



Satellite Applications: NO₂

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Second Joint School on Atmospheric Composition
16-20 November 2020

Satellite instruments measuring NO₂

- * **Past & present:**

25 years of NO₂ observations from space

GOME, SCIAMACHY, GOME-2 A/B/C, OMI, OMPS, TROPOMI (Sentinel-5P)

Increasing the spatial resolution from about 100 km to about 5 km

- * **Future:**

Geostationary: GEMS (launched 2020), TEMPO, Sentinel 4

Sentinel 5

CO2M (2 km resolution), with NO₂ for plume identification

...

Copernicus Sentinel-5P TROPOMI instrument

Dutch instrument Pepijn Veefkind PI (KNMI) Airbus DS, TNO, SRON, KNMI, NSO, ESA, EU

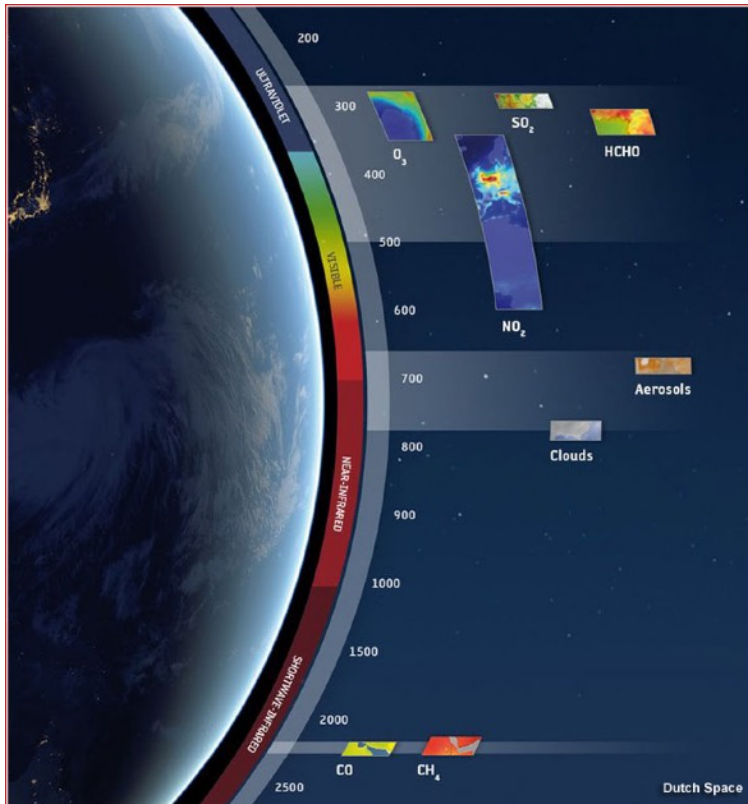
Mission objectives: **Air Quality, Climate Change, Ozone layer**

TROPOMI combines:

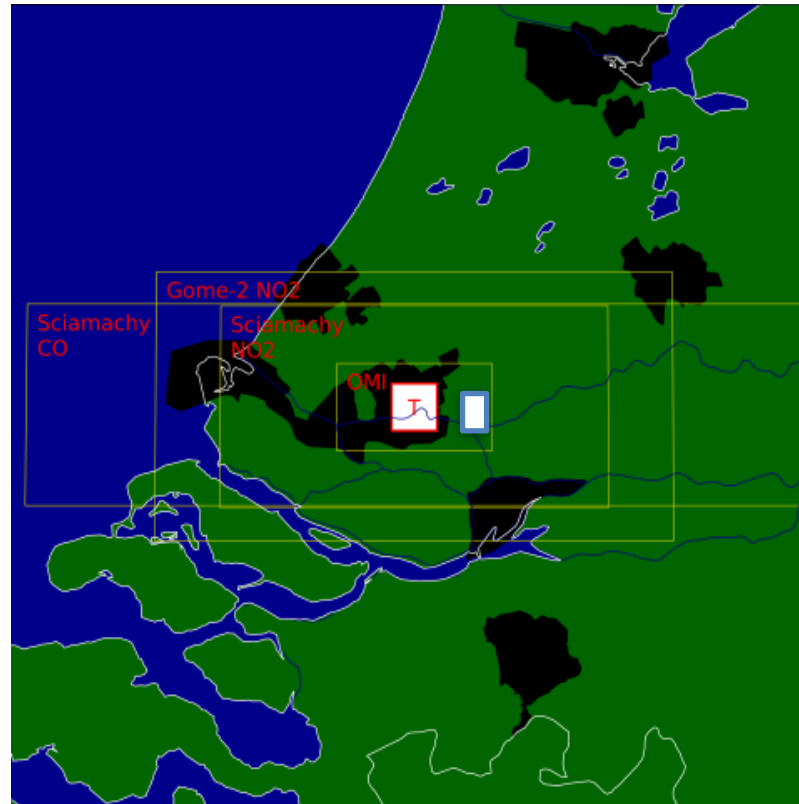
High signal-to-noise

Large spectra range

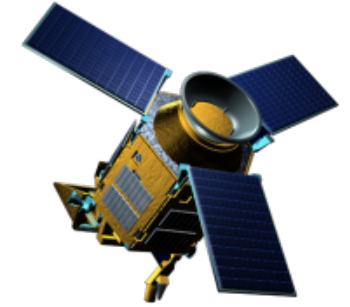
(large number of trace gas species)



High spatial resolution (3.5 x 5.5 km)

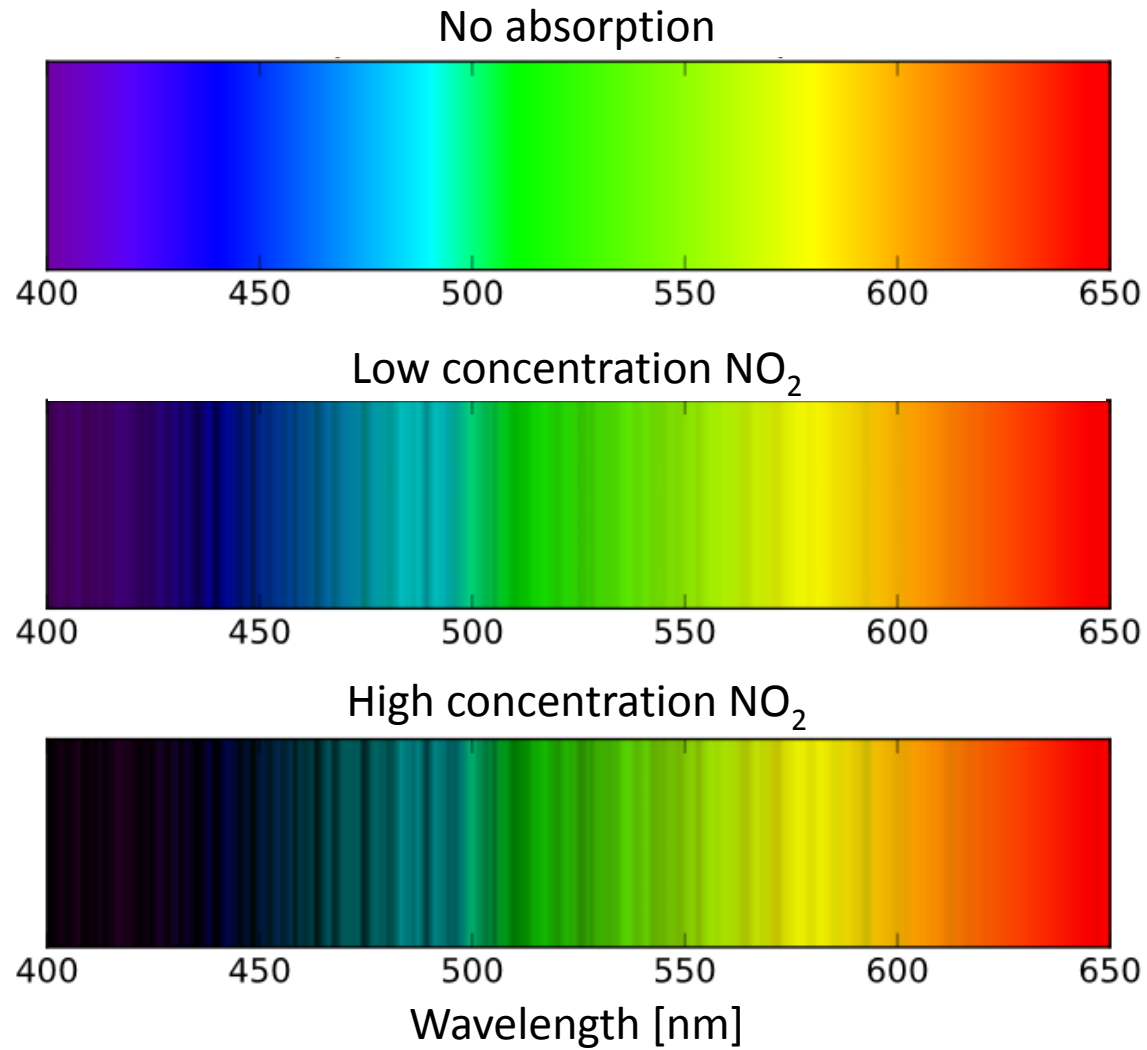


Daily global coverage



Retrieval of NO₂

From spectra to concentrations

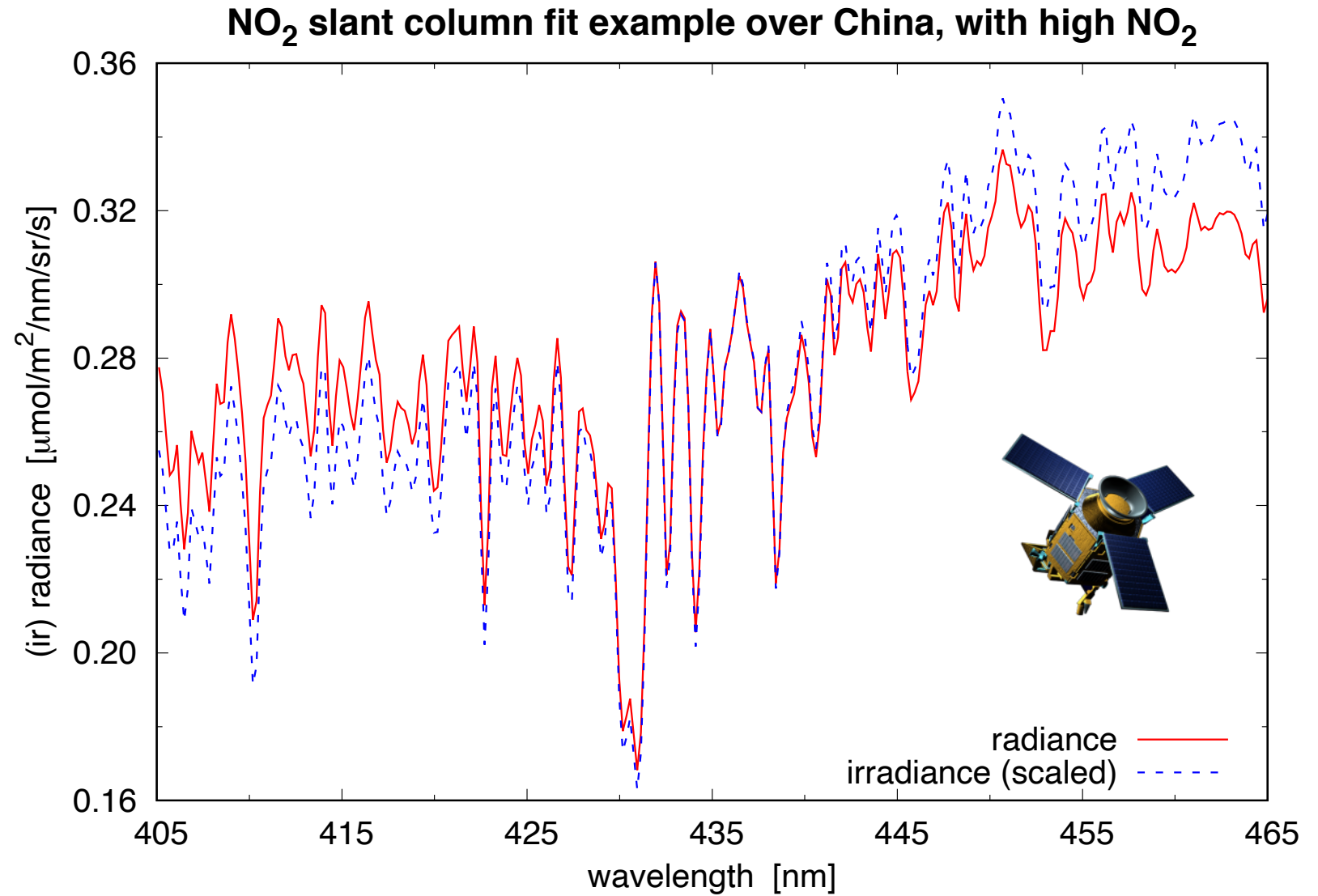


NO₂ typical concentration is
1 molecule per 10⁹ air
molecules: how can we
measure this ??

TROPOMI observations
405-465 spectral range

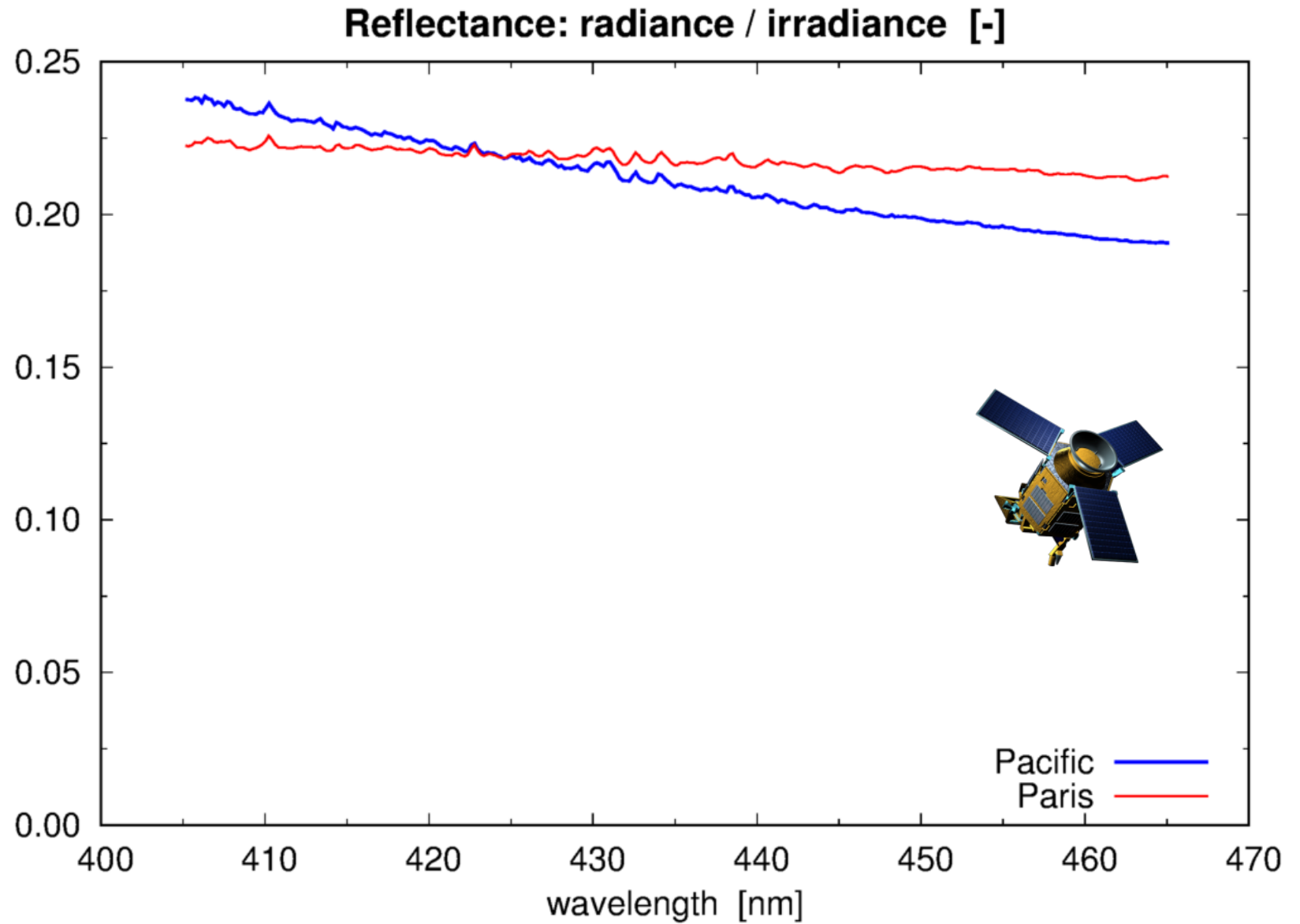
When looking at the Earth
the main spectral features
observed are coming from
the Sun (solar spectrum)

Jos van Geffen, KNMI



TROPOMI observations
405-465 spectral range

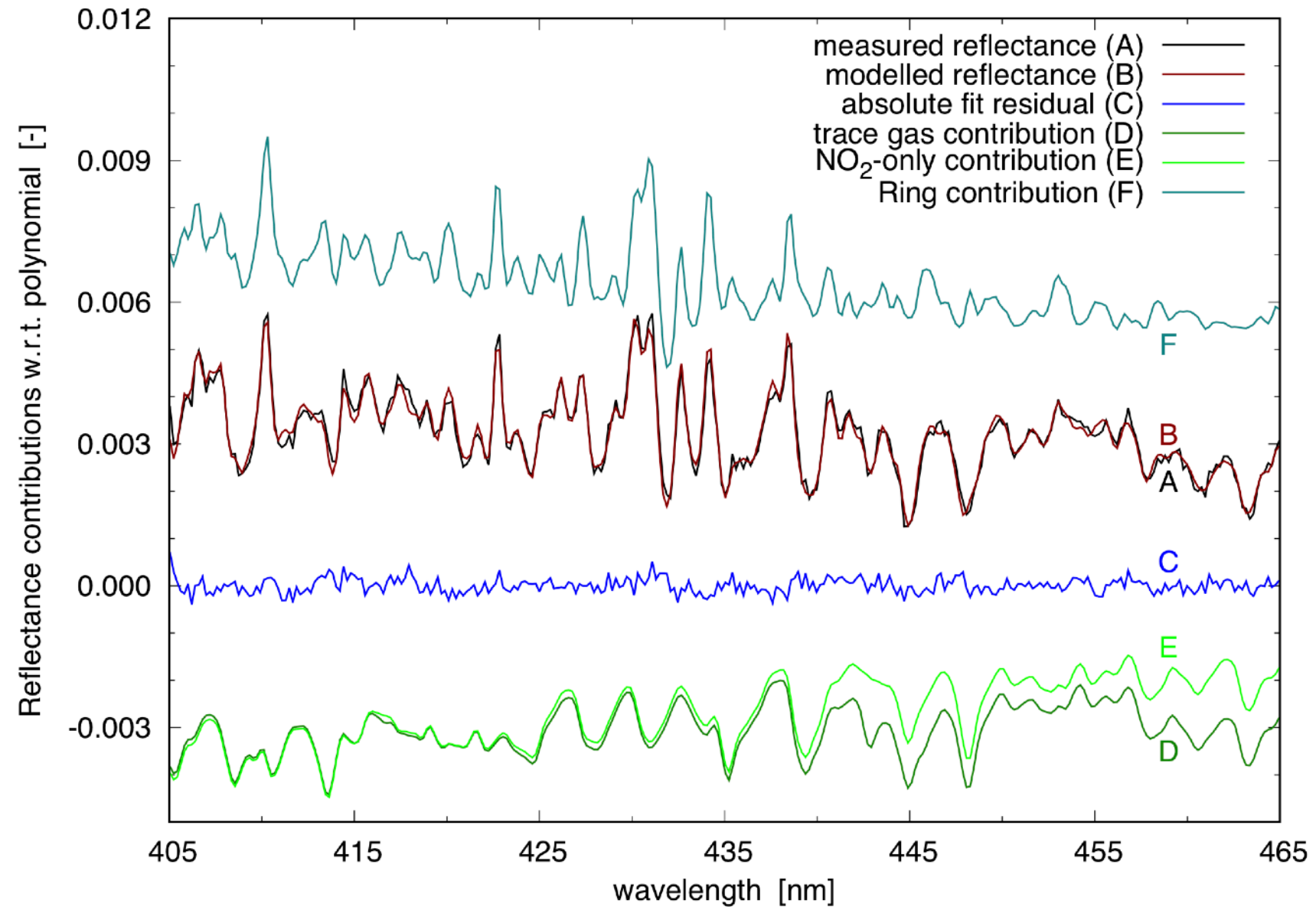
Reflectance is a
“nearly” straight line





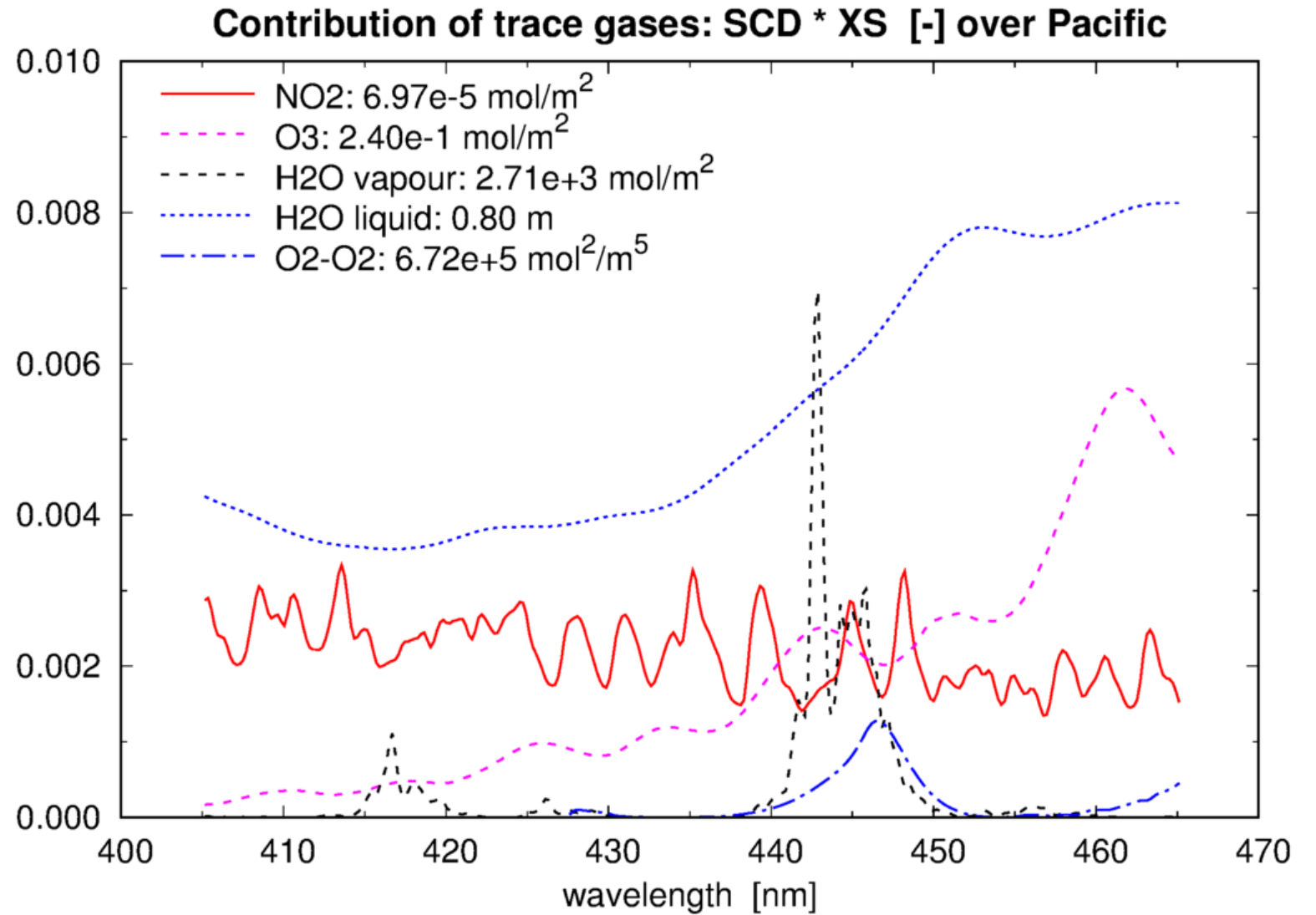
Also in the reflectance
the solar spectral features
are still dominant

Ring effect =
inelastic Raman scattering
of sunlight in the
atmosphere



Absorbers
accounted for:

- NO₂
- Ozone
- Water vapour
- Liquid water
- O₂-O₂



NO₂ spectral fitting: summary

Instrument:

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

Conclusions related to the fits in NO₂ window:

- › We understand the Earth radiance in great detail, residuals $\sim 1\text{e-}4$
- › NO₂ has a very distinct spectral fingerprint and the slant column can be quantified accurately with current instruments.

What did we determine so far?

The amount of NO₂ along the path of the light through the atmosphere:
The “slant column”

What we do not yet know:

How far did the light penetrate into the atmosphere ?

Where is the NO₂ ? (At what altitude?)

Translate “slant column” into vertical column amount

How did the light travel through the atmosphere?

Aspects that influence the light path:

Surface properties (reflection)



Clouds

Aerosols

Air-mass factor



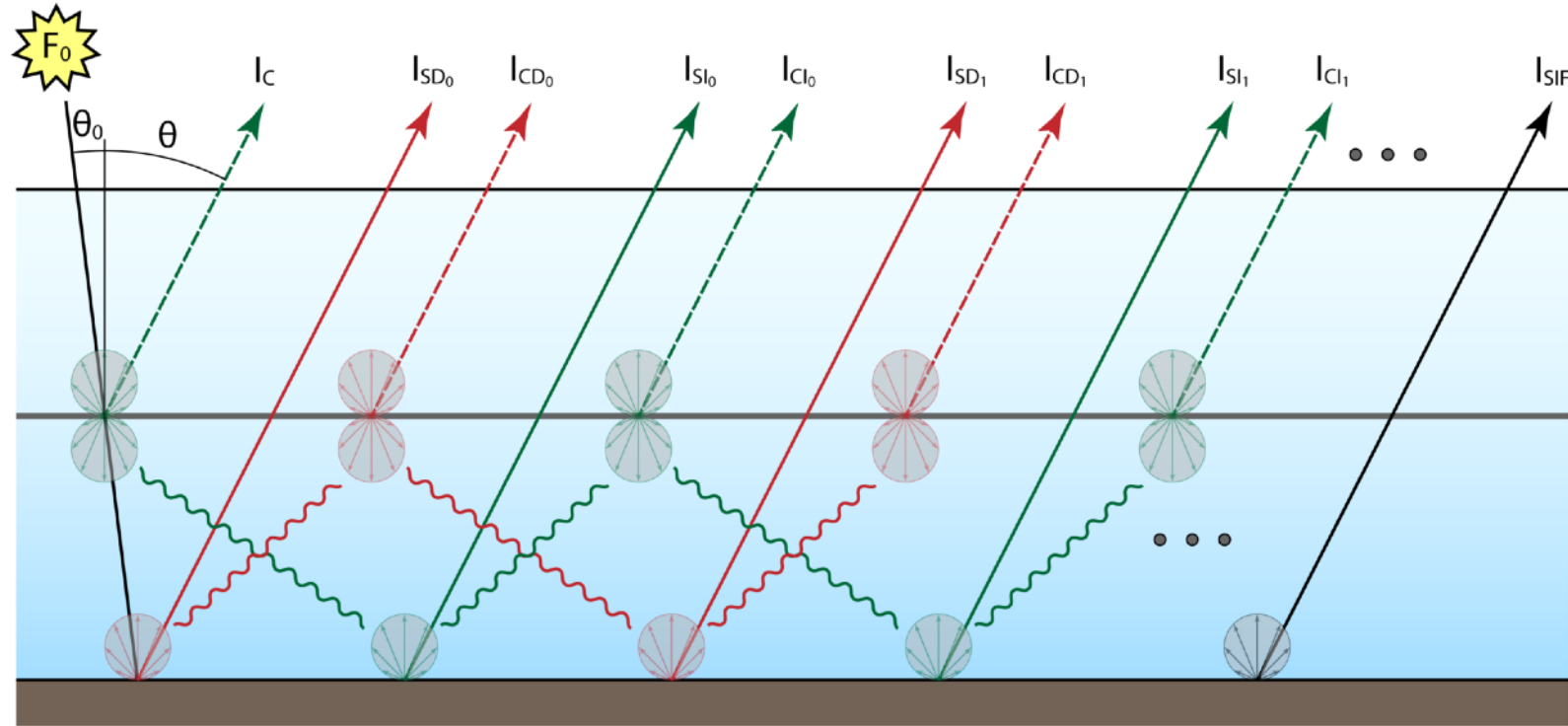
There are substantial uncertainties linked to this (20-60%)!

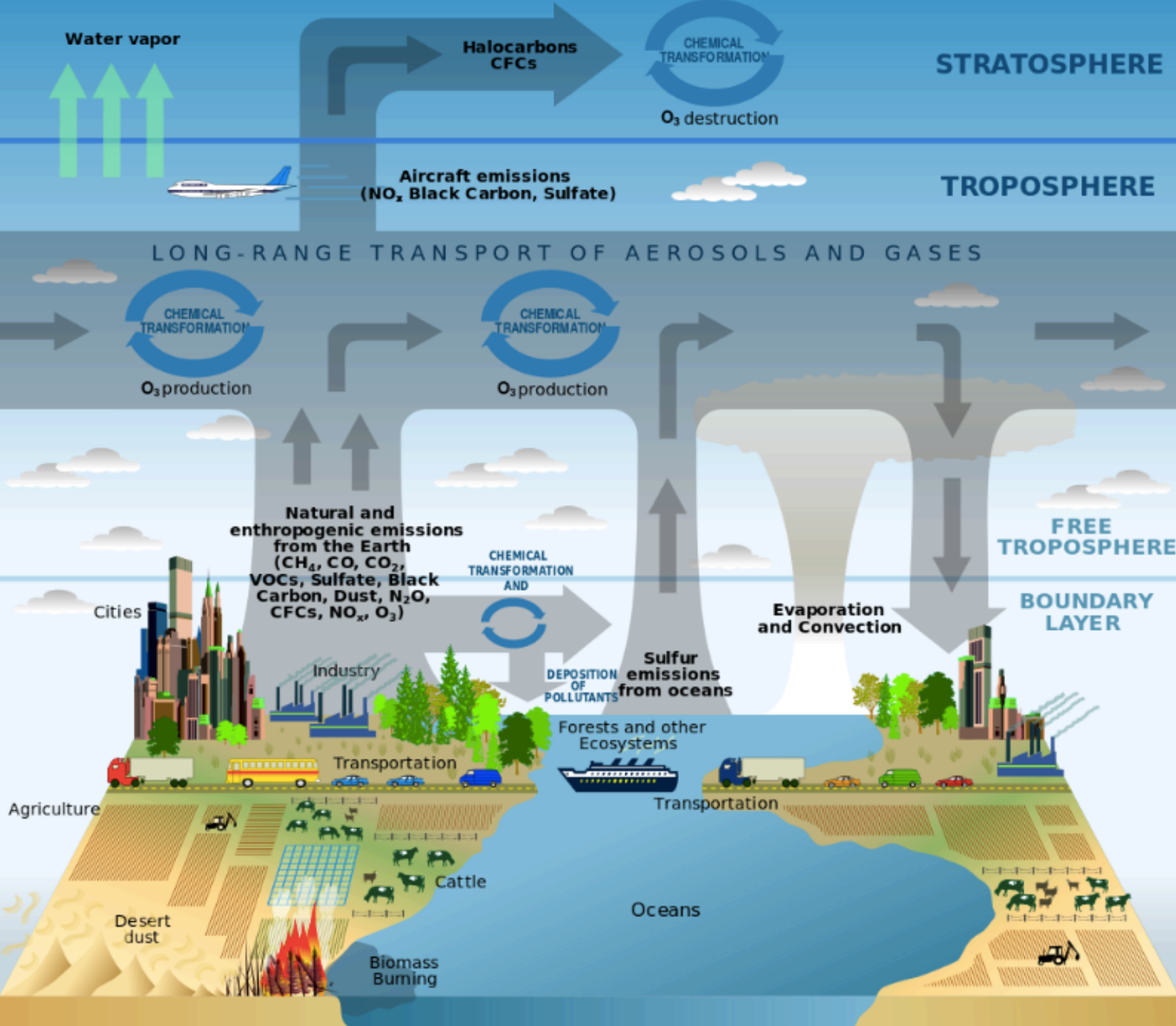
Where did the light travel ?

Radiative transfer models

Depending on
geometry, clouds,
surface albedo,
aerosols

Air-mass factor





Where is the NO₂ ?



Atmospheric model describing chemistry, emissions, transport, deposition.

Most of the NO₂ is in the stratosphere!

The NO₂ data product

Averaging kernels

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

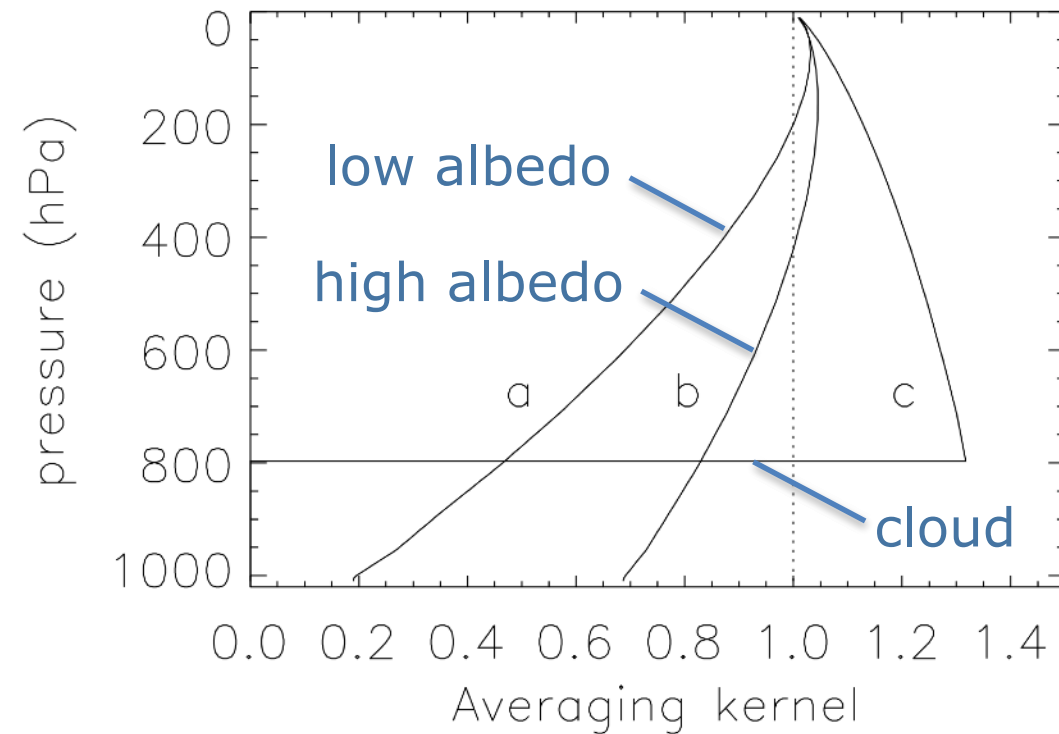


Averaging kernels for DOAS total-column satellite retrievals

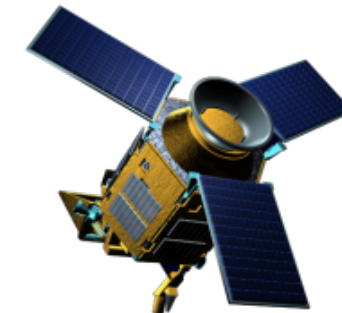
H. J. Eskes and K. F. Boersma

The DOAS retrieval approach may be re-formulated using Rodgers Optimal Estimation formalism.

DOAS averaging kernel profiles: sensitivity of the measurement to NO_2 at a given altitude



Filtering: 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.

Use of the NO₂ product

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

	<i>user application</i>	<i>data sets needed</i>
# 1	Tropospheric chemistry / air quality model evaluation and data assimilation Validation with tropospheric NO ₂ profile measurements (aircraft, balloon, MAX-DOAS)	$N_v^{\text{trop}}, \Delta N_v^{\text{trop, kernel}}$ $M^{\text{trop}}, M, \mathbf{A}^{\dagger}$ $A_l^{\text{TM5}}, B_l^{\text{TM5}}, l_{\text{tp}}^{\text{TM5}}, p_s$
# 2	Tropospheric column comparisons, e.g. with other NO ₂ column retrievals	$N_v^{\text{trop}}, \Delta N_v^{\text{trop}}$
# 3	Stratospheric chemistry model evaluation and data assimilation Validation with stratospheric NO ₂ profile measurements (limb/occultation satellite observations)	$N_v^{\text{strat}}, \Delta N_v^{\text{strat}}$ $M^{\text{strat}}, M, \mathbf{A}^{\ddagger}$ $A_l^{\text{TM5}}, B_l^{\text{TM5}}, l_{\text{tp}}^{\text{TM5}}, p_s$
# 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	$N_v, \Delta N_v^{\text{kernel}} \quad \S$ \mathbf{A} $A_l^{\text{TM5}}, B_l^{\text{TM5}}, l_{\text{tp}}^{\text{TM5}}, p_s$
# 6	Whole atmosphere (troposphere + stratosphere) comparisons with ground-based remote sensing (e.g. Pandora)	$N_v^{\text{sum}}, \Delta N_v^{\text{sum}} \quad \S$
# 7	Visualisation of the NO ₂ product	$N_v^{\text{trop}}, N_v^{\text{strat}}, N_v^{\text{sum}} \quad \S$

[†] 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 $\mathbf{A}^{\text{strat}}$ is derived from the total kernel \mathbf{A} and the air-mass factors M and M^{strat} .

[§] Note that the total NO₂ vertical column $N_v \equiv N_s/M$ is *not* the same as the sum $N_v^{\text{sum}} \equiv N_v^{\text{trop}} + N_v^{\text{strat}}$

Replacing the a-priori using the averaging kernels

The TROPOMI NO₂ 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:

$$N_v^{\text{trop}'} = \frac{M^{\text{trop}}}{M^{\text{trop}'}} N_v^{\text{trop}}$$

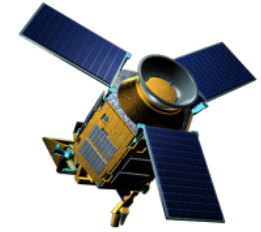
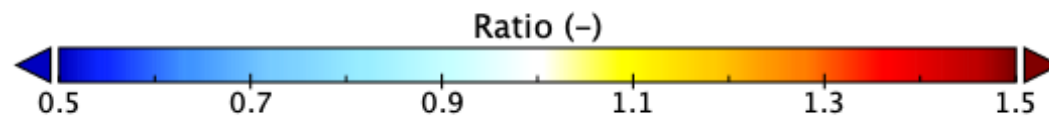
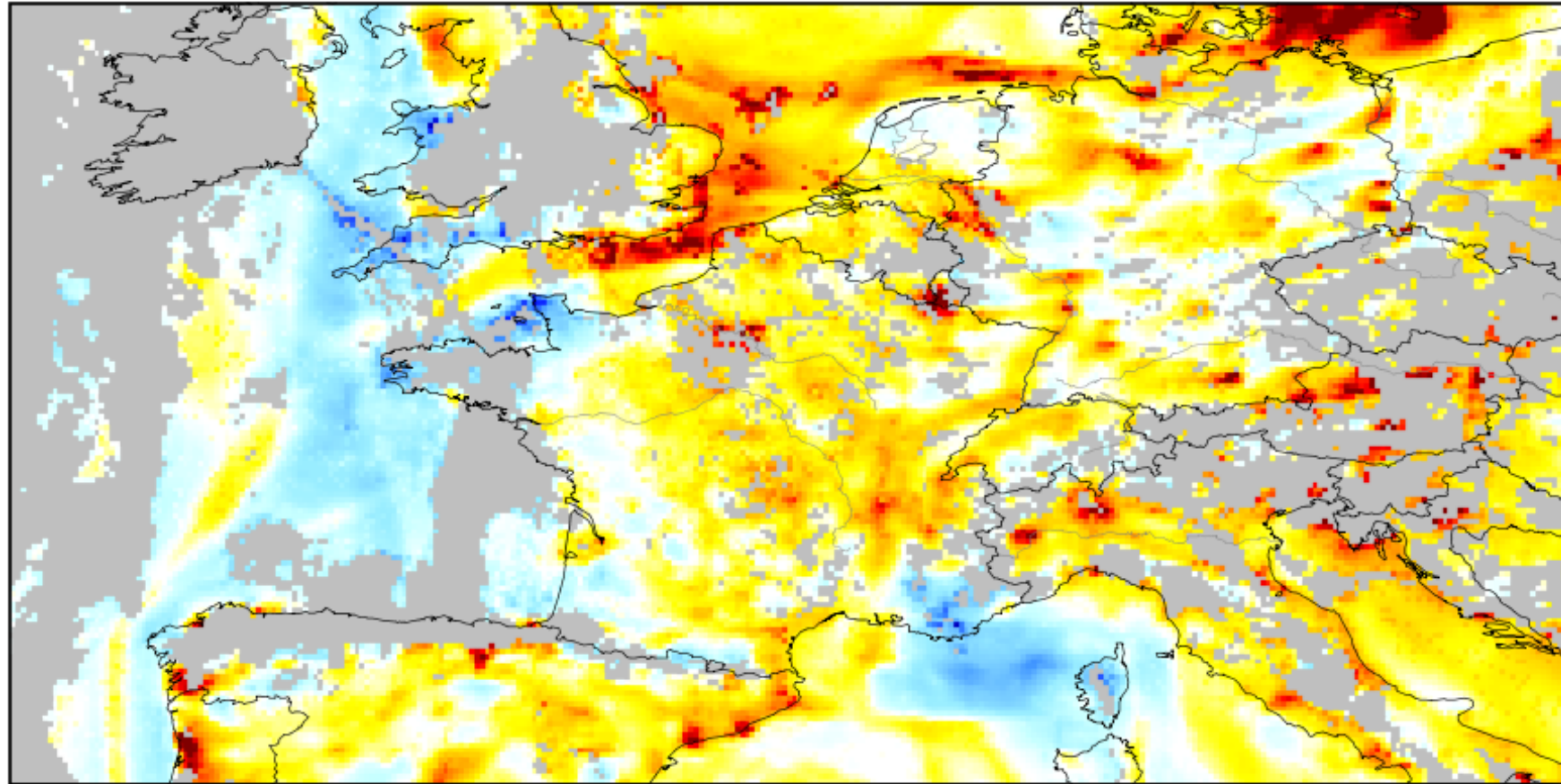
$$\mathbf{A}^{\text{trop}'} = \frac{M^{\text{trop}}}{M^{\text{trop}'}} \mathbf{A}^{\text{trop}}$$

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

All quantities on the left with a prime ' are recomputed using the model NO₂ partial-column profiles $x'_{m,l}$. Other quantities are taken from the S5P_L2_NO2 file.

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

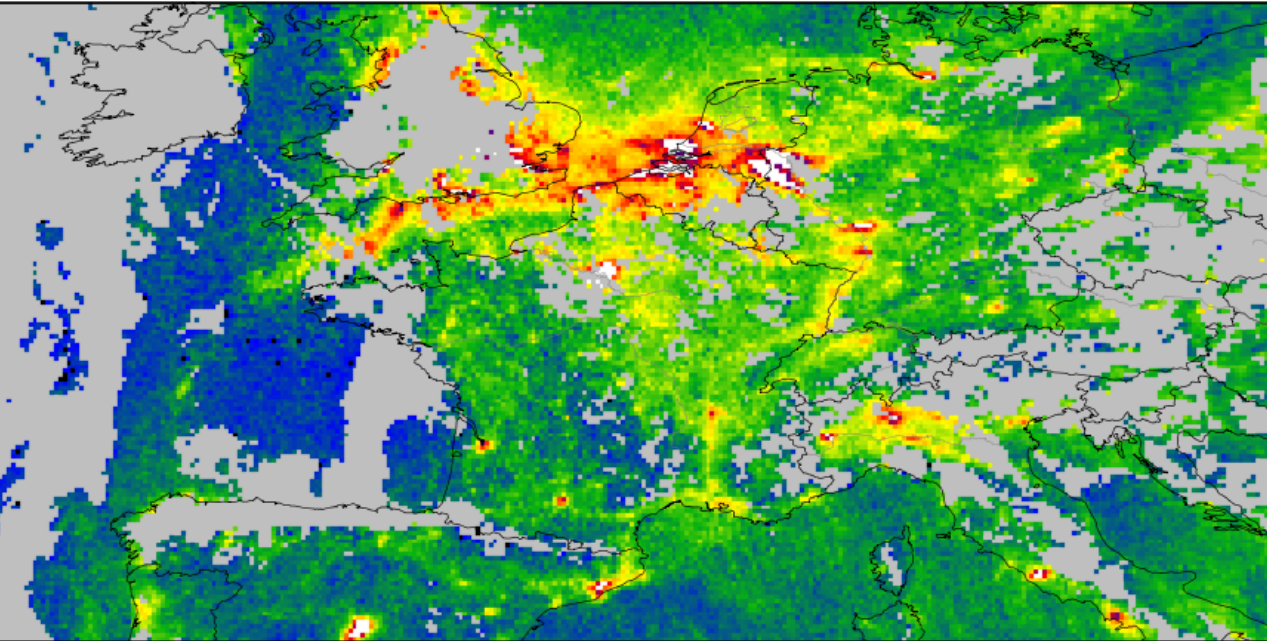
Ratio NO₂ tropospheric column CAMS a-priori / TM5MP a-priori



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

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

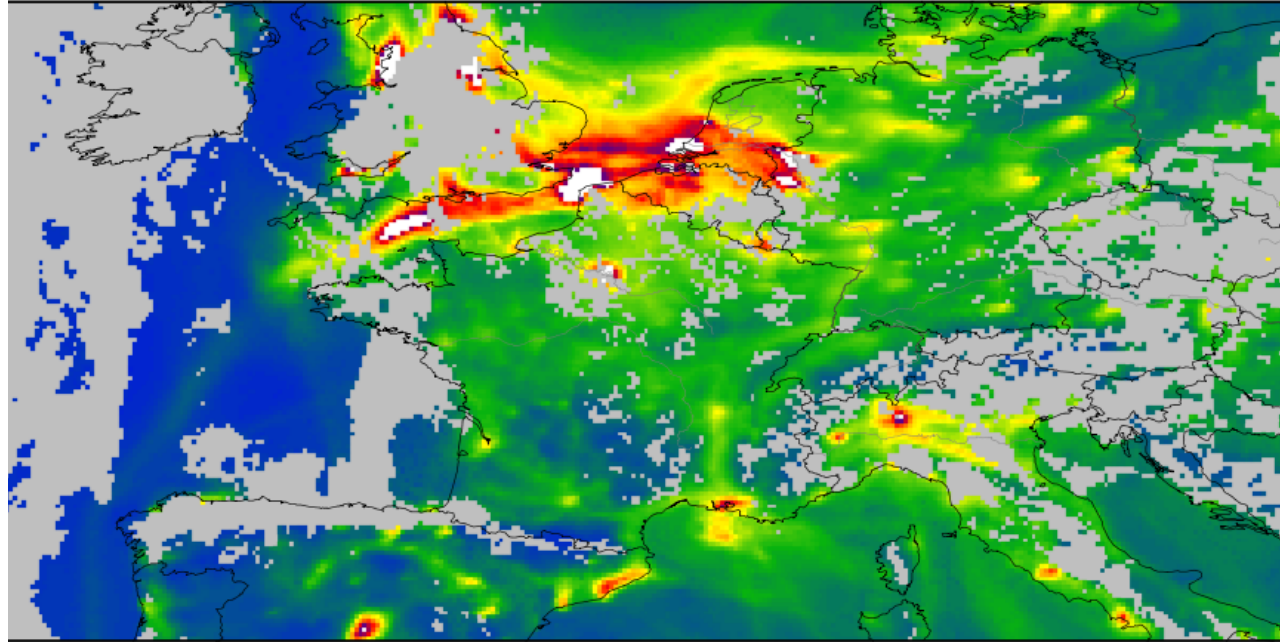
TROPOMI NO₂ based on CAMS-regional a-priori



TROPOMI tropospheric vertical column of nitrogen dioxide using CAMS a-priori profile (10^{15} molecules/c...



CAMS-regional vertical column NO₂



NO₂ tropospheric column ($1e15$ molecules/cm²)



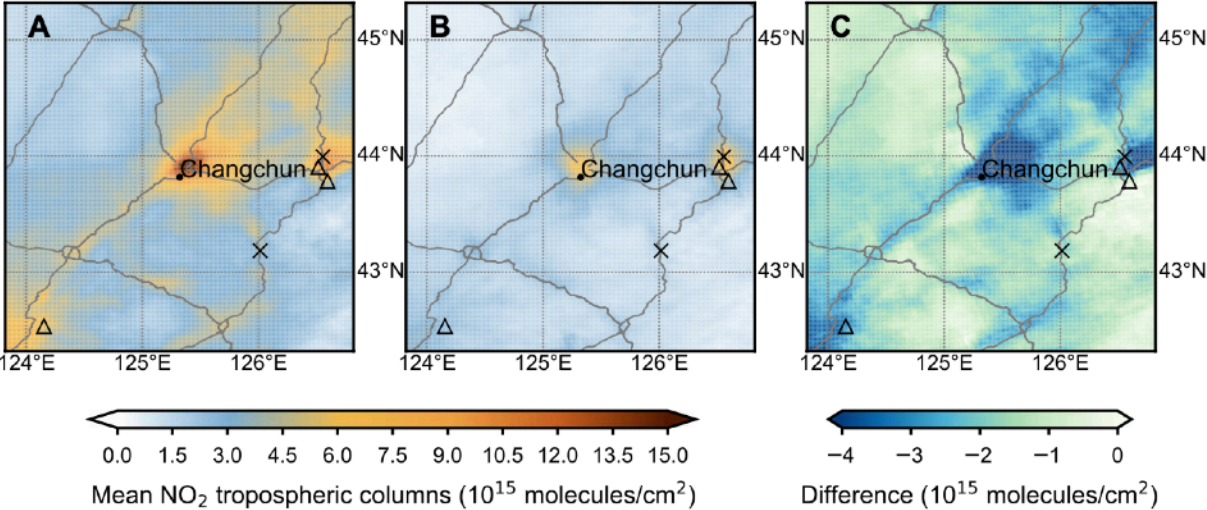
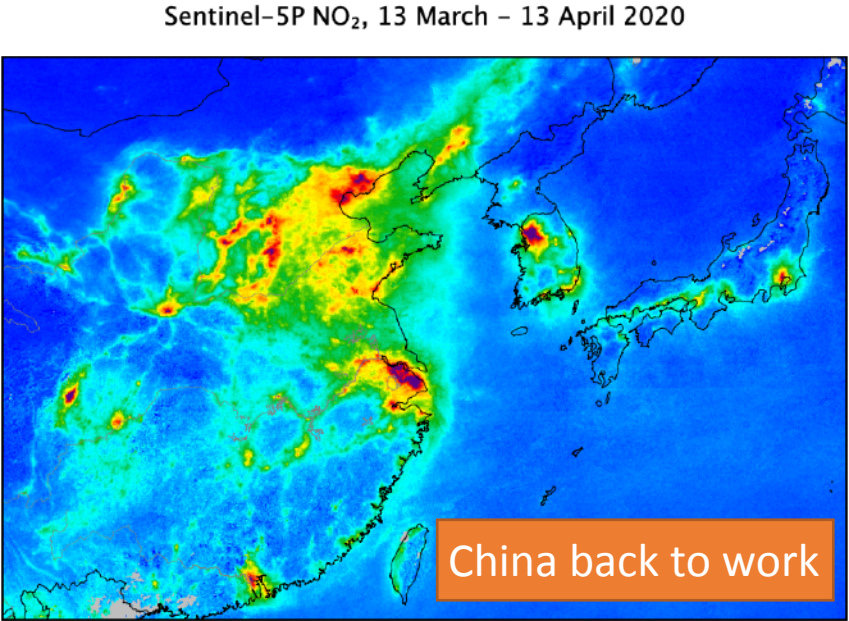
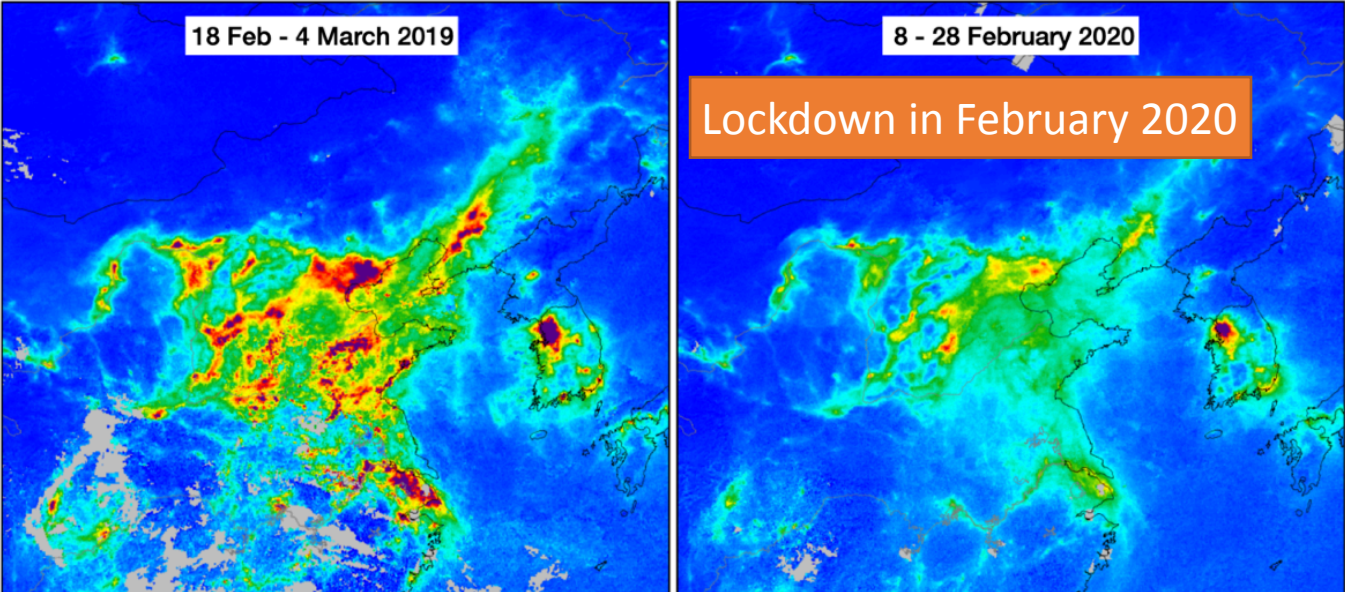
Single overpass, 26 July 2018

Applications

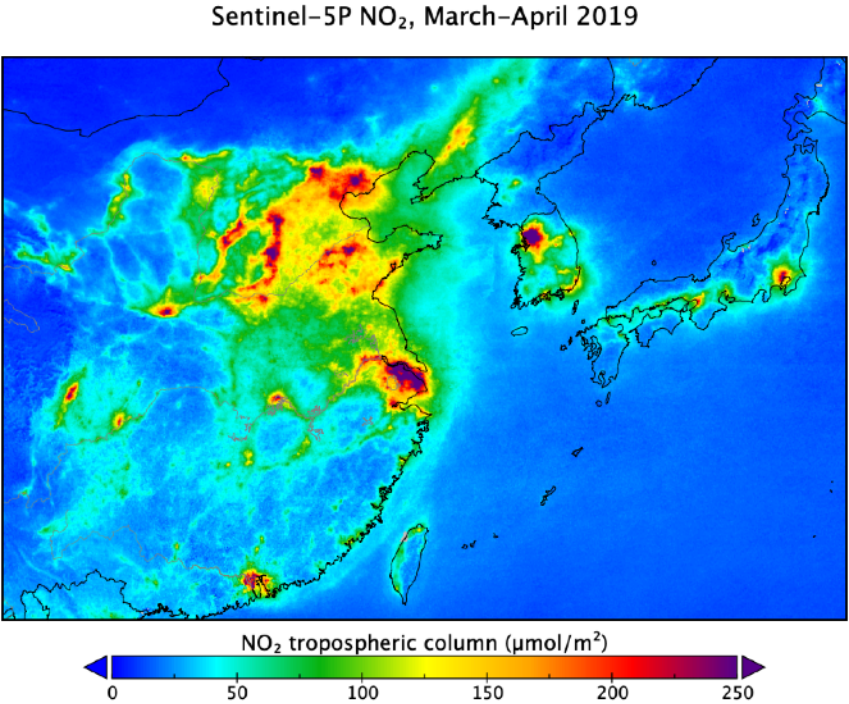
The NO₂ measurements may be used for:

- * Emission estimates
 - Inverse modelling
 - Plume analysis using wind information
 - Flux divergence (Steffen Beirle et al., 2019)
- * Source identification
- * Data assimilation
 - Primary user is CAMS (Copernicus Atmospheric Monitoring Service)
- * Model validation
- * Reactive nitrogen mapping (improving knowledge N-deposition)
- * Trend studies / emission change monitoring
- * Visualisation

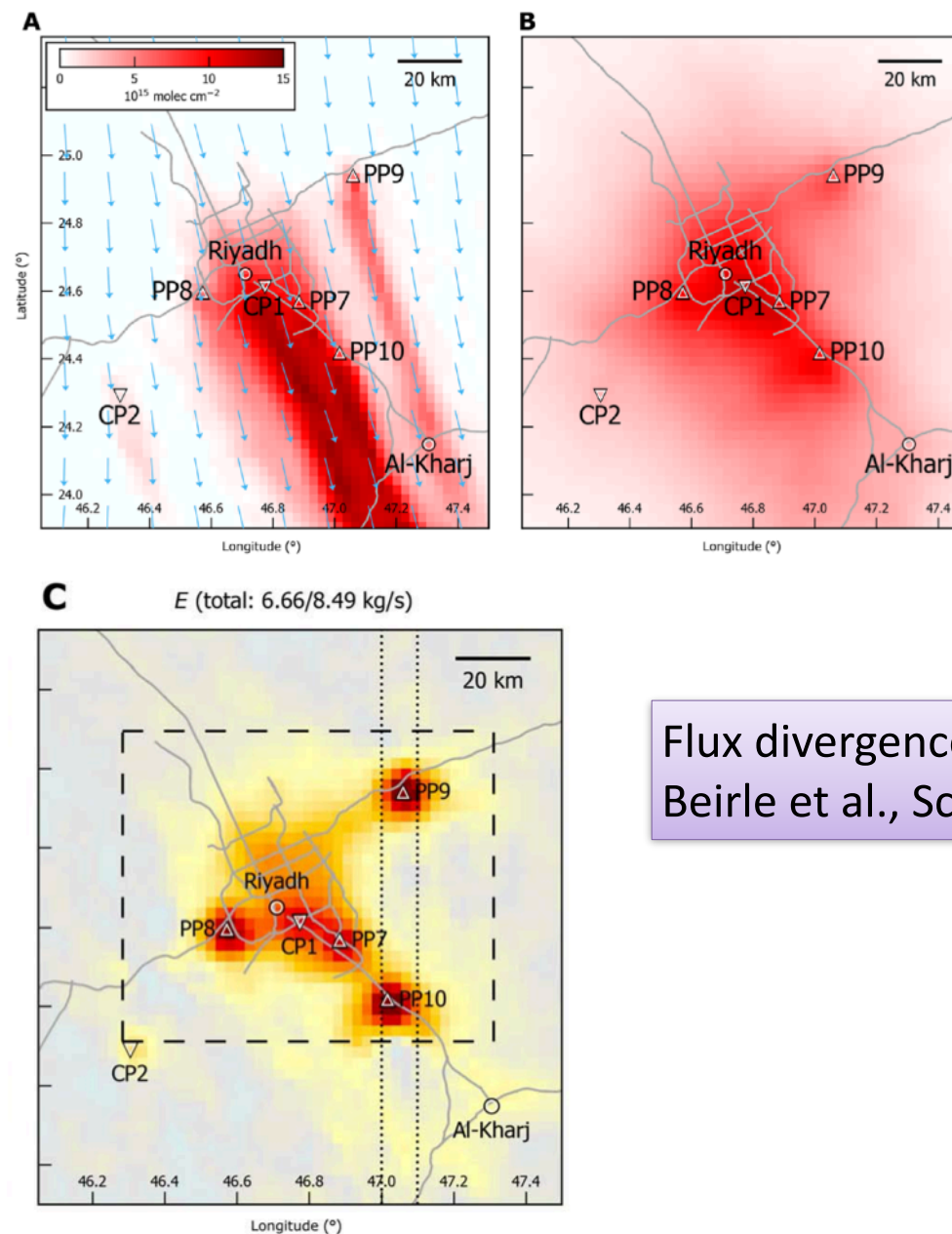
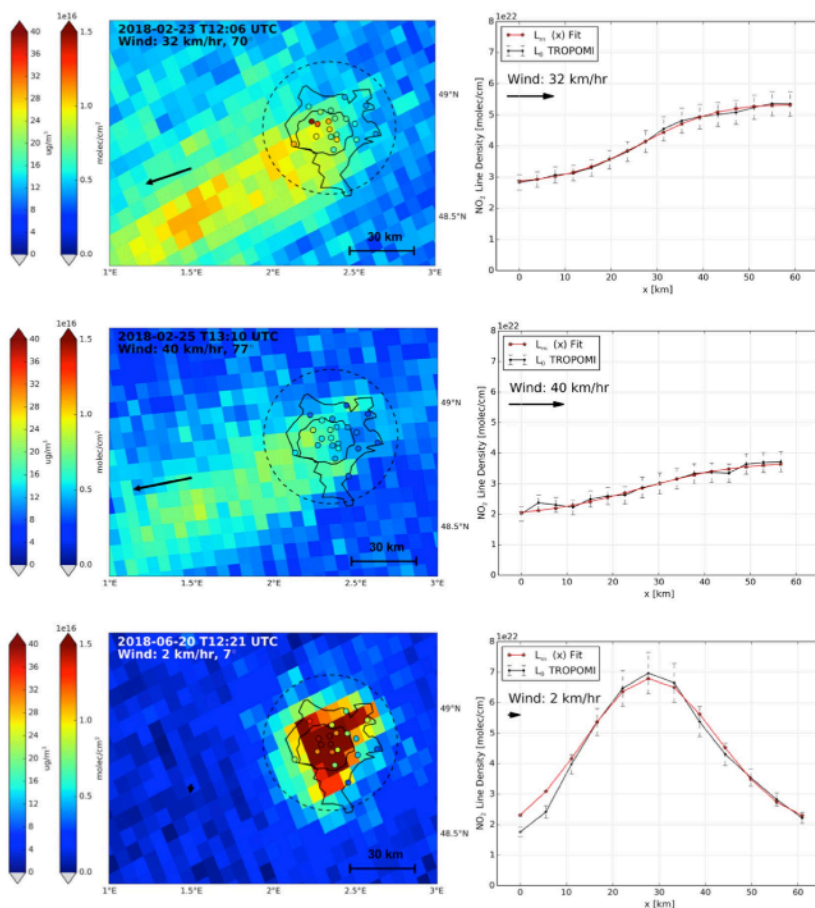
NO2 pollution reductions related to COVID-19 lockdown in China, measured with Sentinel-5P TROPOMI



F. Liu et al.,
Science
Advances
2020



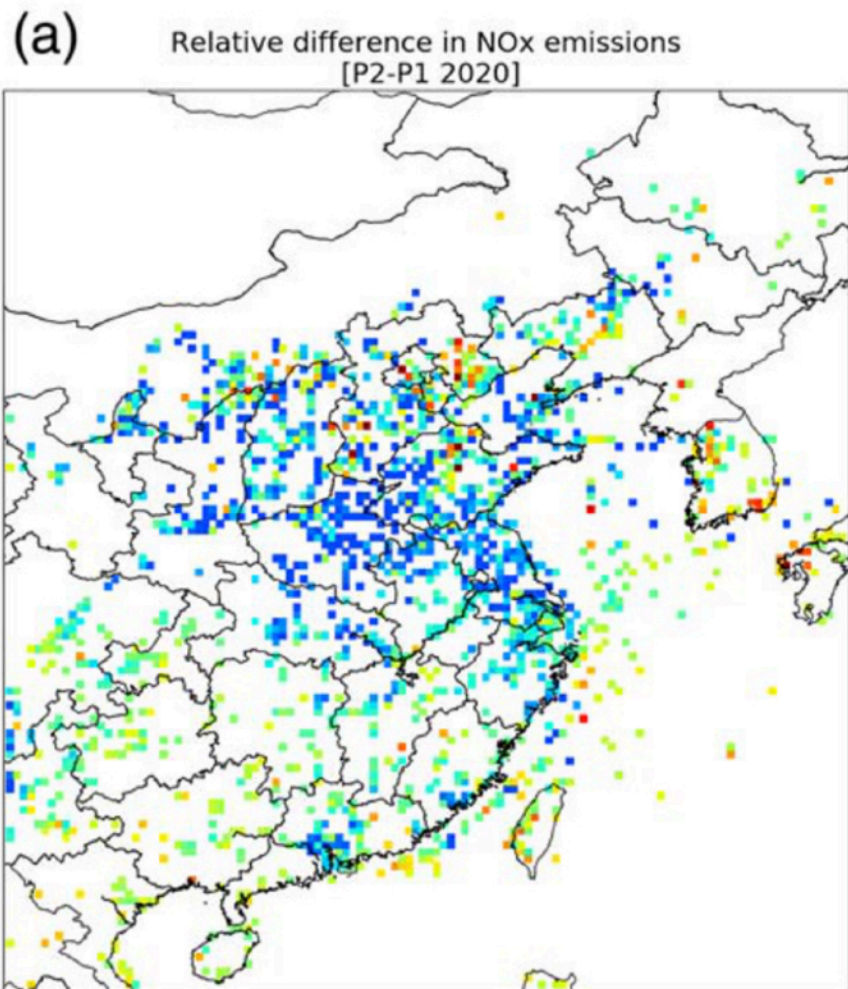
Emission estimates: plume analysis



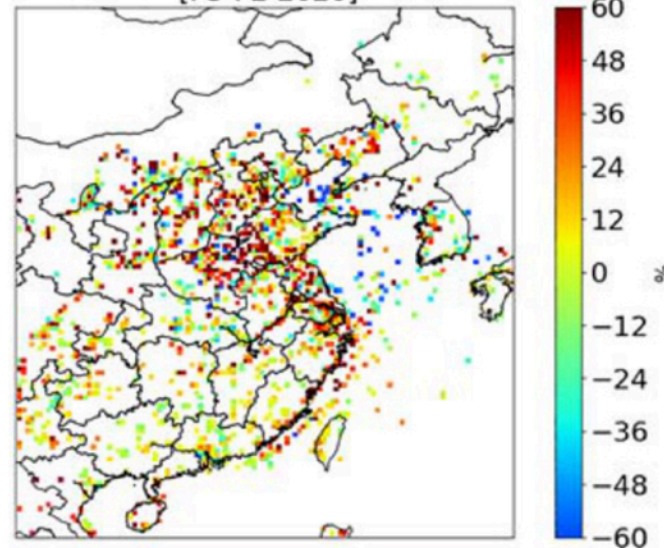
Estimating emissions of Parijs
Combining daily plume observations
with wind information
Lorente et al., Nature Sci. Rep. 2019

Flux divergence method
Beirle et al., Science Adv. 2019

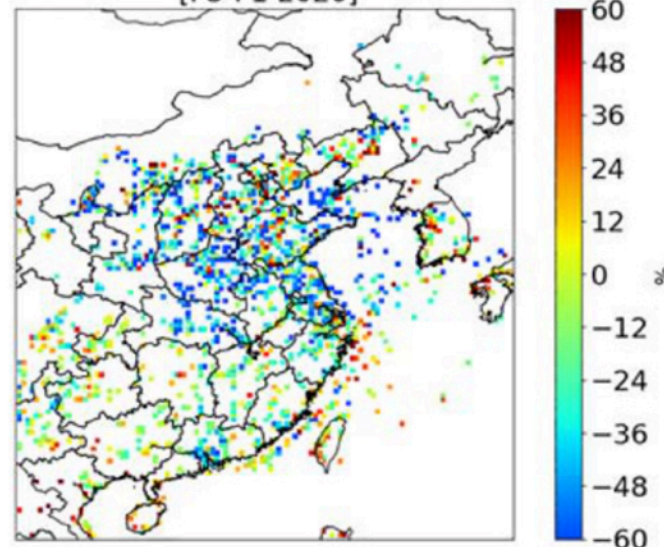
Emissions, using inverse modelling



(b) Relative difference in NO_x emissions
[P3-P2 2020]



(c) Relative difference in NO_x emissions
[P3-P1 2020]



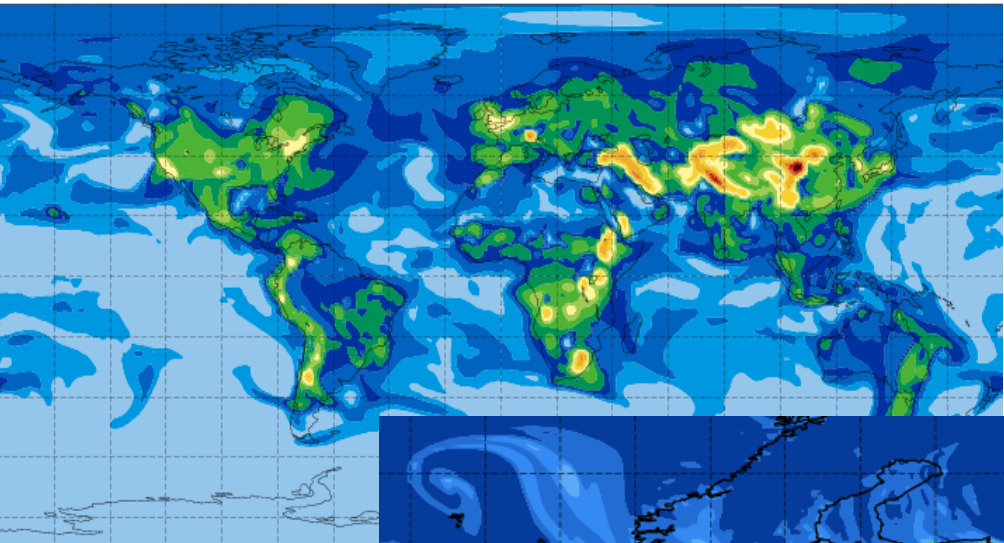
Emissions in China
Ding et al., GRL 2020

P1: Before lockdown

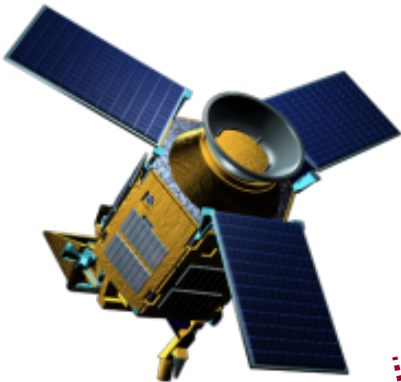
P2: during lockdown

P3: after lockdown

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

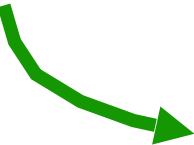
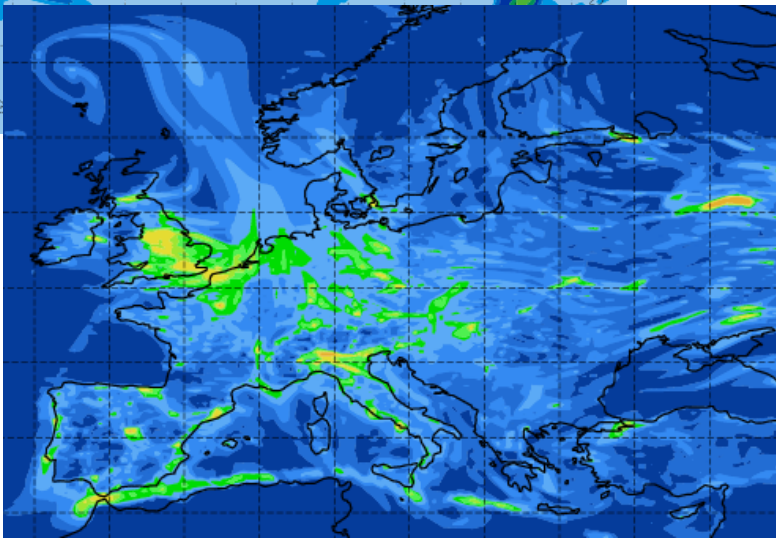


Assimilation
TROPOMI
observations



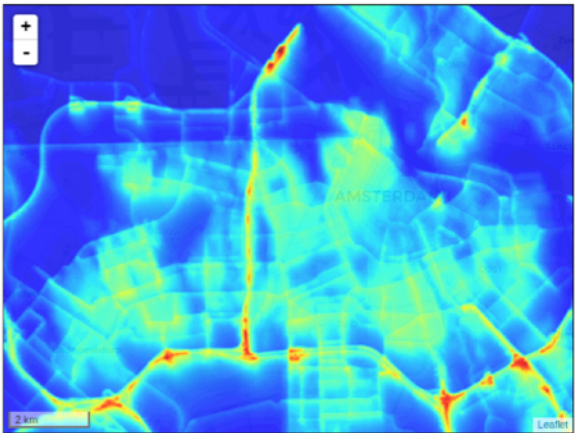
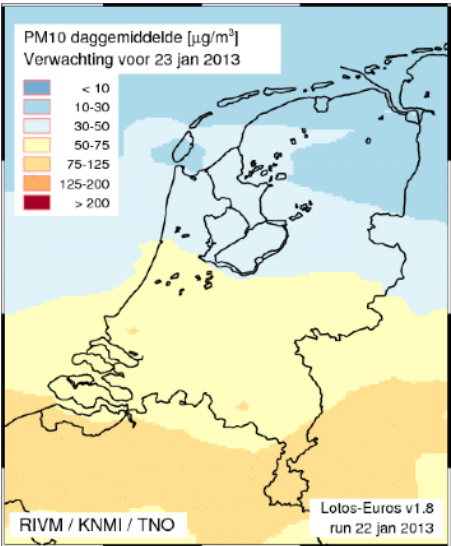
CAMS-Europe as boundary condition for
countries and city regions

Amsterdam



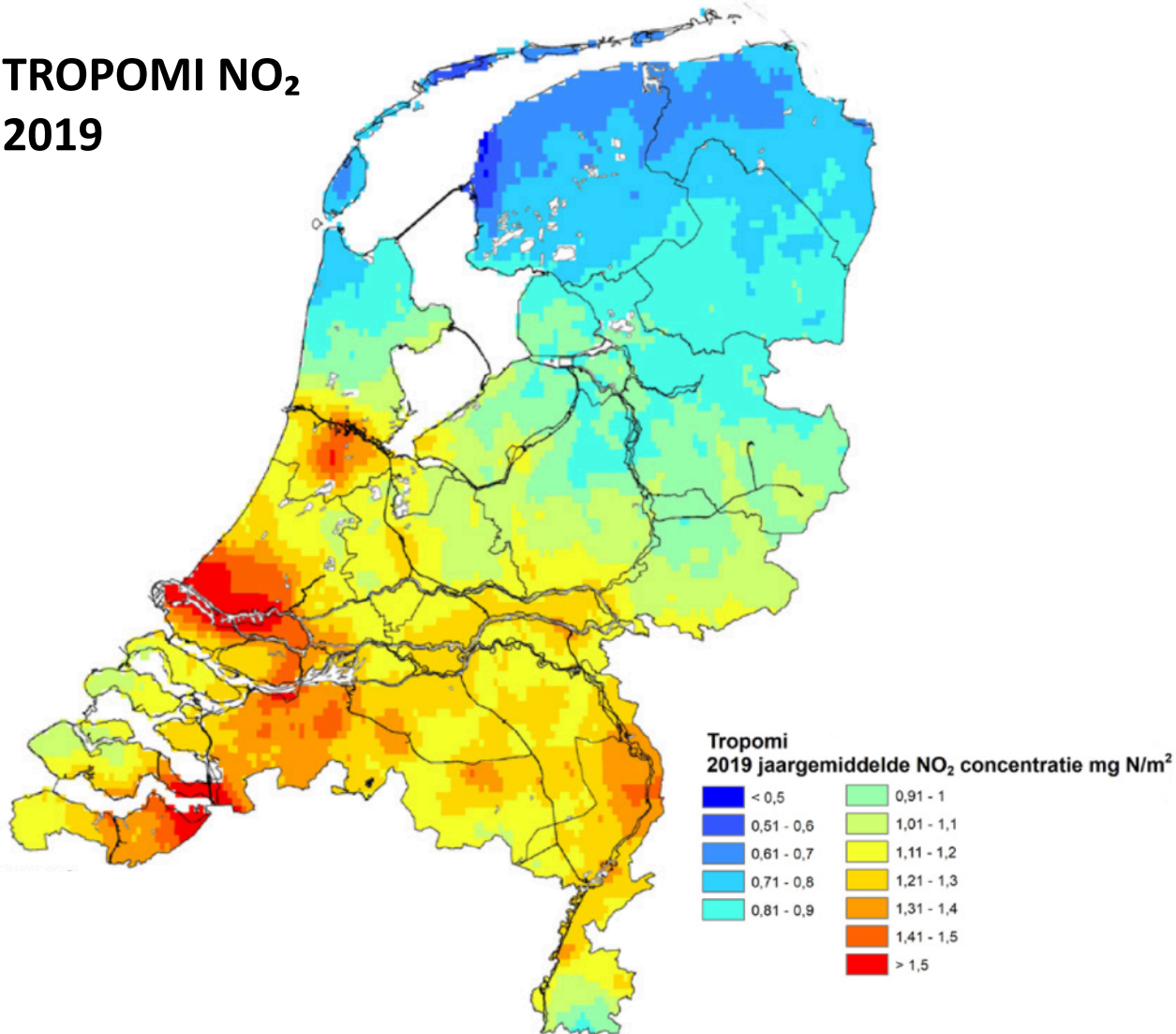
Analyses of CAMS-global as
boundary condition for CAMS-Europe

atmosphere.copernicus.eu

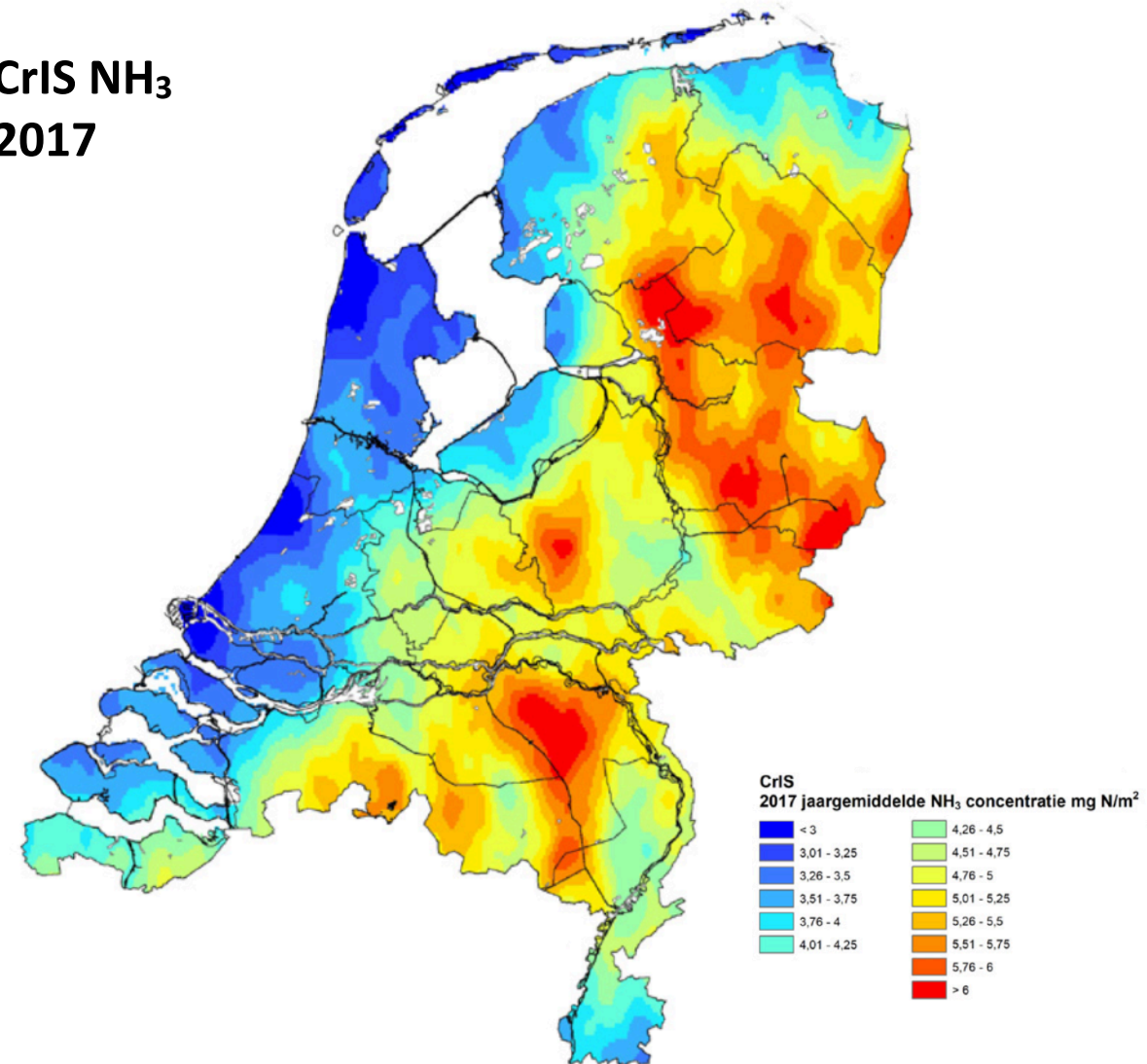


The nitrogen (deposition) problem: loss of biodiversity

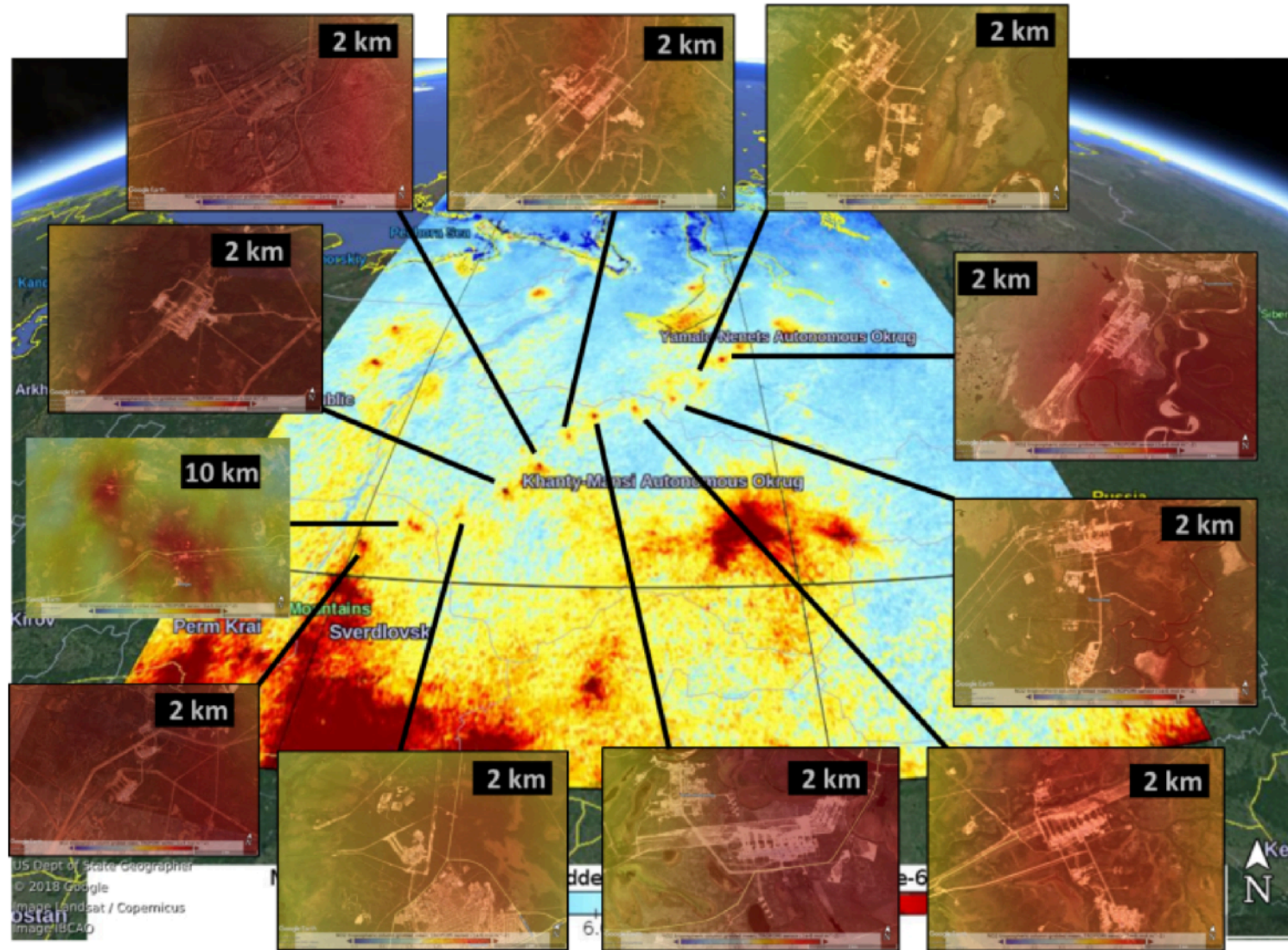
**TROPOMI NO₂
2019**



**CrIS NH₃
2017**

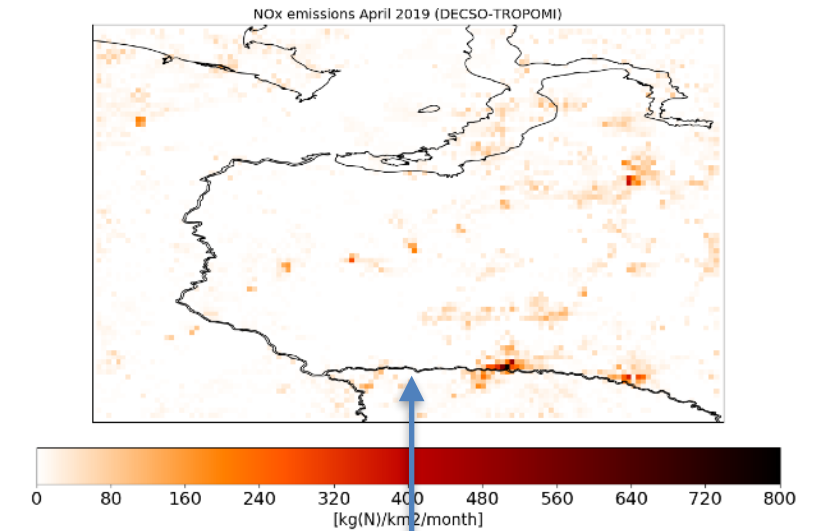


Identification of emission sources

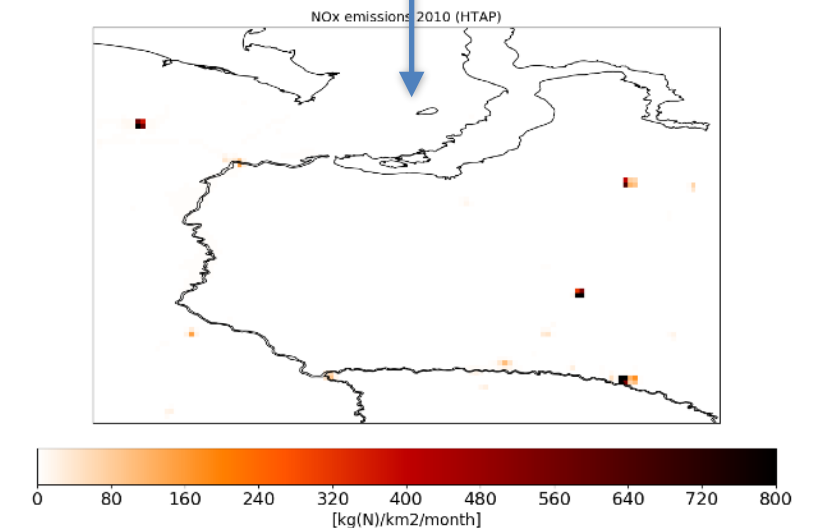


string of gas compressor stations along natural gas pipeline every ≈ 100 km

R. v.d. A et al., NPJ Clim. Atmos. 2020



TROPOMI NO₂ emission inversion
(DECSO) for April 2019
compared with
bottom up emission
inventory (HTAP/EDGAR)



Summary NO₂

- * The NO₂ (tropospheric slant) column can be accurately determined from space with UV-Vis spectrometers, covering a two order of magnitude range of column values, but require high signal-to-noise spectrometers.
- * The air-mass factor, depending on clouds, surface albedo, aerosol, is a major source of uncertainty.
- * The data products are extended, contain intermediate and input products and offer full traceability. Averaging kernels can be used to remove dependence on a-priori, or replace a-priori with high-resolution (regional) model NO₂ profiles.
- * A large range of applications: Emission estimates and source identification, data assimilation and model validation, reactive nitrogen mapping, emission change monitoring (trends, COVID-19 lockdown impacts), visualisation