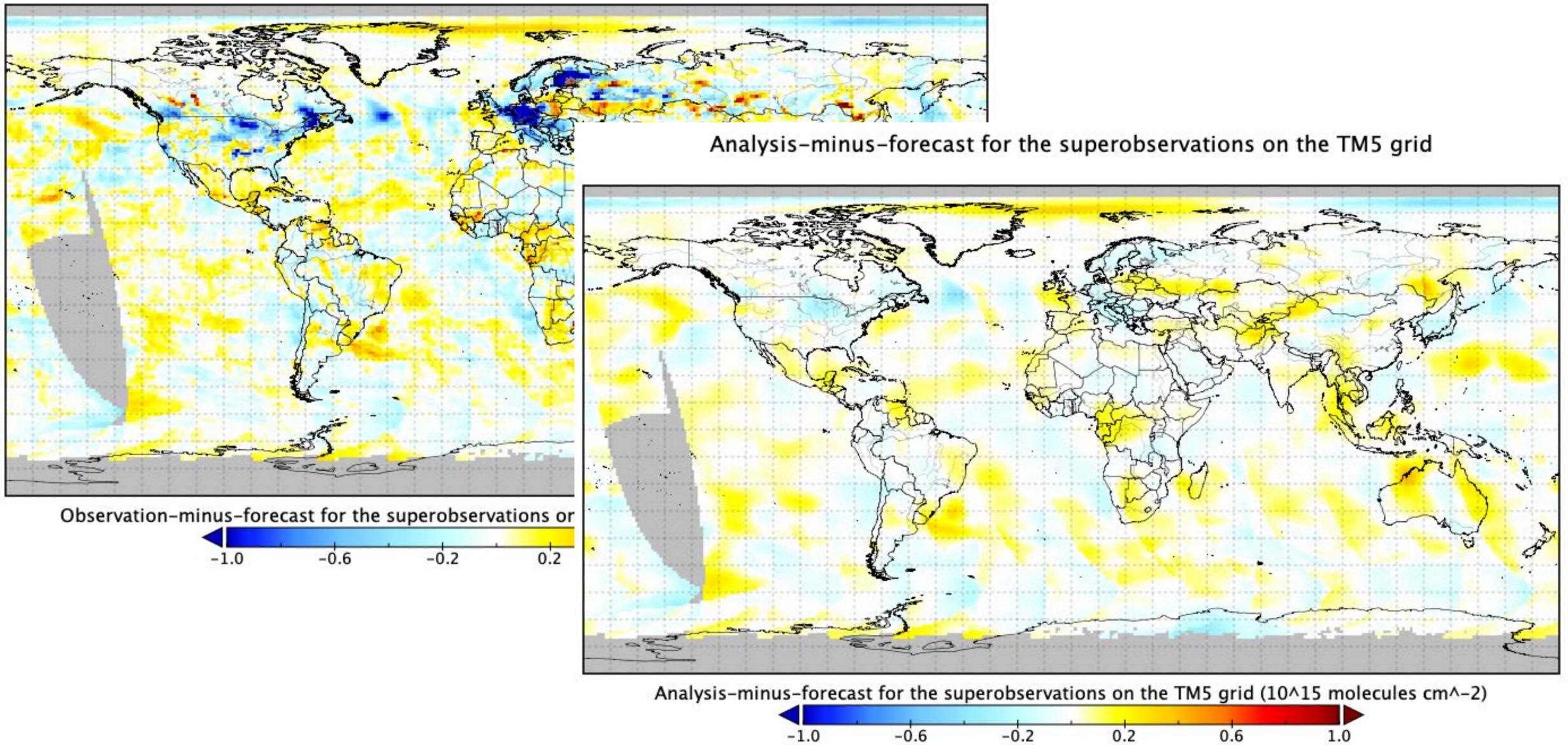
Observation-minus-forecast for the superobservations on the TM5 grid





#### Stratosphere: from assimilation in TM5-MP

Observation-minus-forecast for the superobservations on the TM5 grid



# Validation is crucial to identify biases



#### VALIDATION FACILITY SENTINEL 5P MISSION PERFORMANCE CENTER









#### lost recent contributions

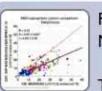


First comparison results for the S5P CH4 product based on correlative reference measurements acquired by FTIR instruments contributing to NDACC and TCCON networks. This VDAF web article gives further details on the first comparison results presented in the CH4 product readme file for the methane data product release (see http://www.tropomi.eu/dataproducts/methane). The main conclusion is that the product quality of this initial L2 CH4 dataset complies with the S5P mission requirements.



Quarterly Validation Report of the Sentinel-5 Precursor Operational Data Products #01: July - October

This document reports consolidated results of the routine operations validation service for the Sentinel-5 Precursor Tronospheric Monitoring



This report describes initial validation results for Sentinel-5p TROPOMI L2\_NO2 tropospheric column, stratospheric column and total column data: tronospheric and

Home VDA Search



#### www.tropomi.eu

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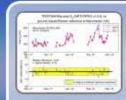








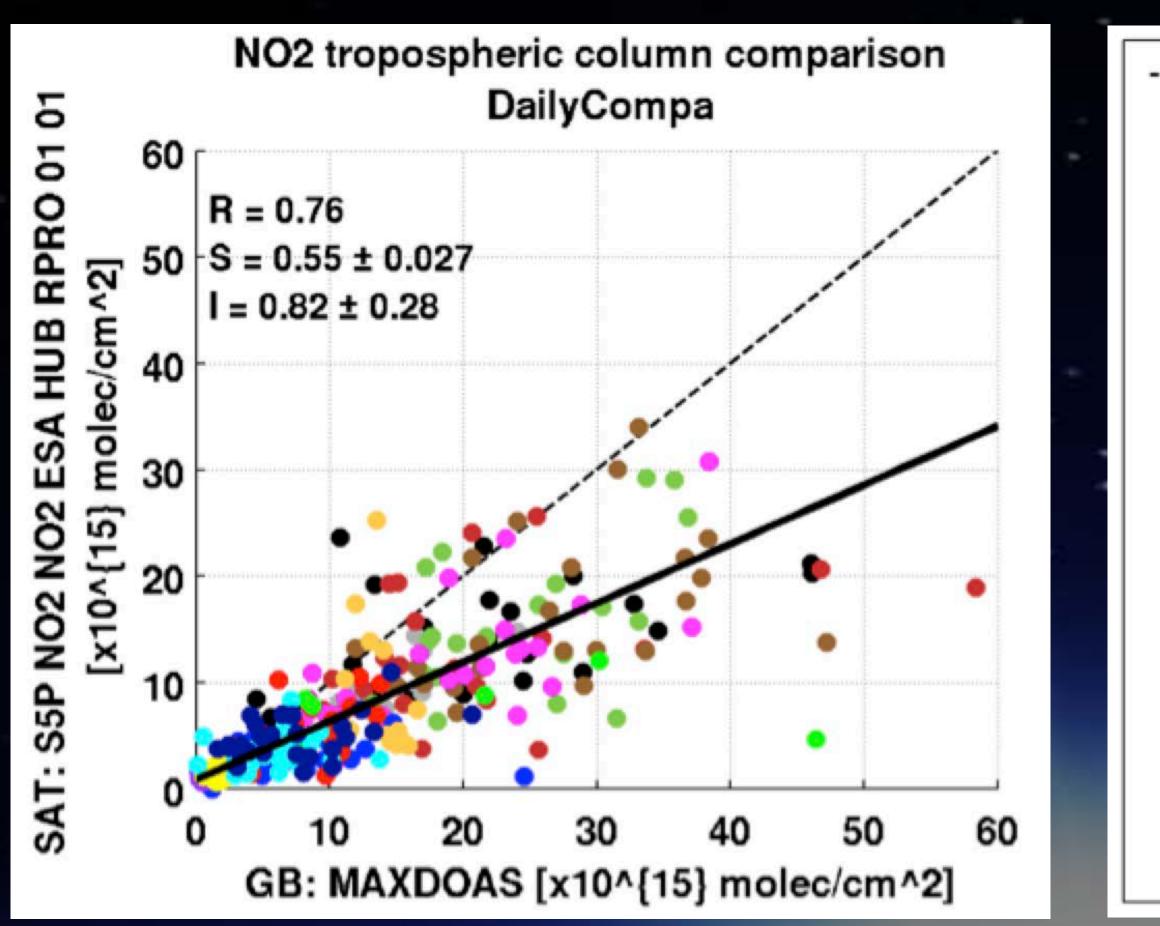
First validation results for Sentinel-5p NO2 column data.



A first validation against NDACC and WOUDC ground-based data confirms that the TROPOMI/S5p NRTI total O3 (L2\_O3) product

meets mission requirements. Initial Sentinel-5p TROPOMI L2\_03 03 column data retrieved with the PDGS NRTI processor (v1 0 0) have been

# TROPOMI vs. MAXDOAS



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





Royal Netherlands Meteorological Institute Ministry of Infrastructure and Water Management





SSP MPC





- Chiba (25)
- uccle (11)
- unam (20)
- vallejo (20)
- xianghe (29)
- yokosuka (31)
- athens (27)
- bremen (30)
- cape\_hedo (21)
- cuautitlan (13)
- fukue (12)
- mainz (7)
- thessaloniki\_ciri (26)
- thessaloniki\_lap (26)

s&]t

Universität Bremen

NILU

# TROPOMI 30% lower than MAXDOAS

#### Bridging the gap ?

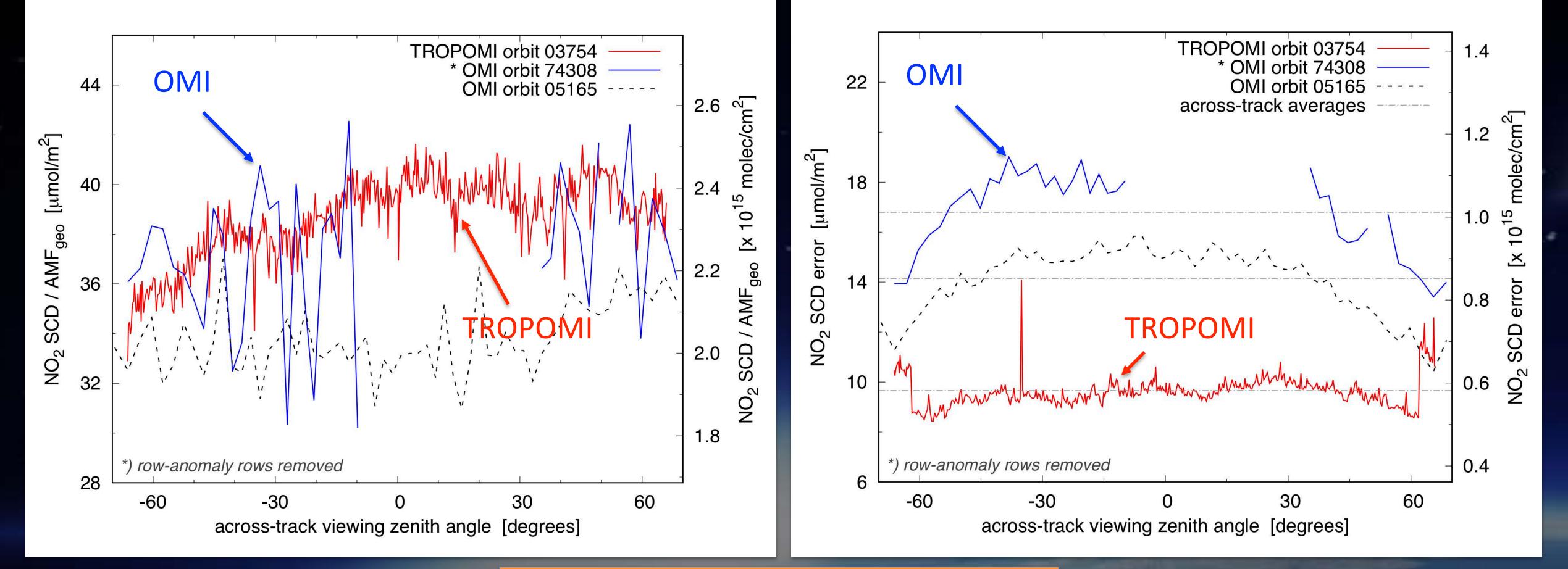
- Profile shape
- Clouds

TROPOMI

- Local situation
- Kernel difference



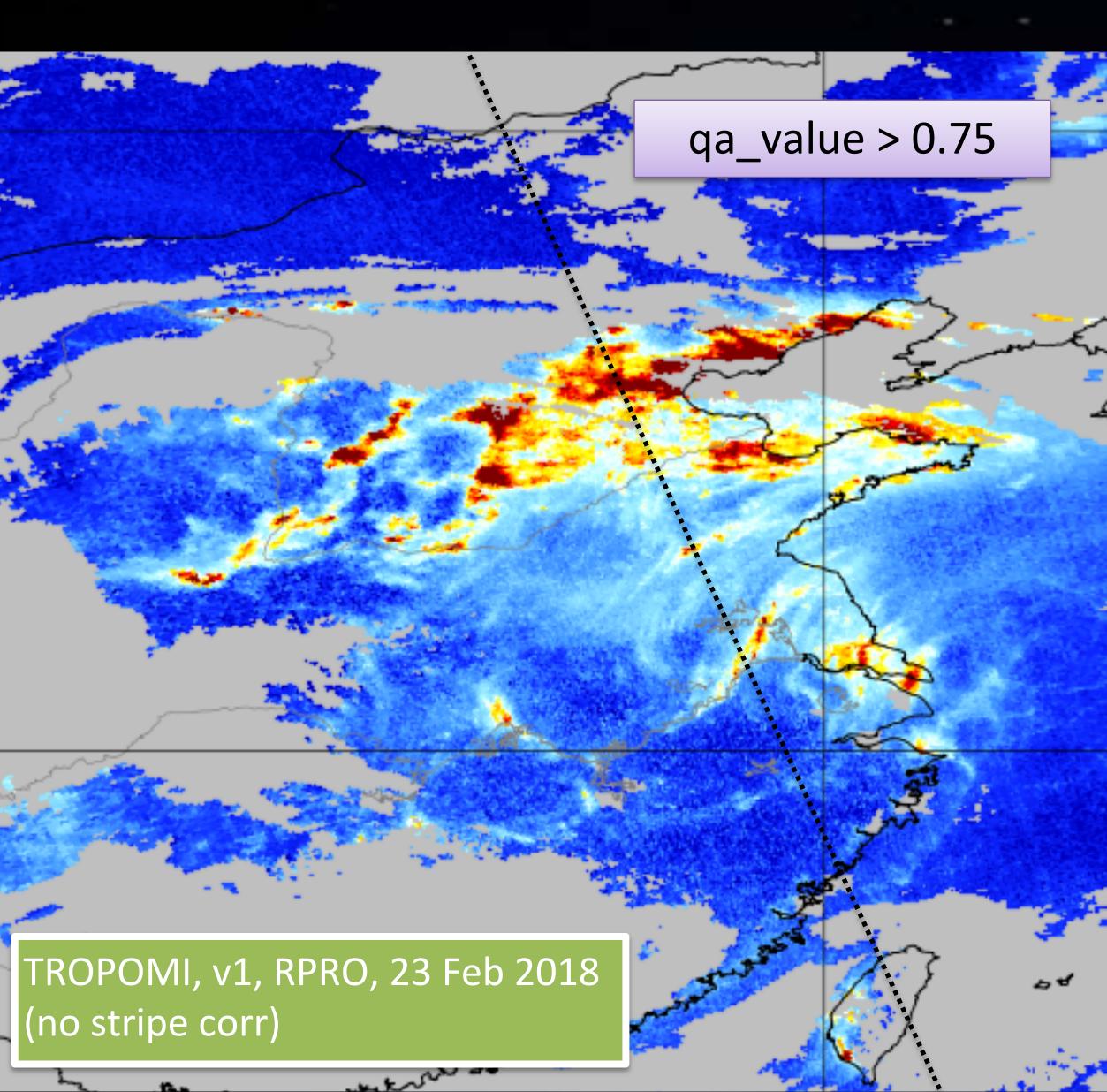
#### Comparison to other satellites: OMI vs. TROPOMI for DOAS slant column fits



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



# **TROPOMI comparison with OMI - China**







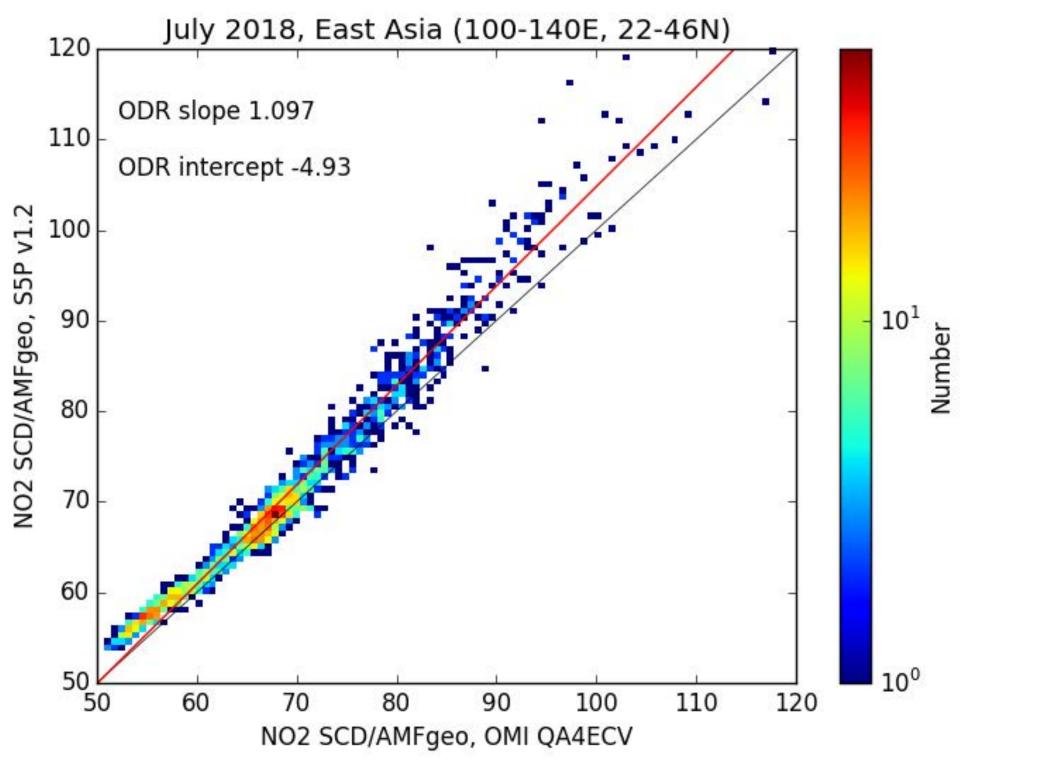
#### OMI, QA4ECV algo, 23 Feb 2018 (stripe corrected)

- EN



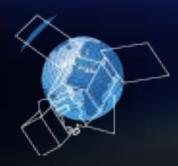
## **Comparison with OMI**

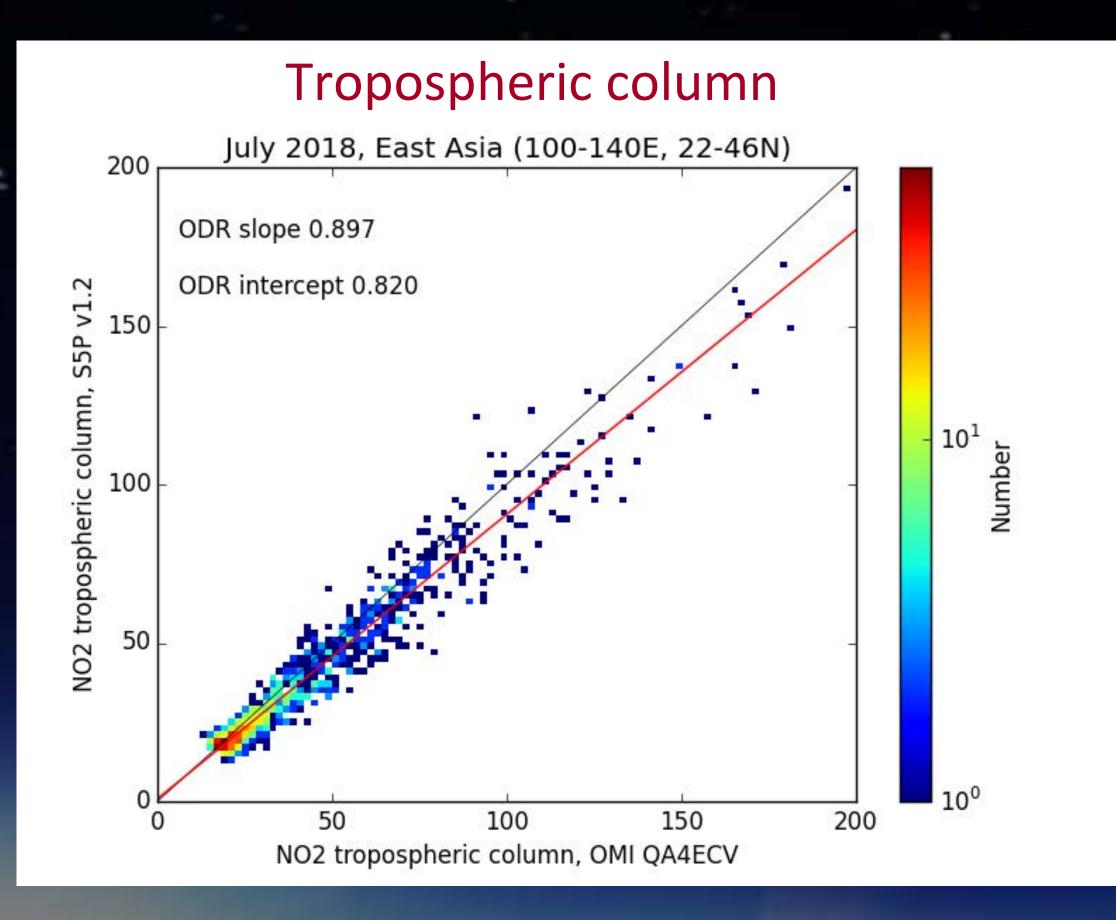
#### SCD / AMFgeo



Differences in AMF?

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



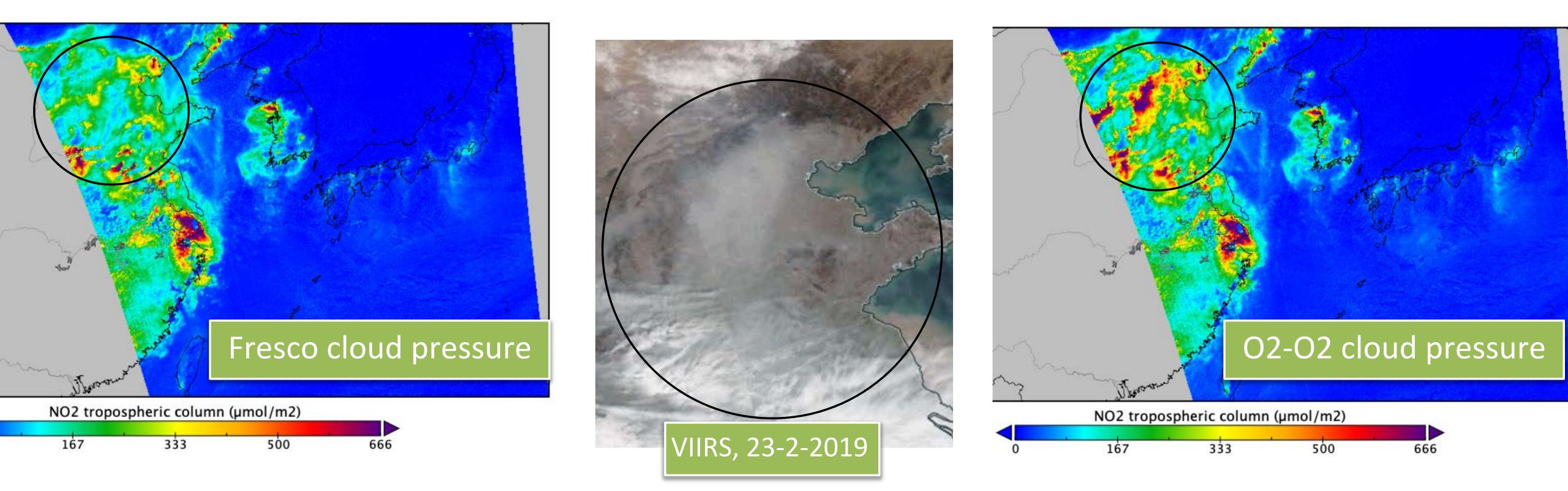








#### Dependence on cloud retrievals: Fresco vs O2-O2



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

#### **Averaging kernels**

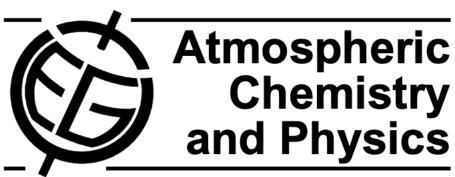
Atmos. Chem. Phys., 3, 1285–1291, 2003 www.atmos-chem-phys.org/acp/3/1285/

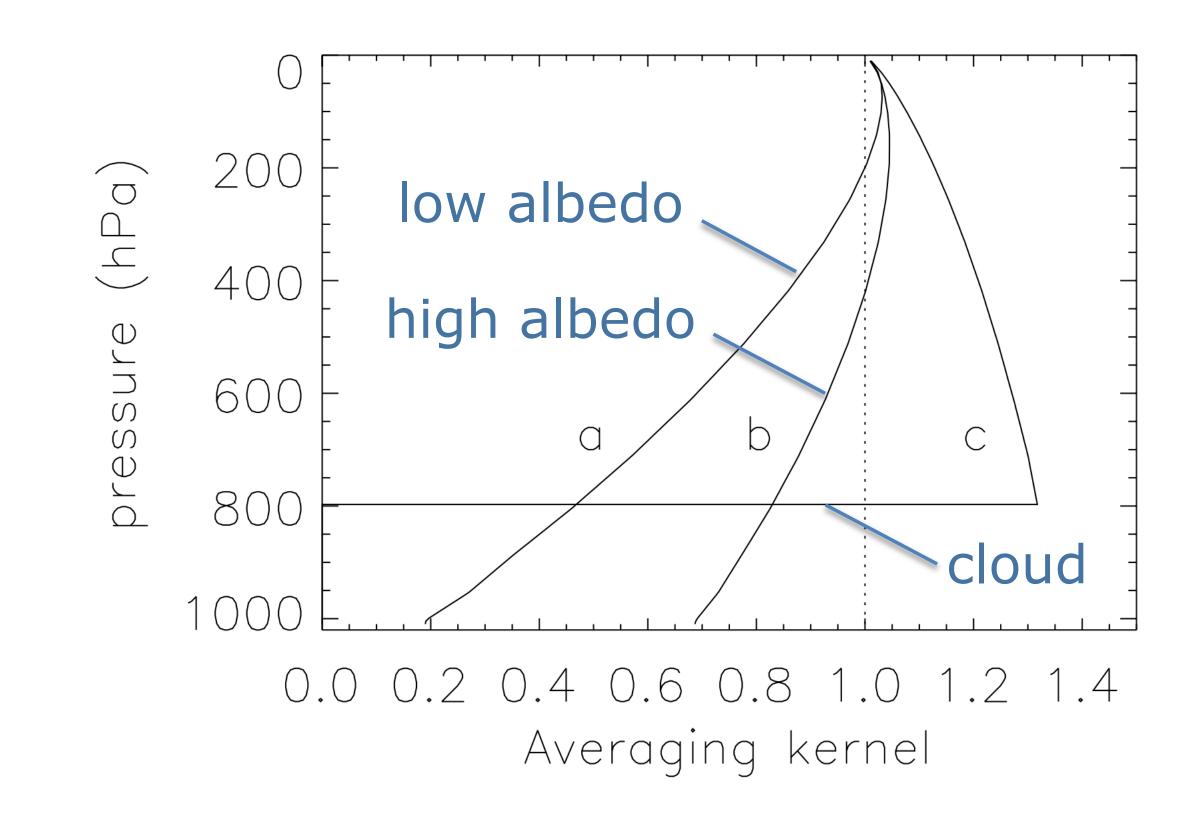
#### Averaging kernels for DOAS total-column satellite retrievals

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<sub>2</sub> 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 <sub>2</sub> profile measurements (aircraft, balloon, MAX-DOAS)	$N_{ m v}^{ m trop}, \Delta N_{ m v}^{ m trop, m kernel}$ $M^{ m trop}, M, {f A}^{\dagger}$ $A_l^{ m TM5}, B_l^{ m TM5}, l_{ m tp}^{ m TM5}, p_{ m s}$
#2	Tropospheric column comparisons, e.g. with other NO <sub>2</sub> column retrievals	$N_{v}^{trop}, \Delta N_{v}^{trop}$
#3	Stratospheric chemistry model evaluation and data assimilation Validation with stratospheric NO <sub>2</sub> profile measurements (limb/occultation satellite observations)	$N_{ m v}^{ m strat}, \Delta N_{ m v}^{ m strat}$ $M^{ m strat}, M, {f A}^{\ \ddagger}$ $A_l^{ m TM5}, B_l^{ m TM5}, l_{ m tp}^{ m TM5}, p_{ m s}$
# 4	Stratospheric column comparisons, e.g. with ground-based remote sensors	$N_{v}^{\text{strat}}, \Delta N_{v}^{\text{strat}}$
# 5	Whole atmosphere (troposphere + stratosphere) data assimilation systems	$N_{ m v}, \Delta N_{ m v}^{ m kernel}$ § A $A_l^{ m TM5}, B_l^{ m TM5}, l_{ m tp}^{ m TM5}, p_{ m s}$
# 6	Whole atmosphere (troposphere + stratosphere) comparisons with ground-based remote sensing (e.g. Pandora)	$N_{ m v}^{ m sum}, \Delta N_{ m v}^{ m sum}$
#7	Visualisation of the NO <sub>2</sub> product	Nv <sup>trop</sup> , Nv <sup>strat</sup> , Nv <sup>sum</sup> §



John Douros (KNMI)

<sup>‡</sup> The stratospheric kernel  $A^{strat}$  is derived from the total kernel A and the air-mass factors M and  $M^{strat}$ . <sup>§</sup> Note that the total NO<sub>2</sub> vertical column  $N_v \equiv N_s/M$  is *not* the same as the sum  $N_v^{sum} \equiv N_v^{trop} + N_v^{strat}$ 



### **Application of the averaging kernels**

The file contains the averaging kernel for the total column. The tropospheric column  $\mathbf{A}^{trop}$  is obtained in the following way

$$egin{array}{lll} \mathbf{A}^{ extsf{trop}} = & rac{M}{M^{ extsf{trop}}} \mathbf{A} &, \ l <= l_{ extsf{tp}}^{ extsf{TM5}} \ \mathbf{A}^{ extsf{trop}} = & 0 &, \ l > l_{ extsf{tp}}^{ extsf{TM5}} \end{array}$$

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

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

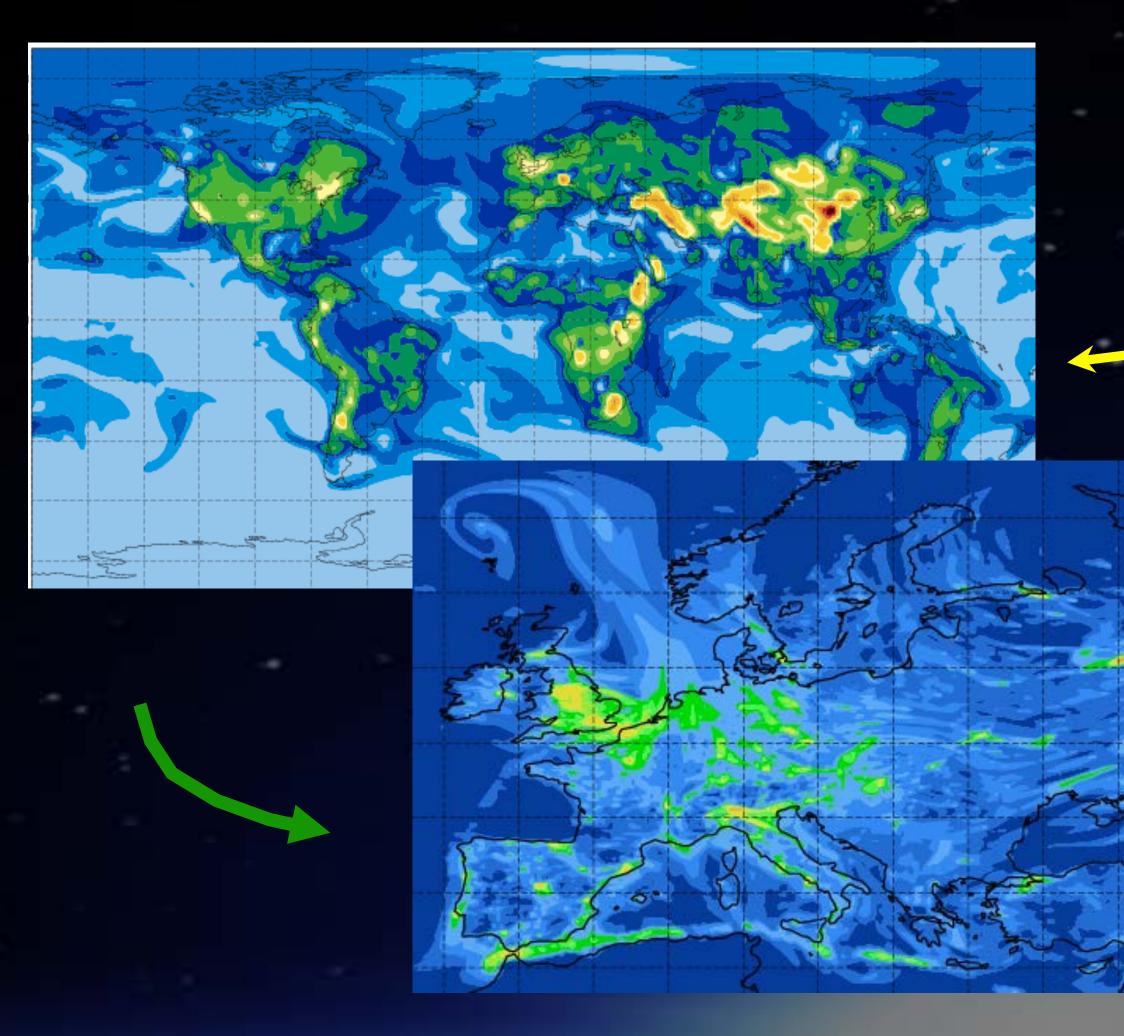
### **Replacing the a-priori using the averaging kernels**

The TROPOMI NO<sub>2</sub> 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:

$$N_{v}^{\text{trop}'} = \frac{M^{\text{trop}}}{M^{\text{trop}'}} N_{v}^{\text{trop}}$$
$$\mathbf{A}^{\text{trop}'} = \frac{M^{\text{trop}}}{M^{\text{trop}'}} \mathbf{A}^{\text{trop}}$$
$$M^{\text{trop}'} = M^{\text{trop}} \sum_{l} A_{l}^{\text{trop}} x'_{m,l} / \sum_{l} x'_{m,l}$$

All quantities on the left with a prime ' are recomputed using the model NO<sub>2</sub> 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



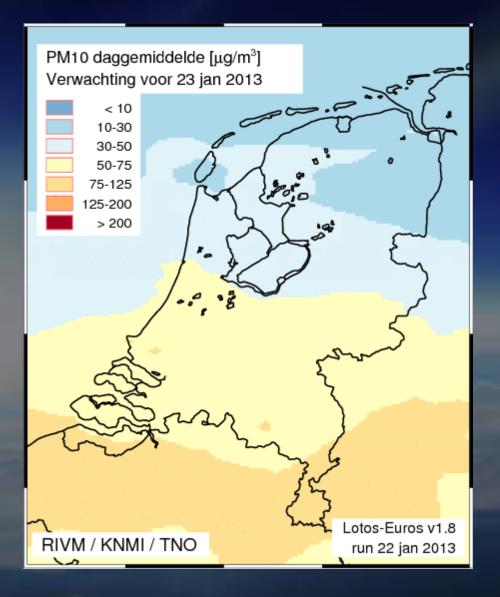
Analyses of CAMS-global as boundary condition for CAMS-Europe

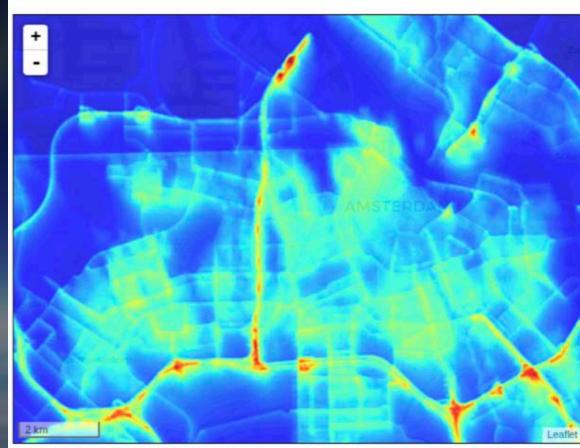
atmosphere.copernicus.eu

Assimilation TROPOMI observations

# CAMS-Europe as boundary condition for countries and city regions

#### Amsterdam



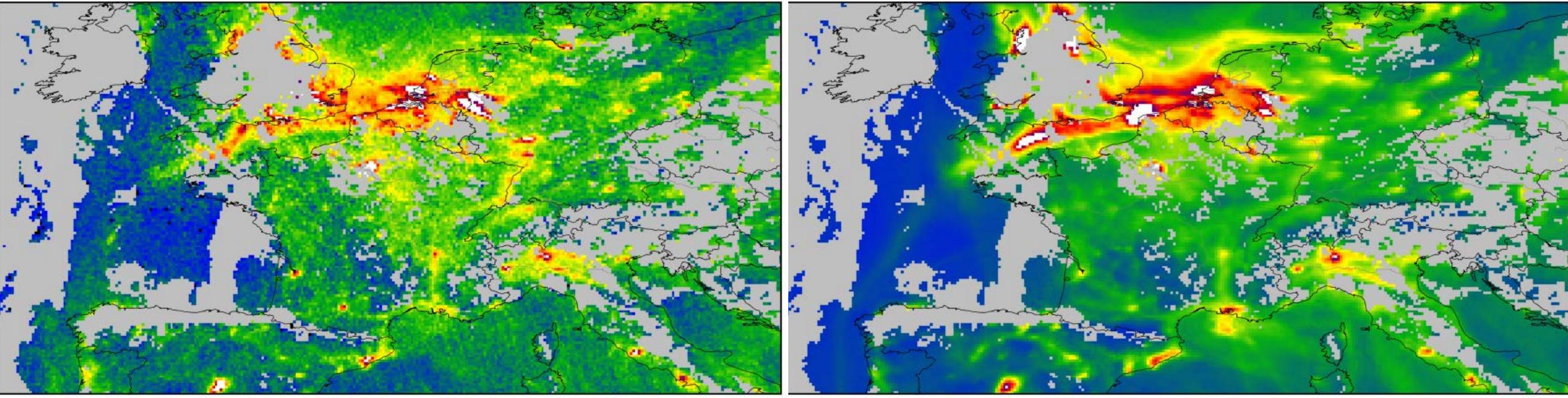






### Using a-priori profiles from CAMS-regional AQ forecasts for Europe

#### TROPOMI NO2 based on CAMS-regional a-priori

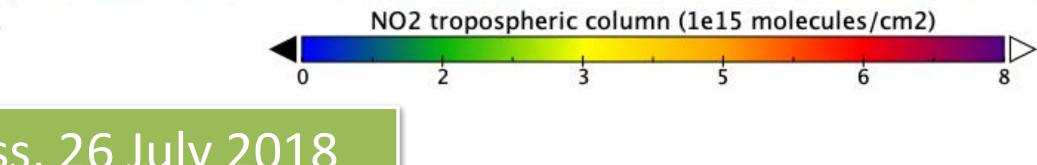


TROPOMI tropospheric vertical column of nitrogen dioxide using CAMS a-priori profile (10^15 molecules/c... Single overpass, 26 July 2018

John Douros, KNMI

John Douros (KNMI)

#### CAMS-regional vertical column NO2



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

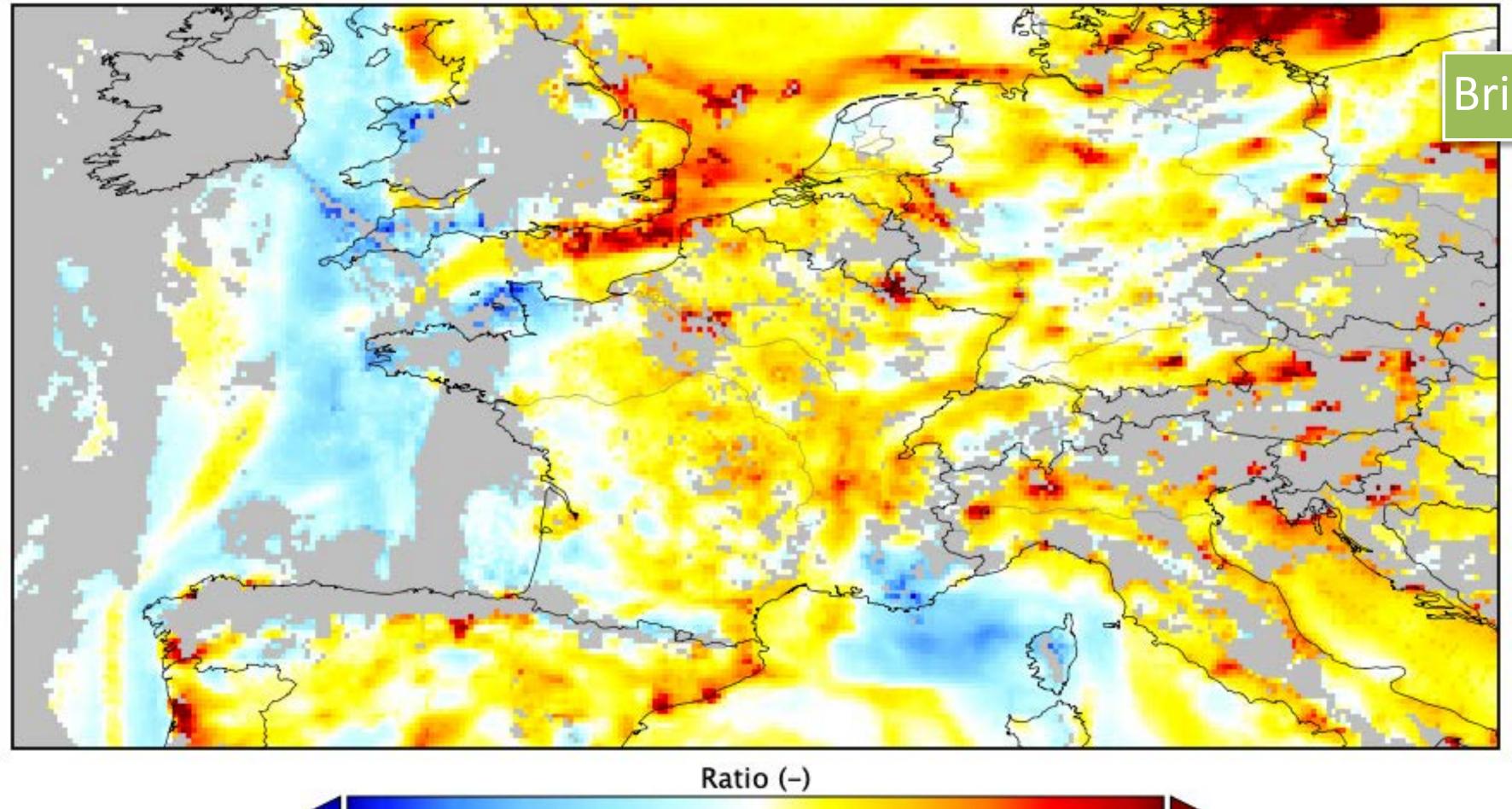
#### Ratio NO2 tropospheric column CAMS a-priori / TM5MP a-priori

0.7

0.5

0.9

1.1



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

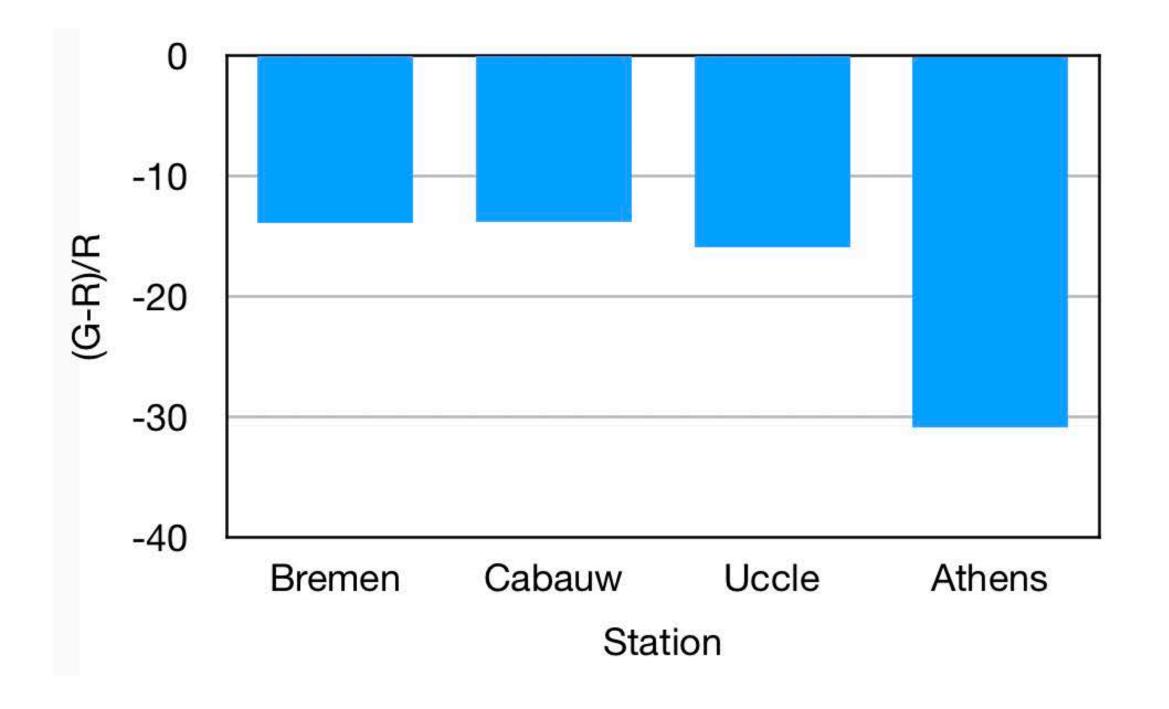
1.3 1.5

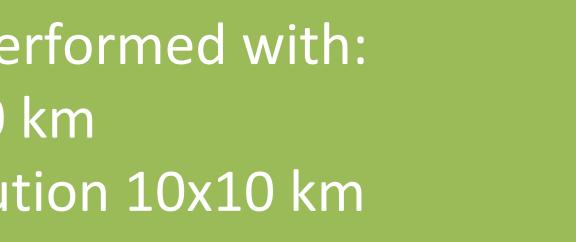


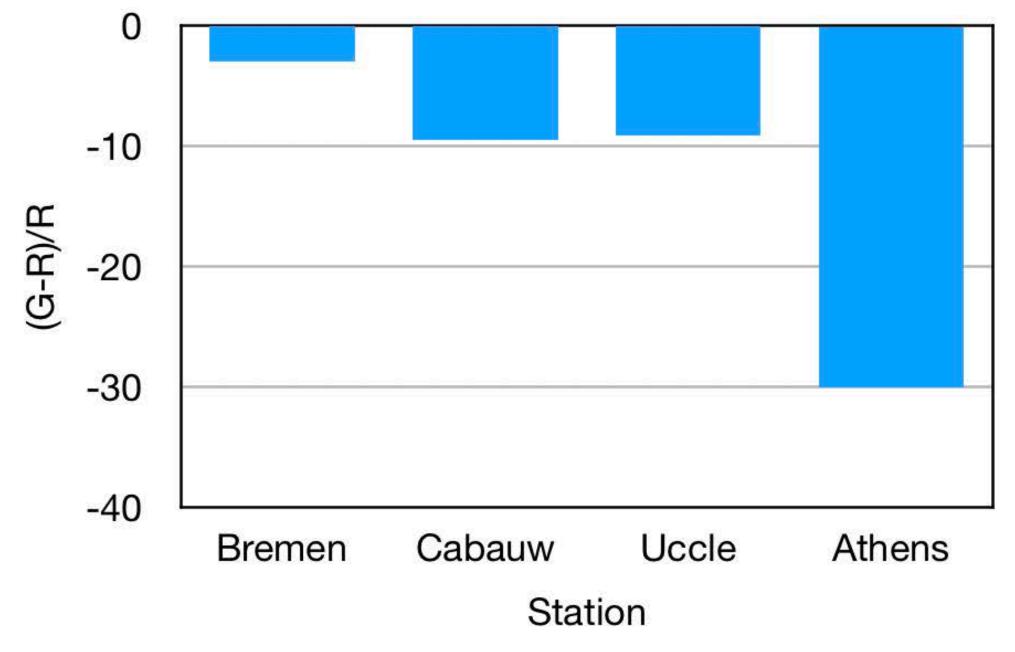


### Using a-priori profiles from CAMS-regional AQ forecasts for Europe

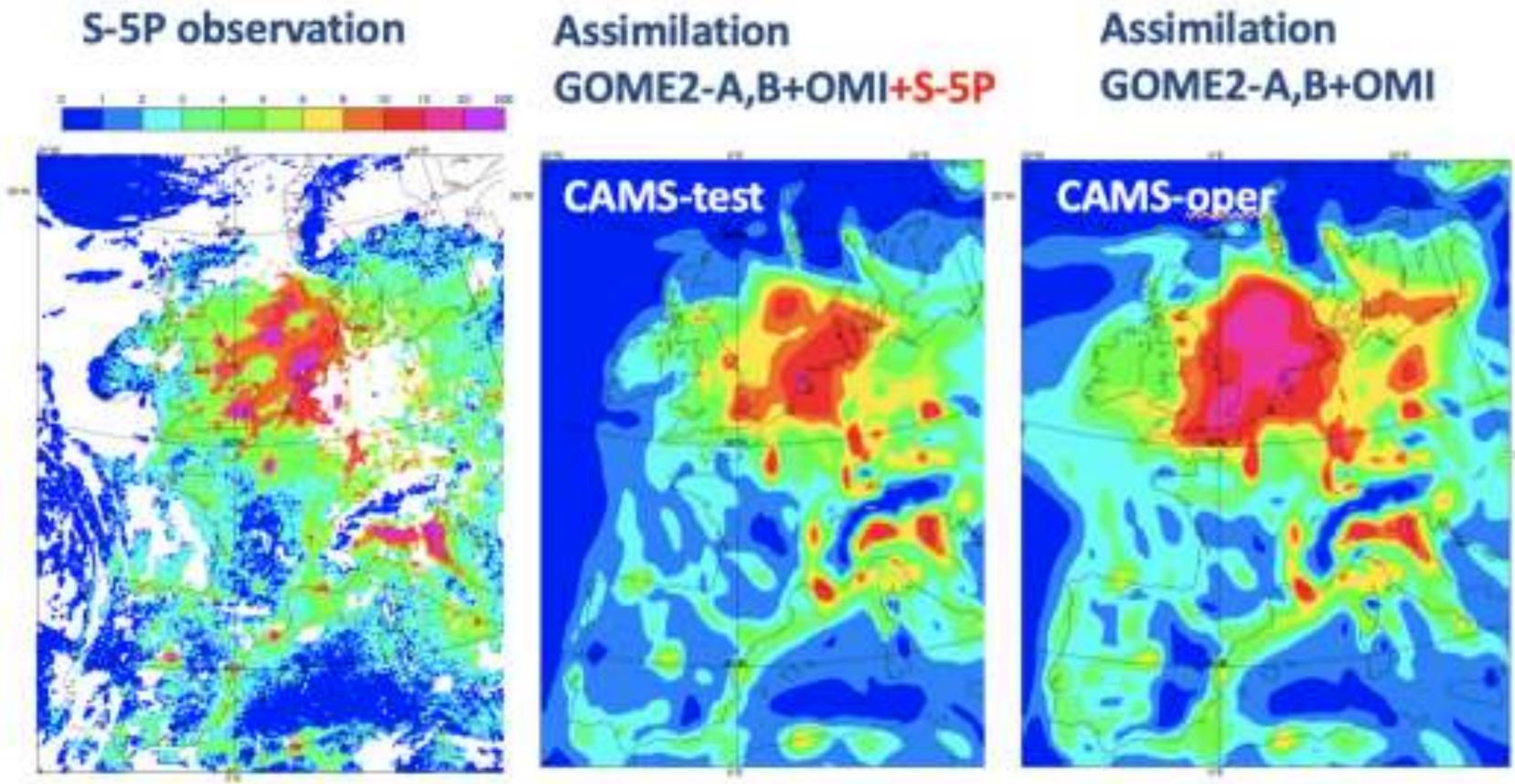
Ratio of retrievals @ MAX-DOAS stations, performed with: • TM5-MP at a resolution of about 100x100 km • CAMS-regional (European domain), resolution 10x10 km







# **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

- A game changer in spatial resolution and signal-to-noise!
- NO<sub>2</sub> 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<sub>2</sub> 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



www.tropomi.eu

www.temis.nl

sentinels.copernicus.eu

#tropomi, @tropomi



# EXTRA SLIDES





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

24 km

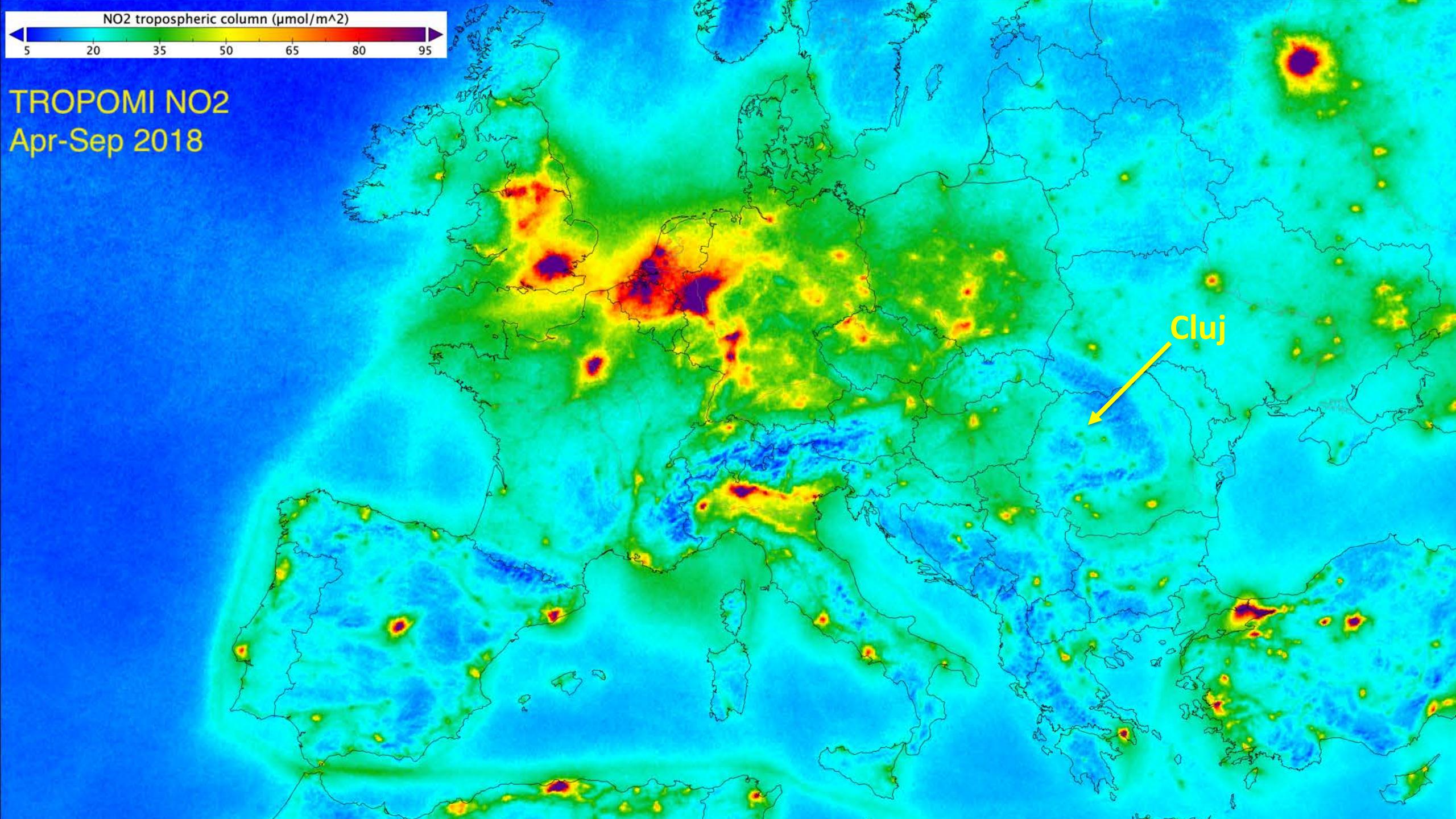
5,63 m diameter,

ent (TROPOMI)

) and Kiruna

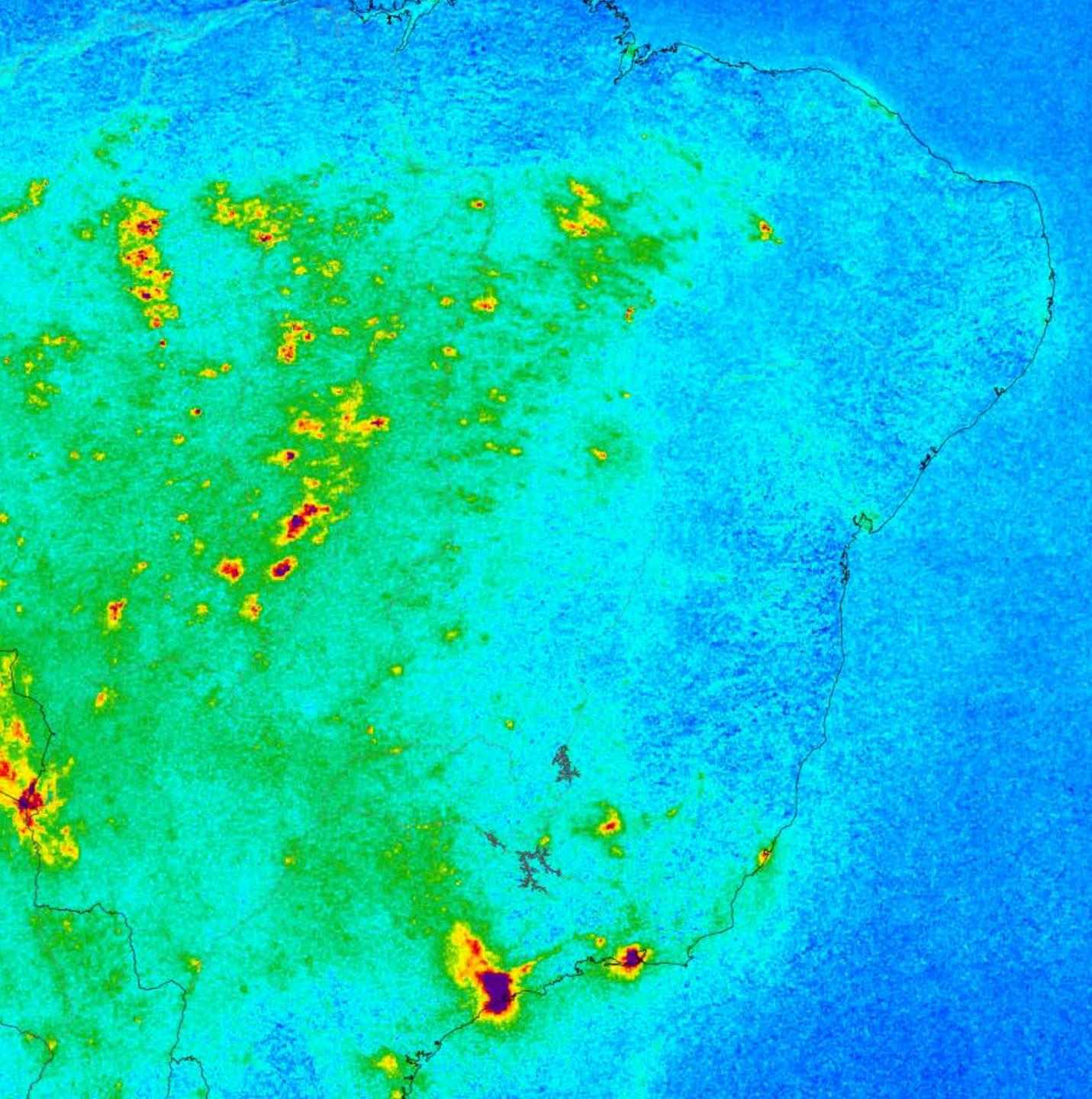


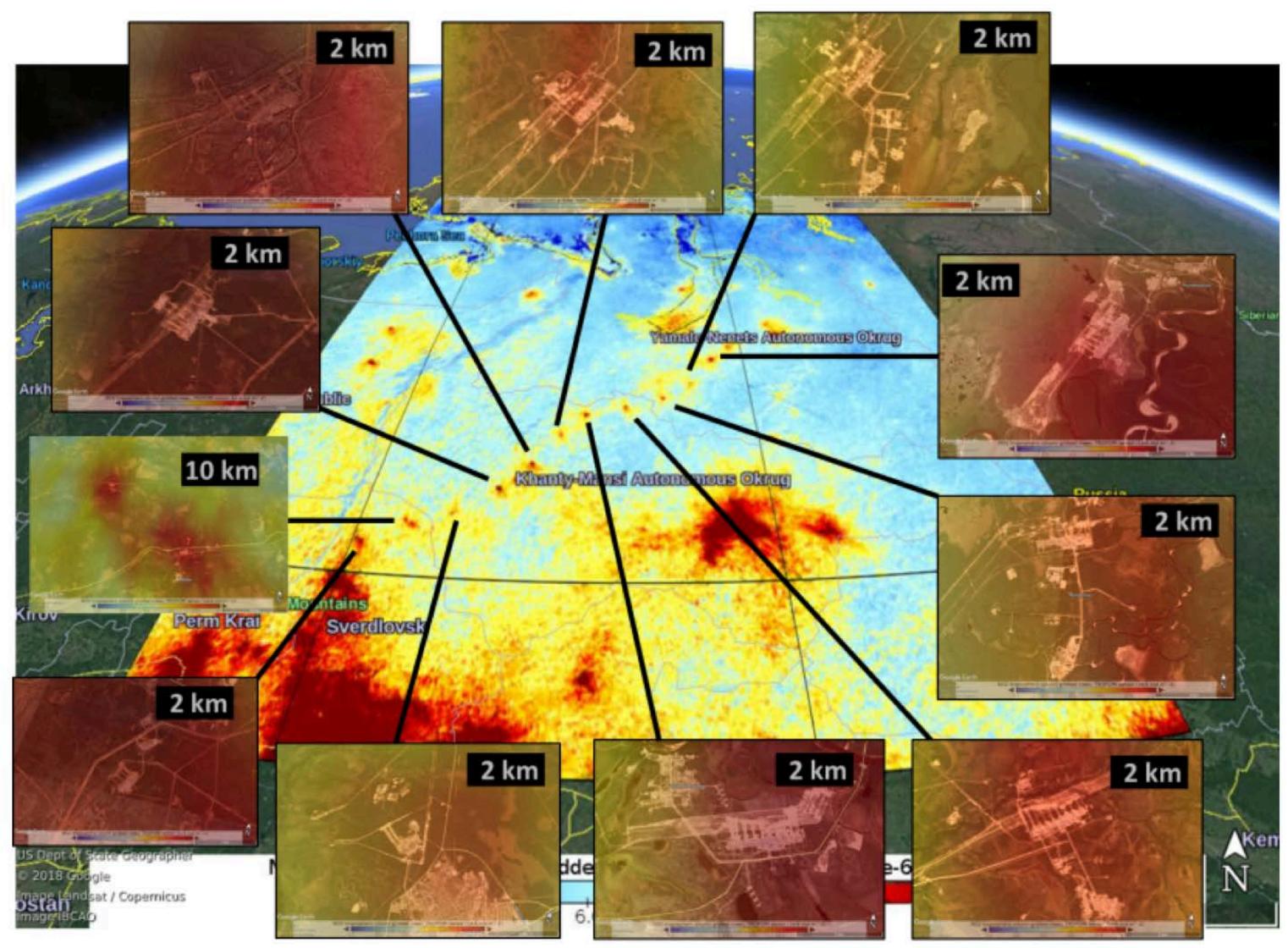




#### South America, August 2019

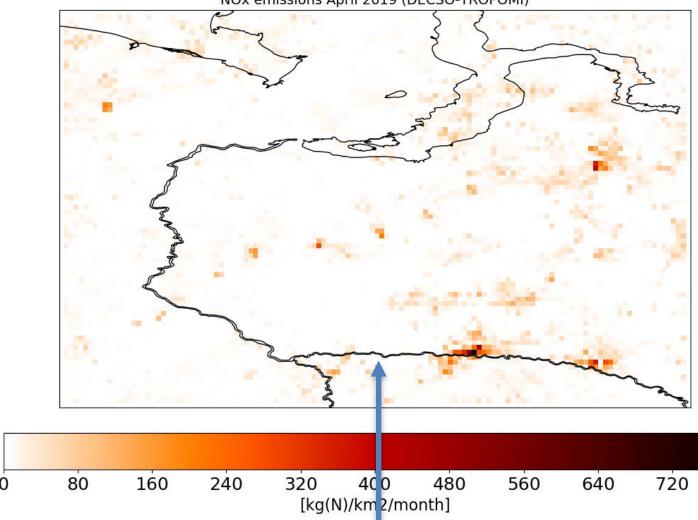
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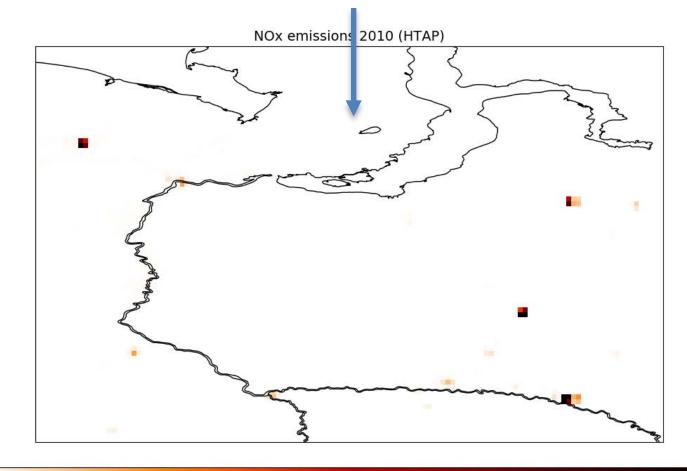


string of gas compressor stations along natural gas pipeline every ≈ 100 km

NOx emissions April 2019 (DECSO-TROPOMI)



#### TROPOMI NO<sub>2</sub> emission inversion (DECSO) for April 2019 compared with bottom up emission inventory (HTAP/EDGAR)









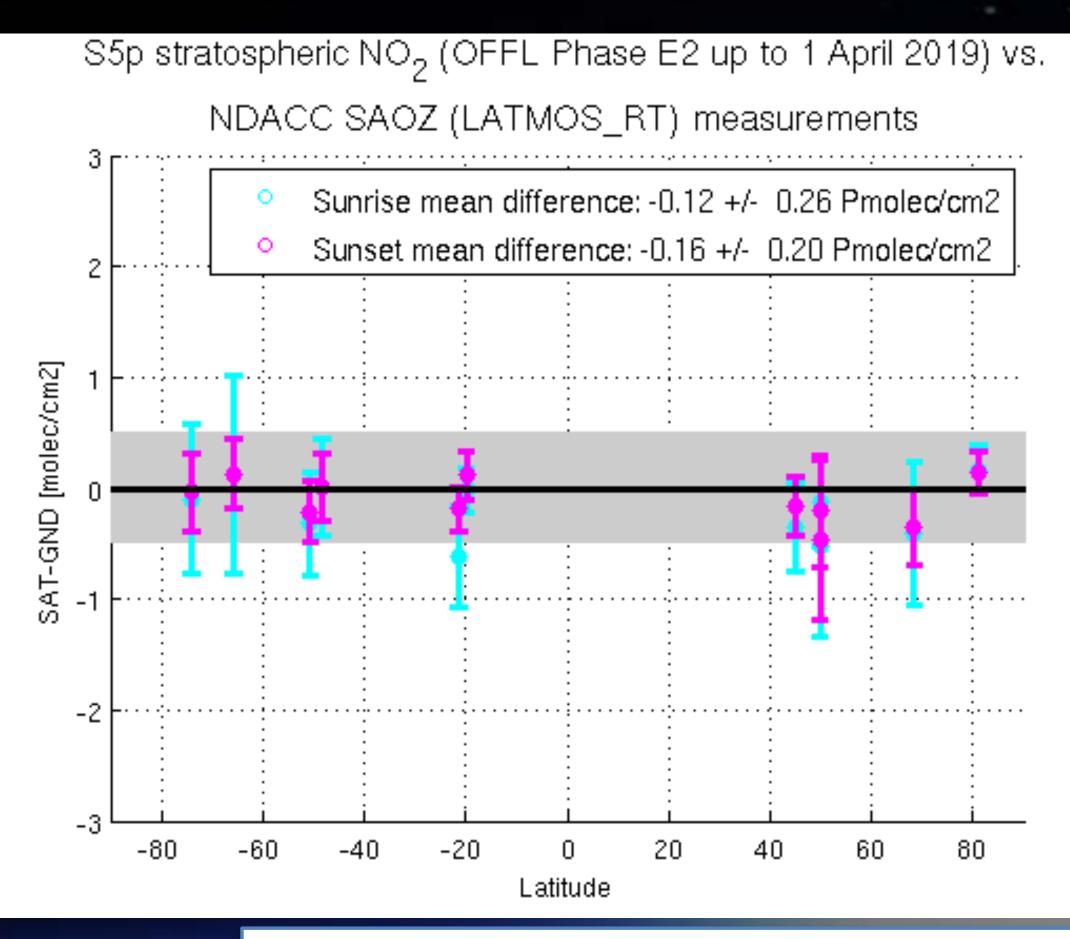
# **NO2: upgrades and reprocessing**

				ly 2018:	+ 24 C	October 2	ase (NR7 2018: v1. g v1.2.2 (	2 releas	e			
								+ 27 Ⅳ	larch 20	19: v1.3	release	
			-> Pha	se E2 (E	Data ava	ilable fro	om 30 Ap	oril 2018)		<ul> <li>6 Aug</li> </ul>	2019: sn	nall pixels
Jan 2018	Mar 2018	May 2018	Jul 2018	Sep 2018	Nov 2018	Jan 2019	Mar 2019	May 2019	Jul 2019	Sep 2019	Nov 2019	

Each of these releases accompanied with documentation updates:

- **ReadMe (PRF)** 0
- **Product User Manual (PUM)**  $\bigcirc$
- **Algorithm description (ATBD)**  $\bigcirc$

# S5P MPC: TROPOMI vs SAOZ



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

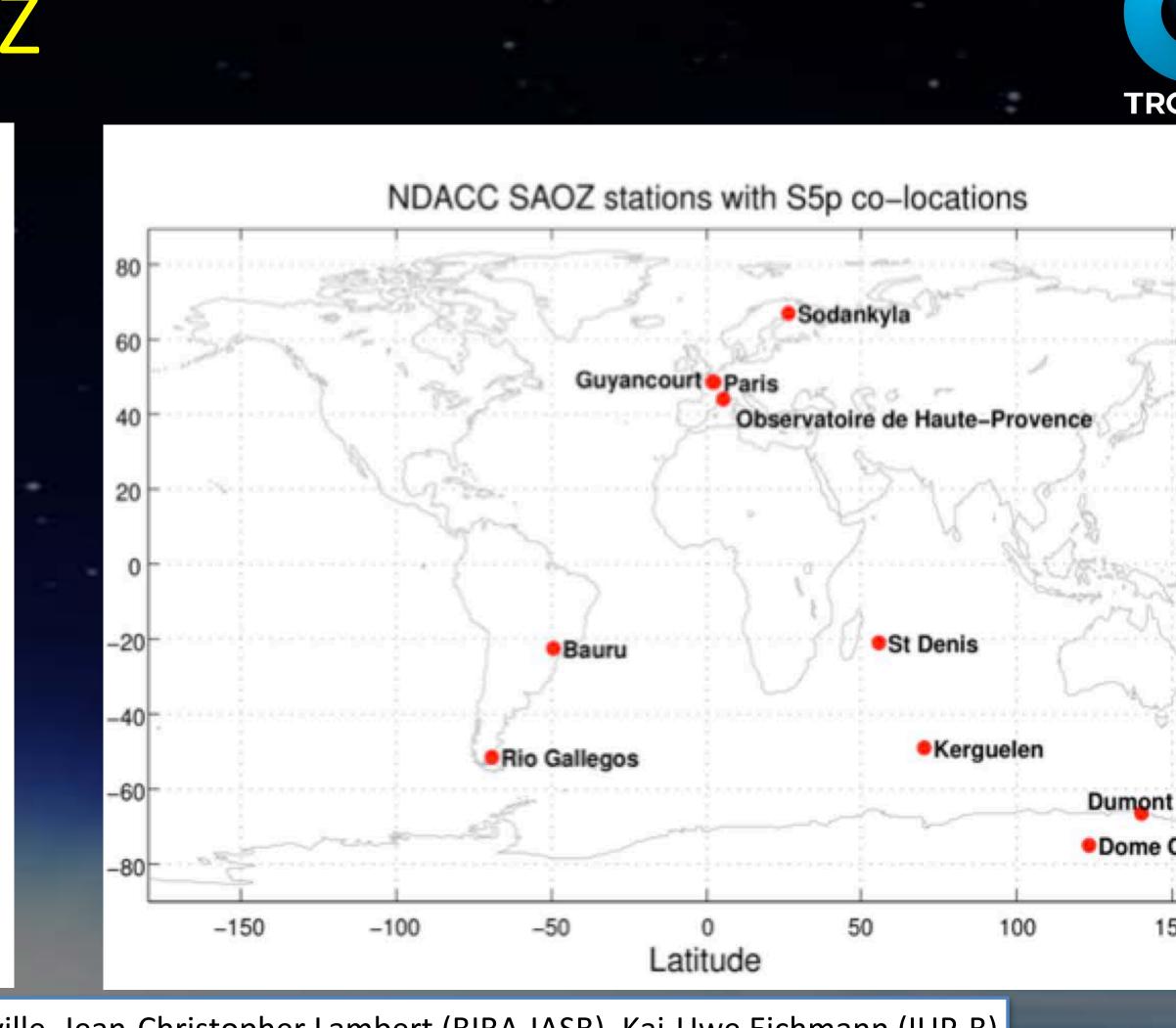




**Royal Netherlands** Meteorological Institute Ministry of Infrastructure and Water Management











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