SPECATMOS : "Spectroscopy and Atmosphere: Measurements and Modelling" International Summer School

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Multispectral synergism for observing atmospheric ozone pollution

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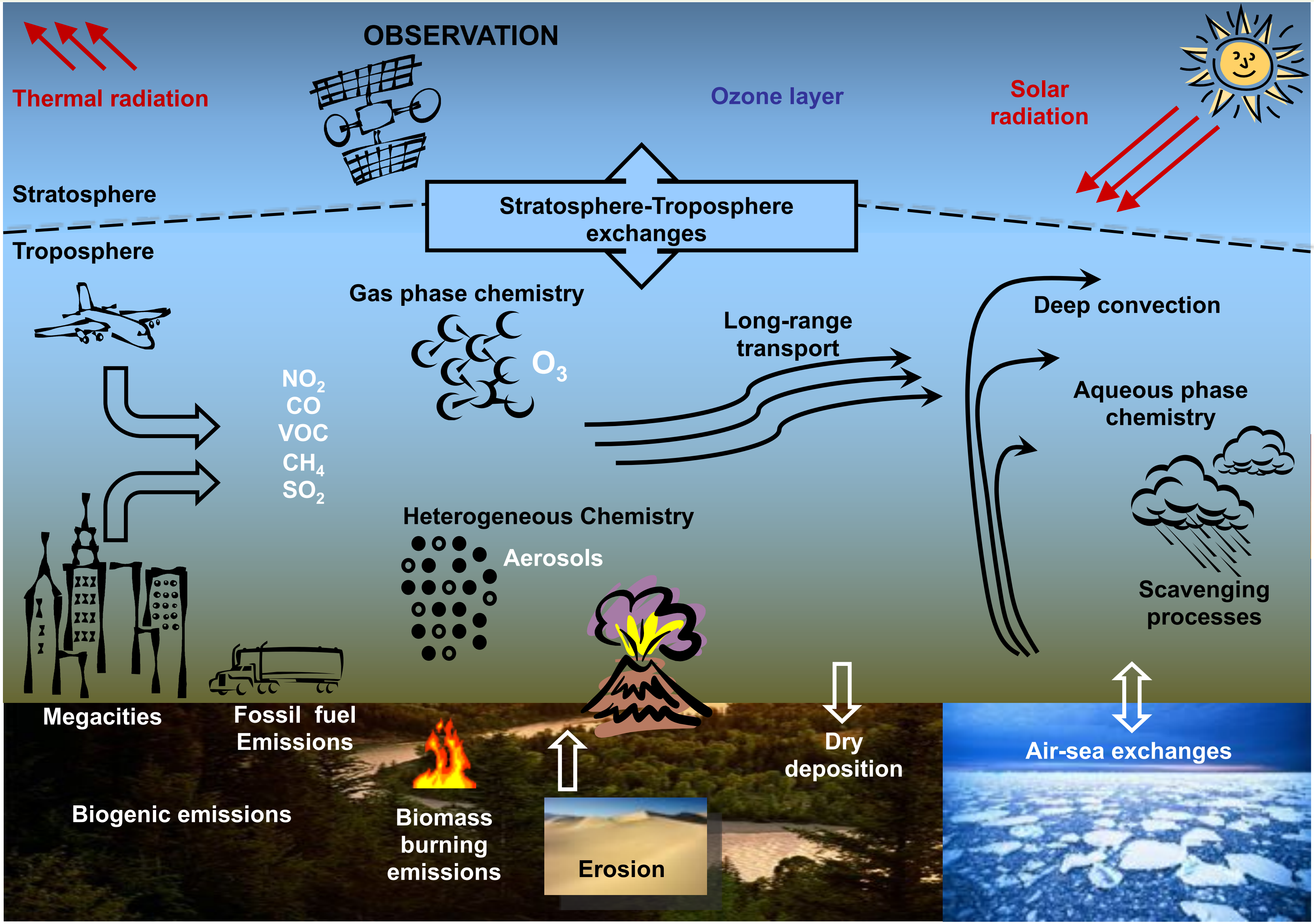
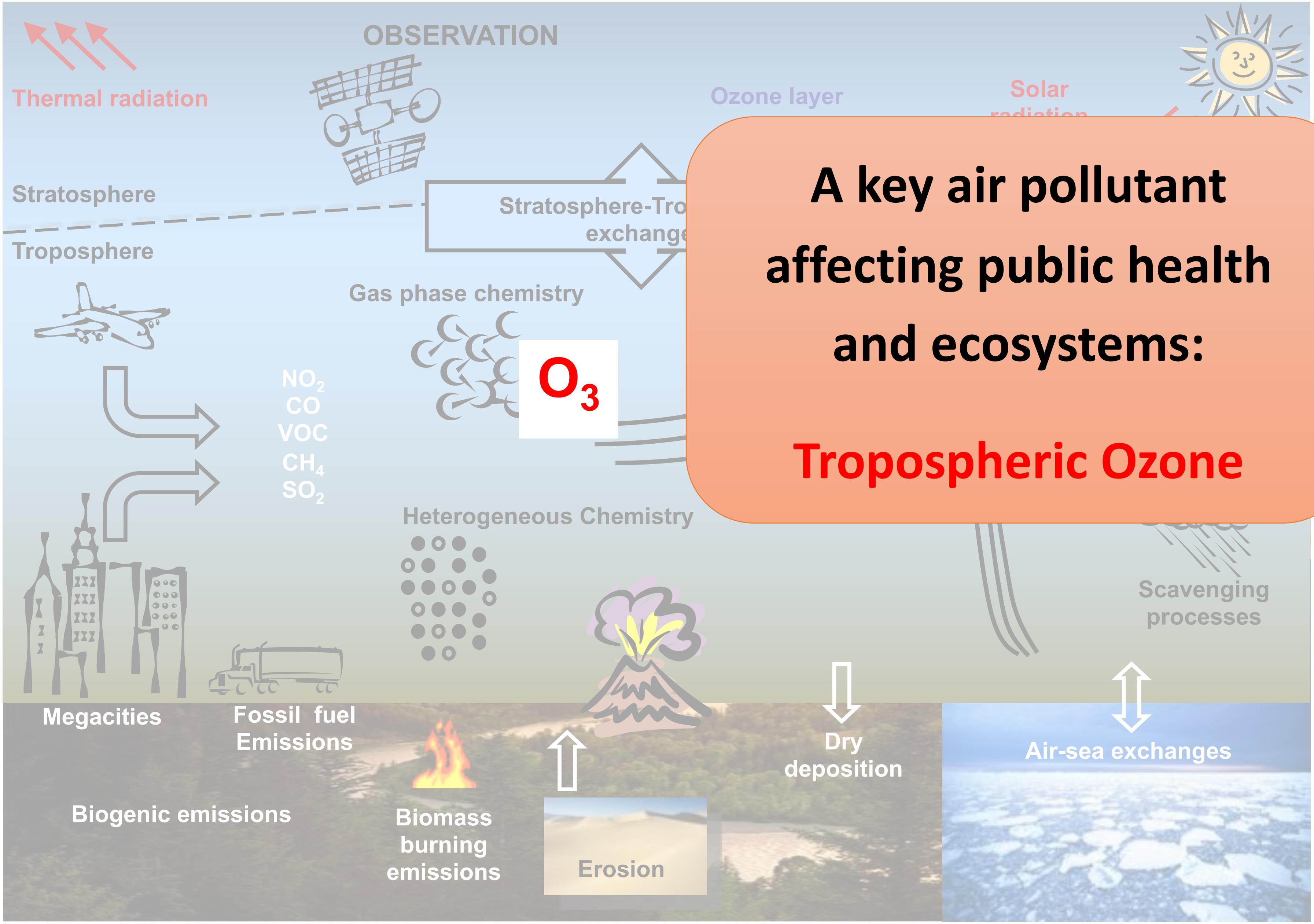
Processes affecting tropospheric chemistry



Processes affecting tropospheric chemistry

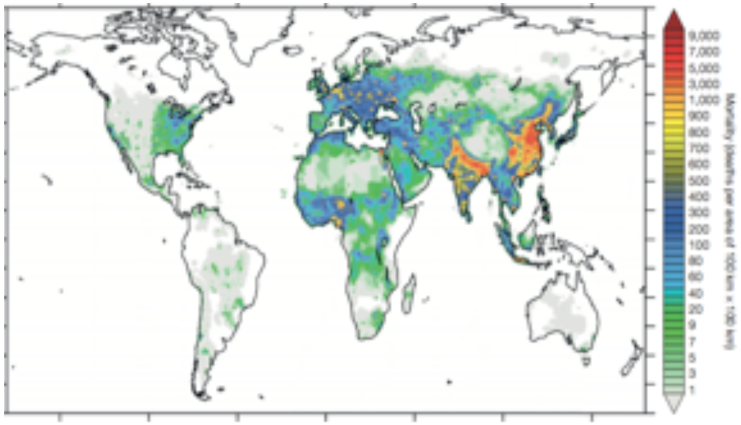


A key air pollutant affecting public health and ecosystems:

Tropospheric Ozone

Observing air pollutants from space

- Major impact of air pollution on public health and ecosystems



Mortality associated to Ambient Air Pollution in 2010
Lelieveld et al., 2015

- Better knowledge of atmospheric chemistry and its environmental impacts

→ Only satellites can observe pollutants at the regional and global scales

✧How to observe air pollutants near the surface from space ?

✧How to improve chemistry-transport models using satellite observations ?

Ozone Pollution

- Severe impact on public health and ecosystems

Irritation of respiratory system

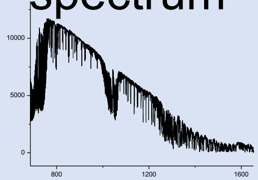
Limitation of photosynthesis

Necrosis on leaves

Remote sensing of the atmospheric composition

PASSIVE spectrally-resolved measurements

Atmospheric spectrum



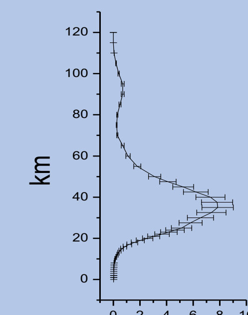
Atmospheric radiative transfer calculation

Spectroscopic databases

Retrieval approach : Iterative minimization of a cost function :

$$\left\|\mathbf{y}-\mathrm{F}(\mathbf{x})\right\|_{S_y}+\left\|\mathbf{x}-\mathbf{x}_a\right\|_{R}$$

Atmospheric profile



- **Constrained fit** of calculated spectra with respect to atmospheric measurements
- Constraints *R*: control of **resemblance** between **a priori** knowledge of the atmosphere and the retrieved profiles
- Other approaches also exist (neural networks, look-up-tables, DOAS)

Inversion method

Minimization of the following function:

Variance-covariance matrix of radiometric noise

Radiative transfer model

Climatological average a priori

$$\chi^2 = \|F(\hat{x}) - y\|_{\varepsilon} + \|\hat{x} - x_a\|_R$$

Calculated spectrum

Satellite measurement

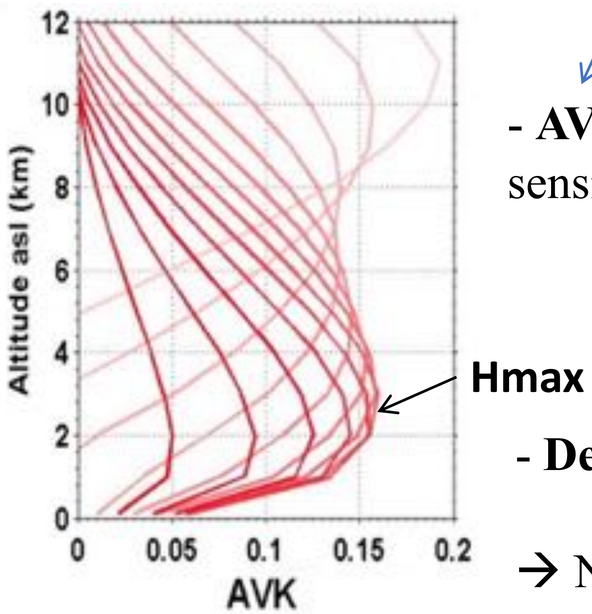
Constraint matrix

O_3 profile in the atmosphere

Inversion method

$$\chi^2 = \|F(\hat{x}) - y\|_\varepsilon + \|\hat{x} - x_a\|_R$$

→ **Retrieved O_3 profile :** $\hat{x} = A(x - x_a) + Err$



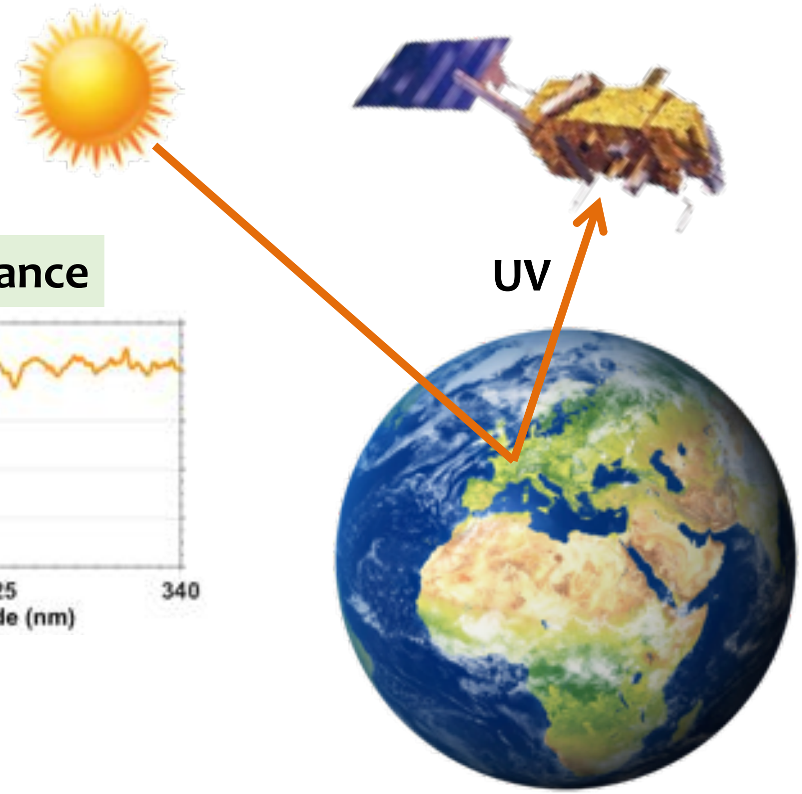
- **AVK** → Averaging Kernels allow the evaluation of the sensitivity of the retrieved profile with respect to the real profile

- **Degree of freedom (DOF)** $DOF = Trace(AVK)$

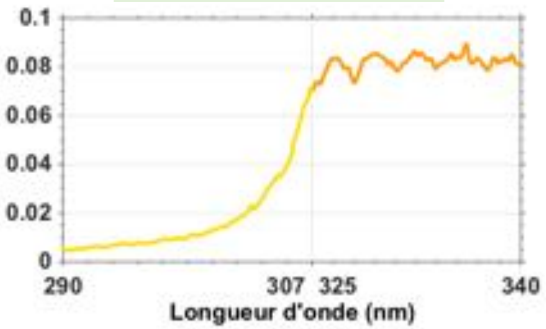
→ Number of independent points on the vertical (sensitivity to O_3)

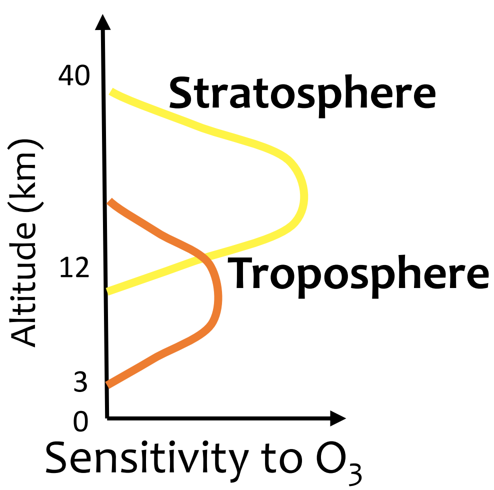
- **Maximum sensitivity height (Hmax)** : Altitude of the maximum AVK value (i.e. the maximum sensitivity)

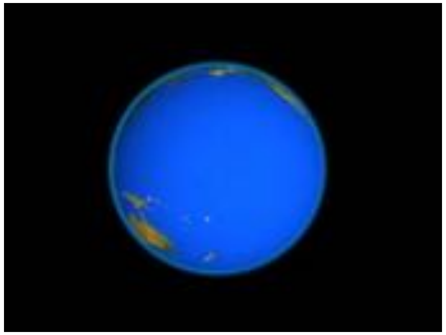
Ozone remote sensing from space



UV reflectance





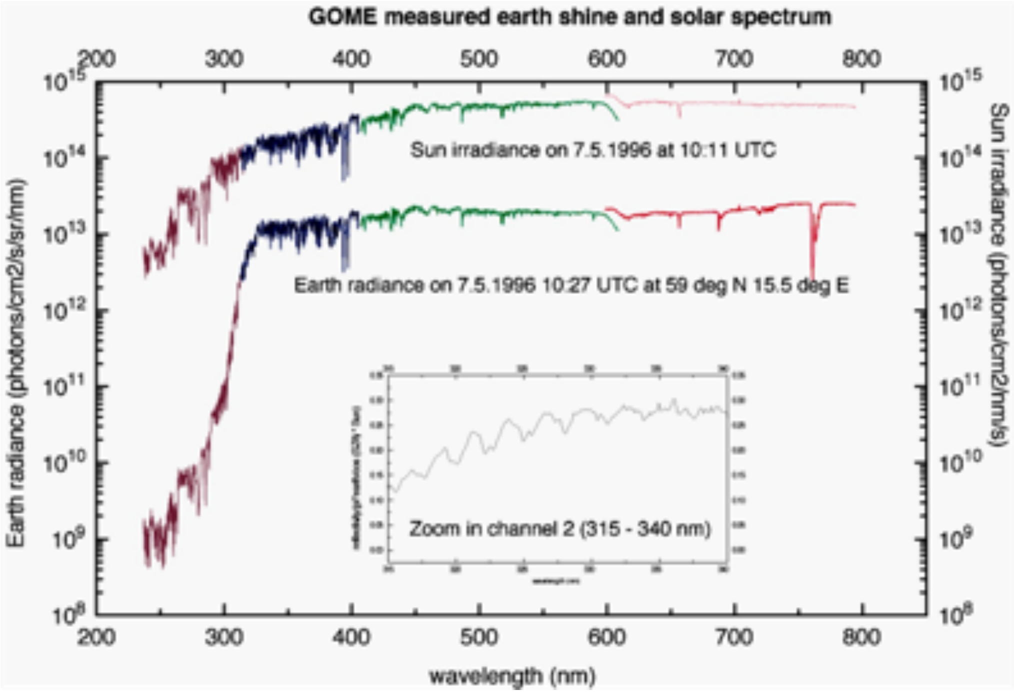


Nadir atmospheric spectrum at the UV/Visible

Spectra from GOME satellite radiometer:

1) Directly pointing the sun (Sun irradiance ➔ once a day)
2) Backscattered light from Earth (Earth radiance➔ every pixel)

The ratio is **reflectance**

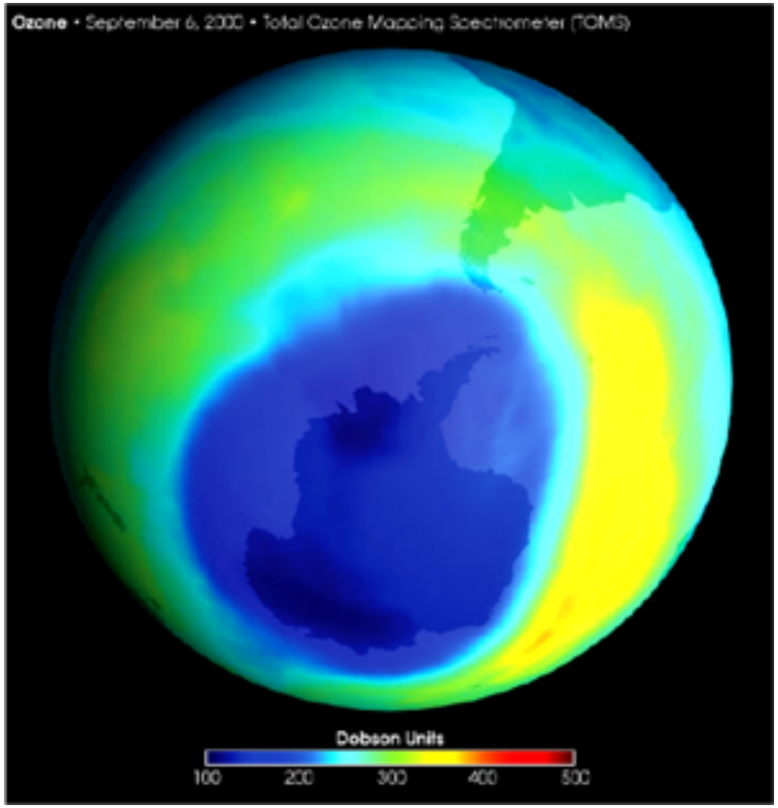


Units

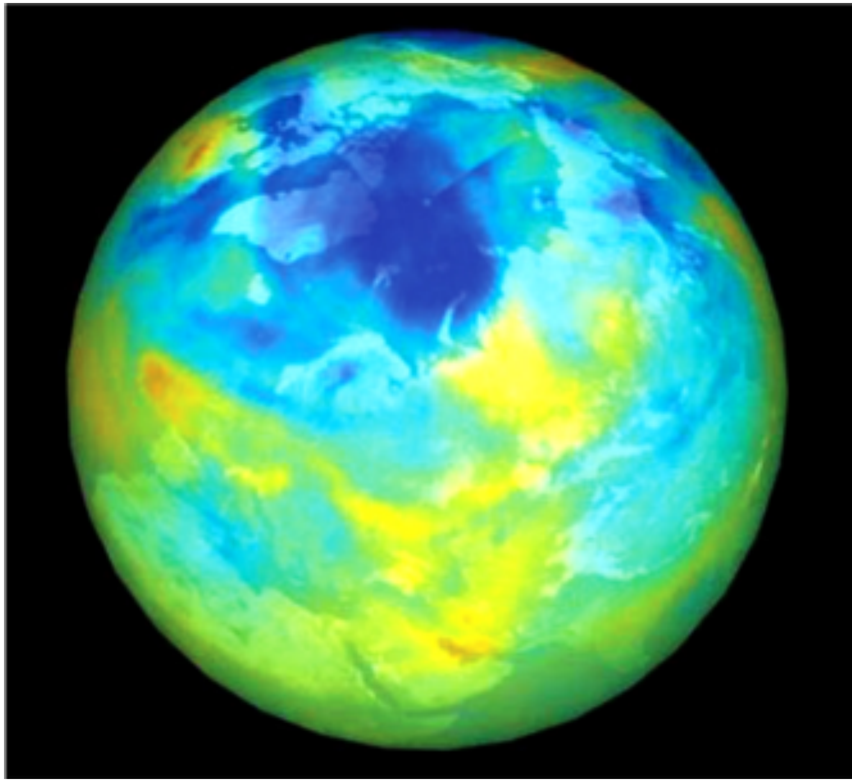
TOMS: Total Ozone Mapping Spectrometer

1978 –
Based on the UV backscattered radiations

Ozone total column



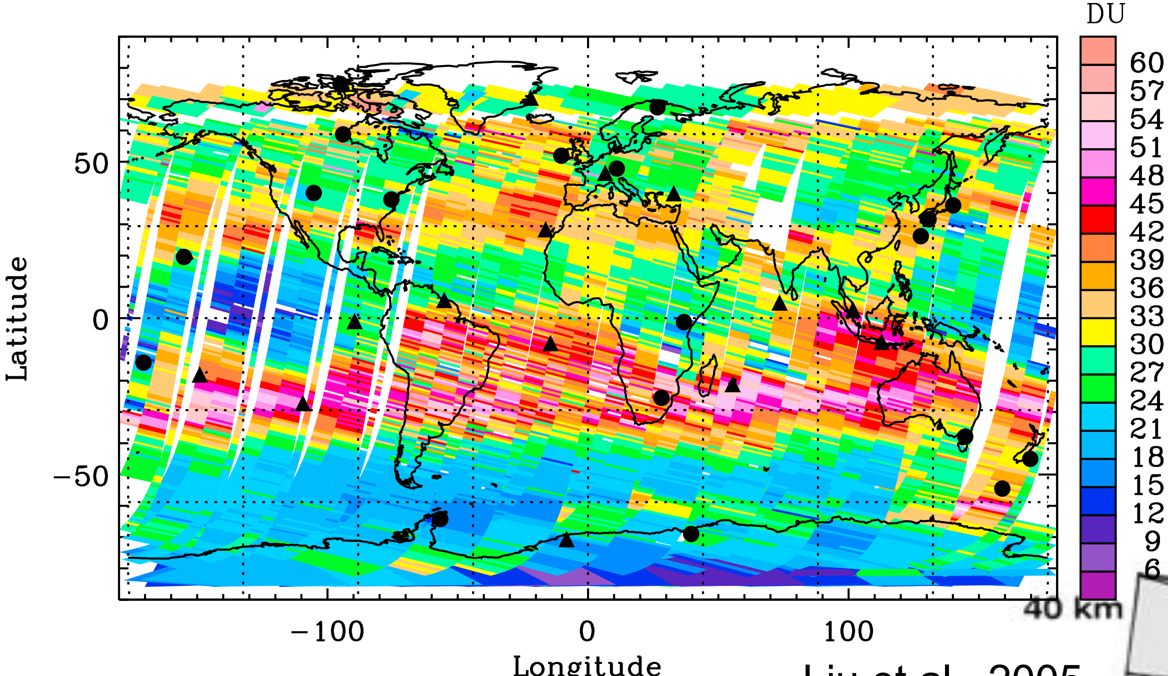
Antarctique



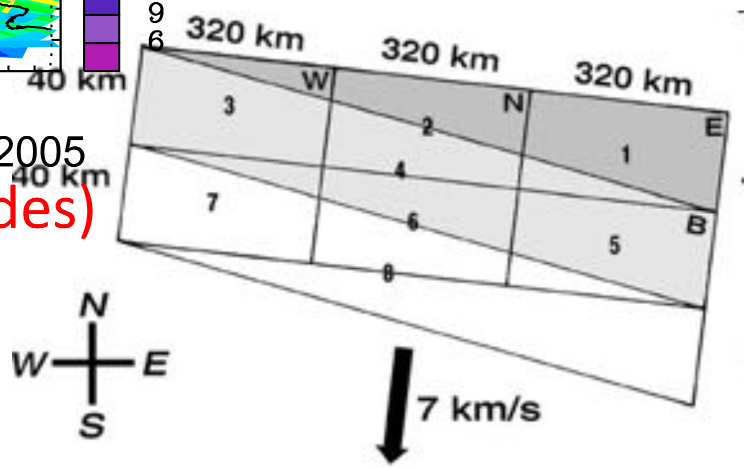
Arctique

GOME: Global Ozone Monitoring Experiment

Ozone tropospheric column

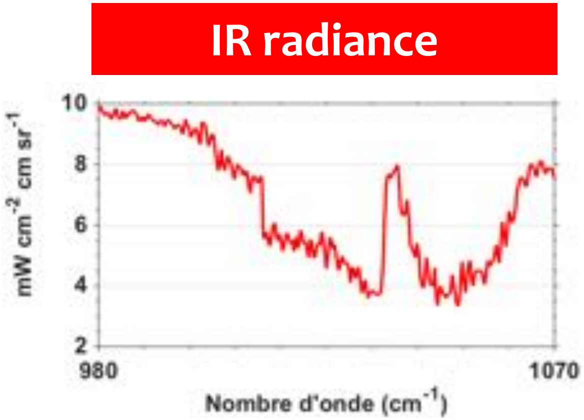


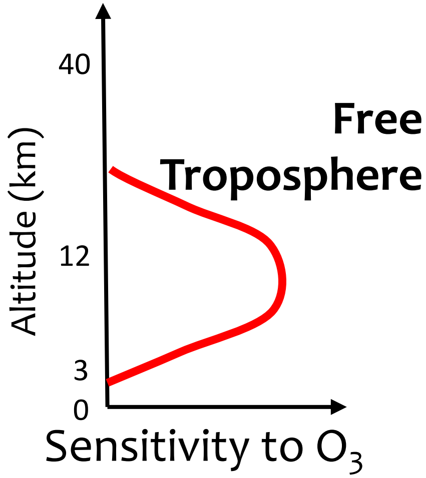
Liu et al., 2005



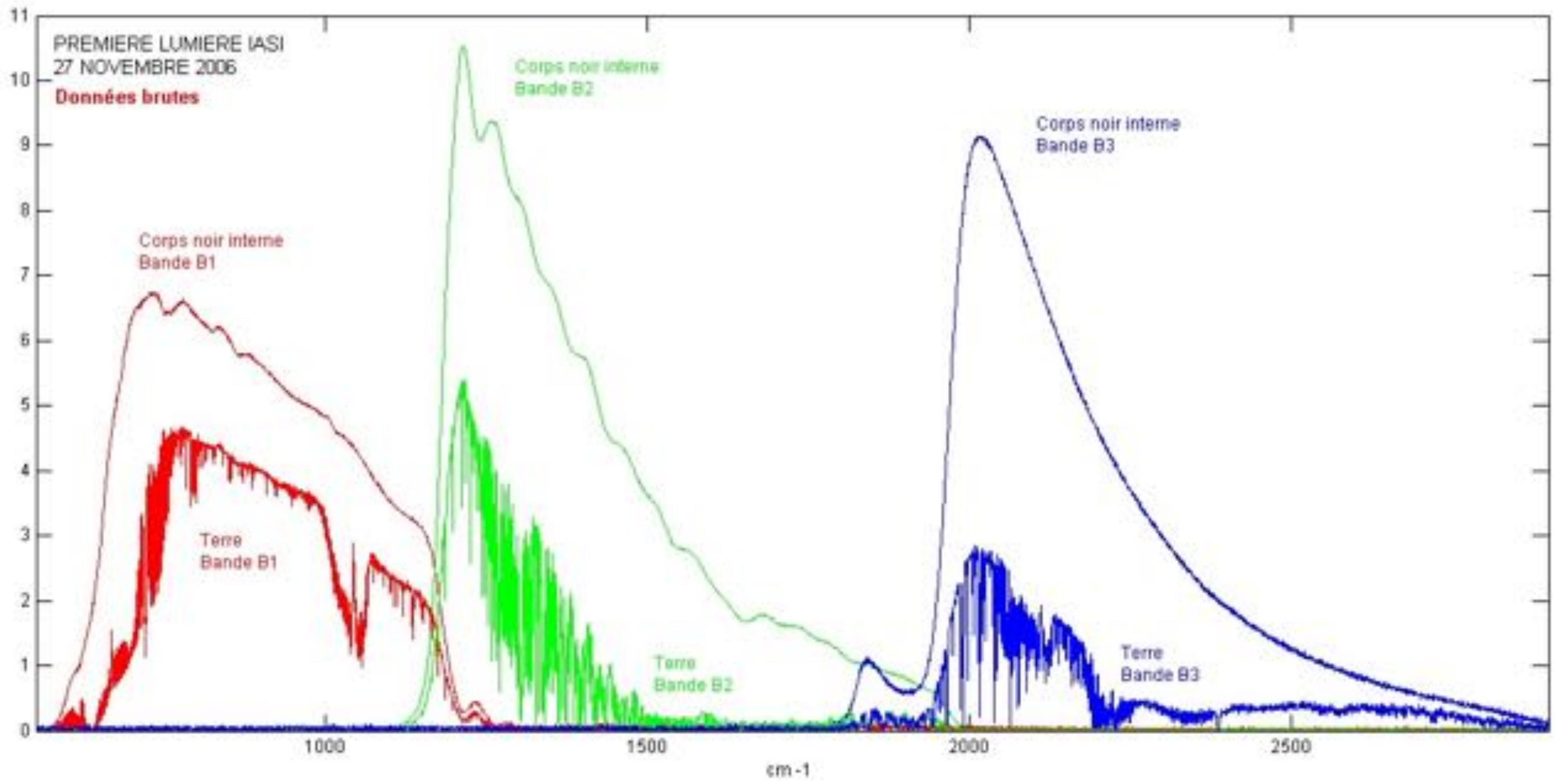
(up to about 12 km at mid-latitudes)

Satellite remote sensing of Ozone

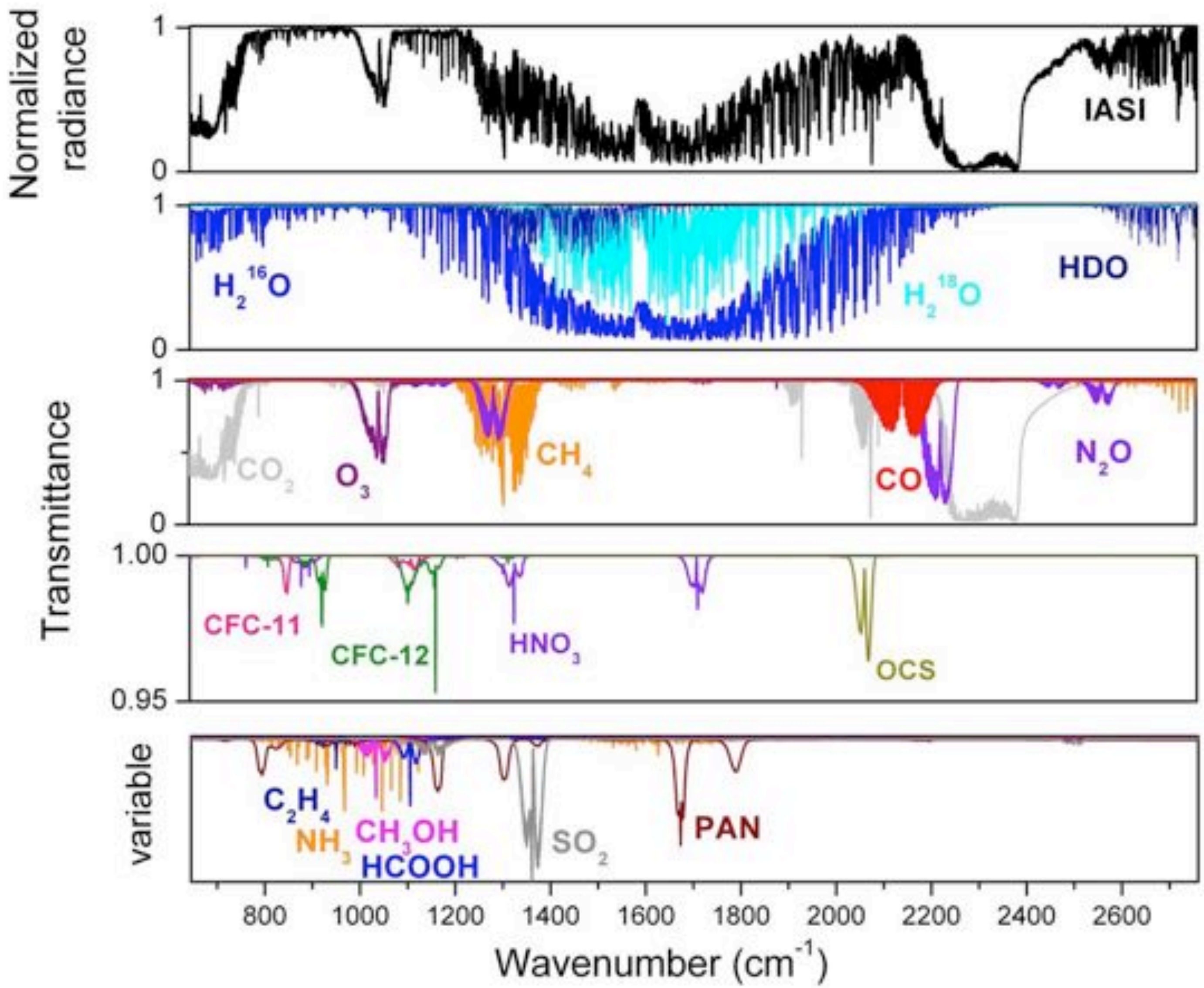




Earth thermal infrared spectrum measured by IASI



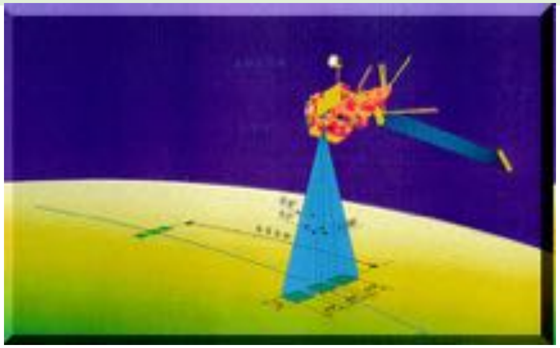
Which information from the infrared spectrum?



Clerbaux et al., 2009

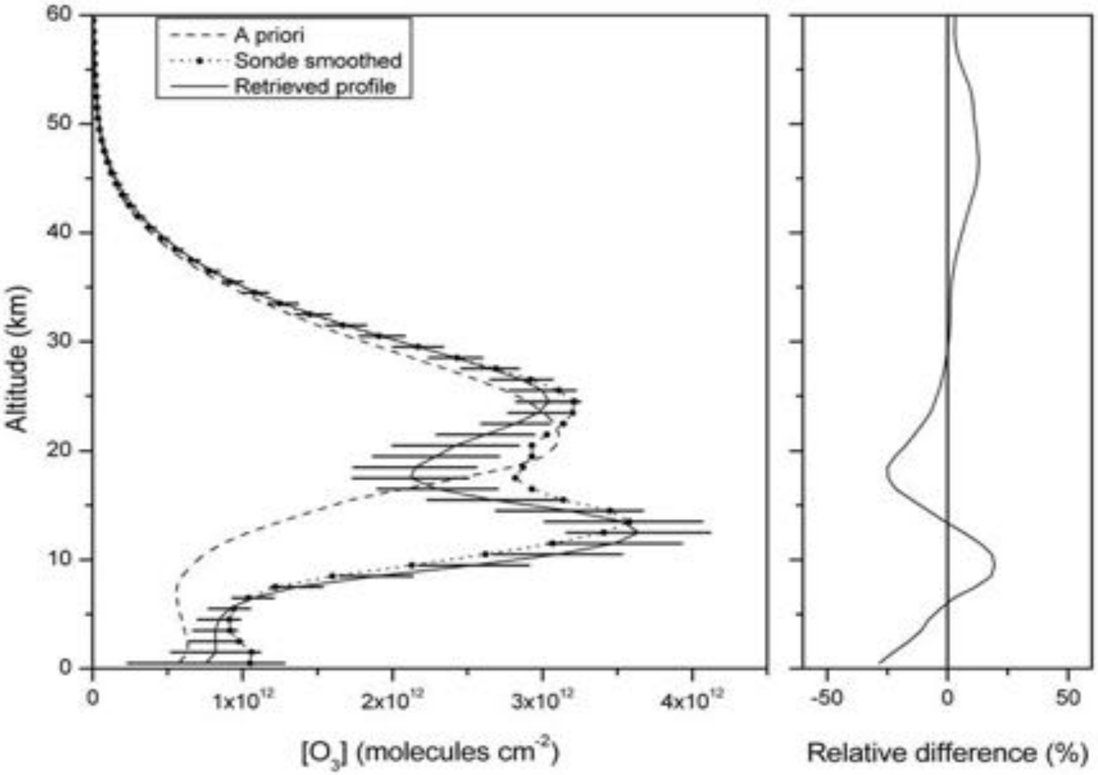
IMG: Interferometric Monitor for Greenhouse gases

- Japanese mission ADEOS
- Launch in August 1996
- Michelson Interferometer
  - Spectral range 740-3030 cm^{-1}
  - Spectral Resolution 0.1 cm^{-1}
  - Spatial Resolution - 3 pixels of 8km*8km



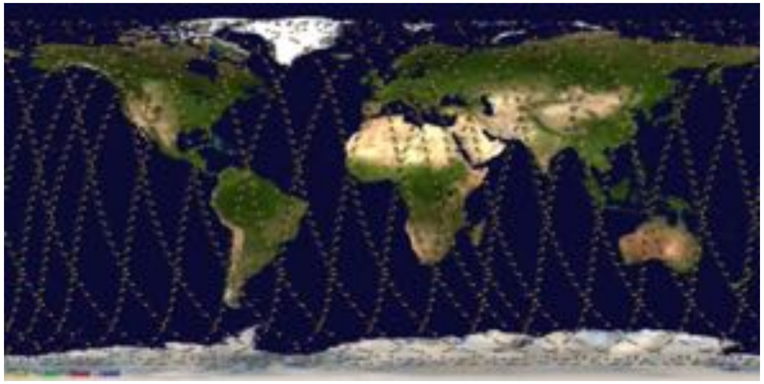
Coheur et al., 2005

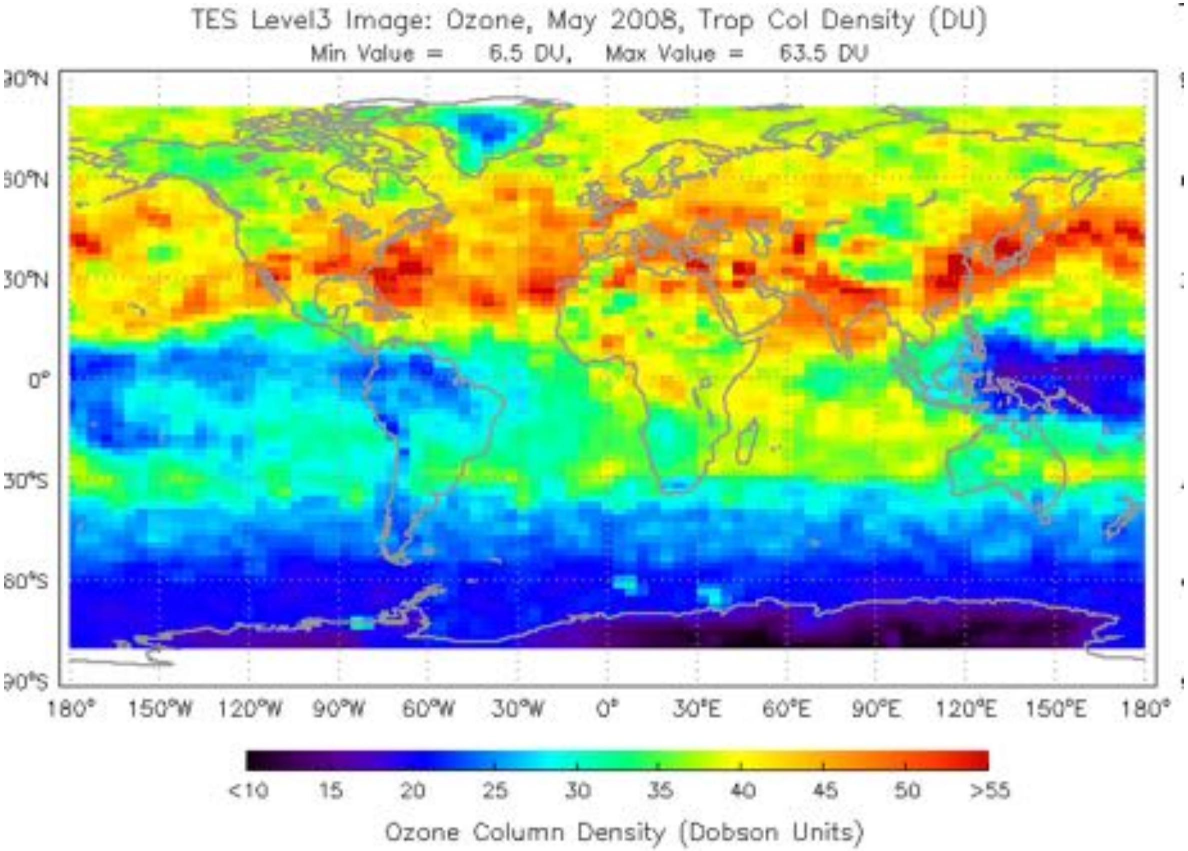
Ozone vertical profile



TES/Aura: Tropospheric Emission Spectrometer

Spectral Resolution at Nadir : 0.1 cm^{-1}
But no across-track scanning





MetOp satellites ➔ New performances to observe ozone pollution

- In orbit since 2006 aboard MetOp-A and expected for at least **15 years** with MetOp-B and MetOp-C
- **Global coverage twice daily** (morning ~ 9:30 LT, evening ~ 21:30 LT)

IASI (IR)

GOME-2 (UV-Vis)

- Spatial resolution : 25 km (at nadir)
- Across track swath : ~ 2000 km
- Spectral resolution : 0.5 cm^{-1}

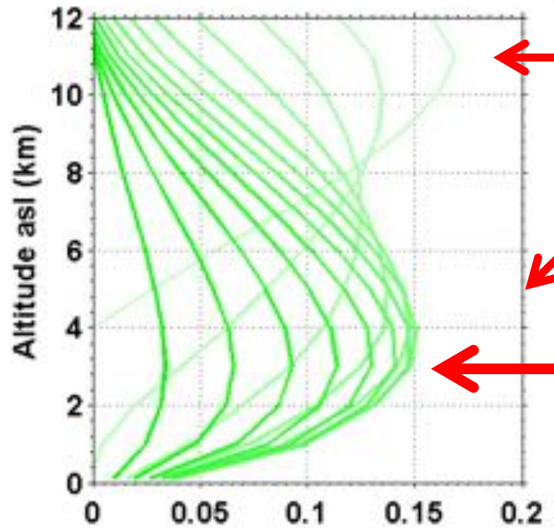
- Spatial resolution : 40 x 80 km^2
- Across track swath : ~ 1920 km
- Spectral resolution : ~ 0.24 nm

And after 2020, A New Generation of satellites : EPS-SG with IASI-NG and UVNS

Sensitivity of IASI retrievals of ozone

IASI → Lower tropospheric ozone

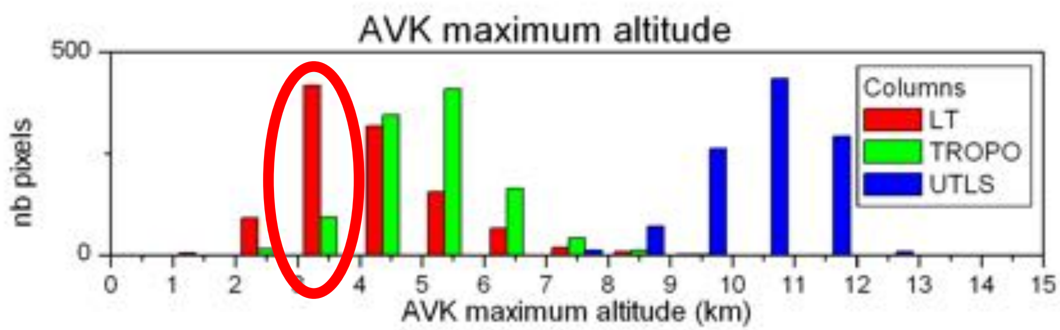
IASI (IR)



Averaging kernels

Possibility to discriminate between **Lower Troposphere and Upper Troposphere** when thermal conditions are favorable

LT sensitivity maximum around 3 km



Over land DOFs up to 6 km : ~ 0.6
up to 12 km : ~ 1.2

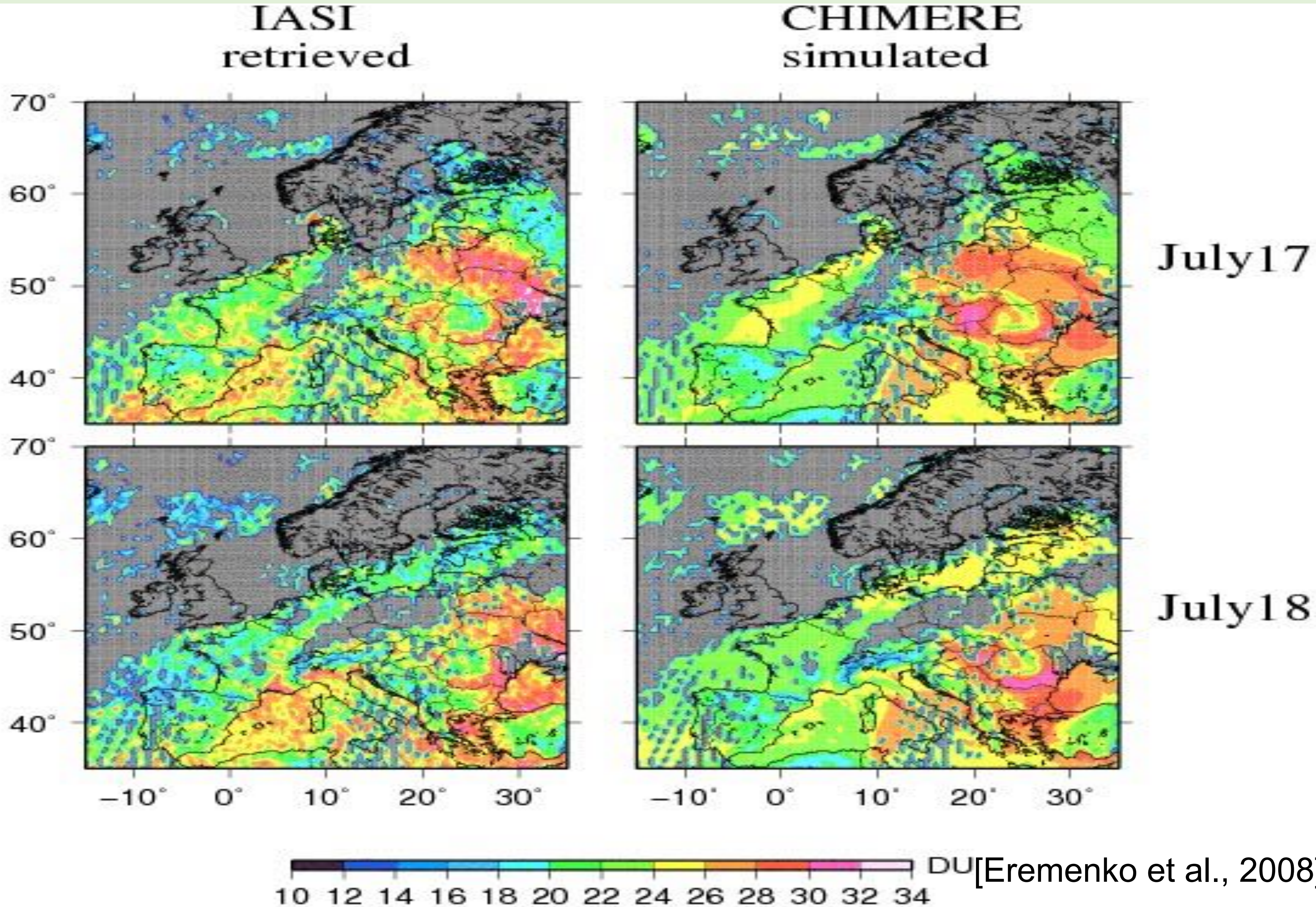
Validation against ozonesondes:

Mid-latitudes bias : < 2.5%

Precision : ~15%

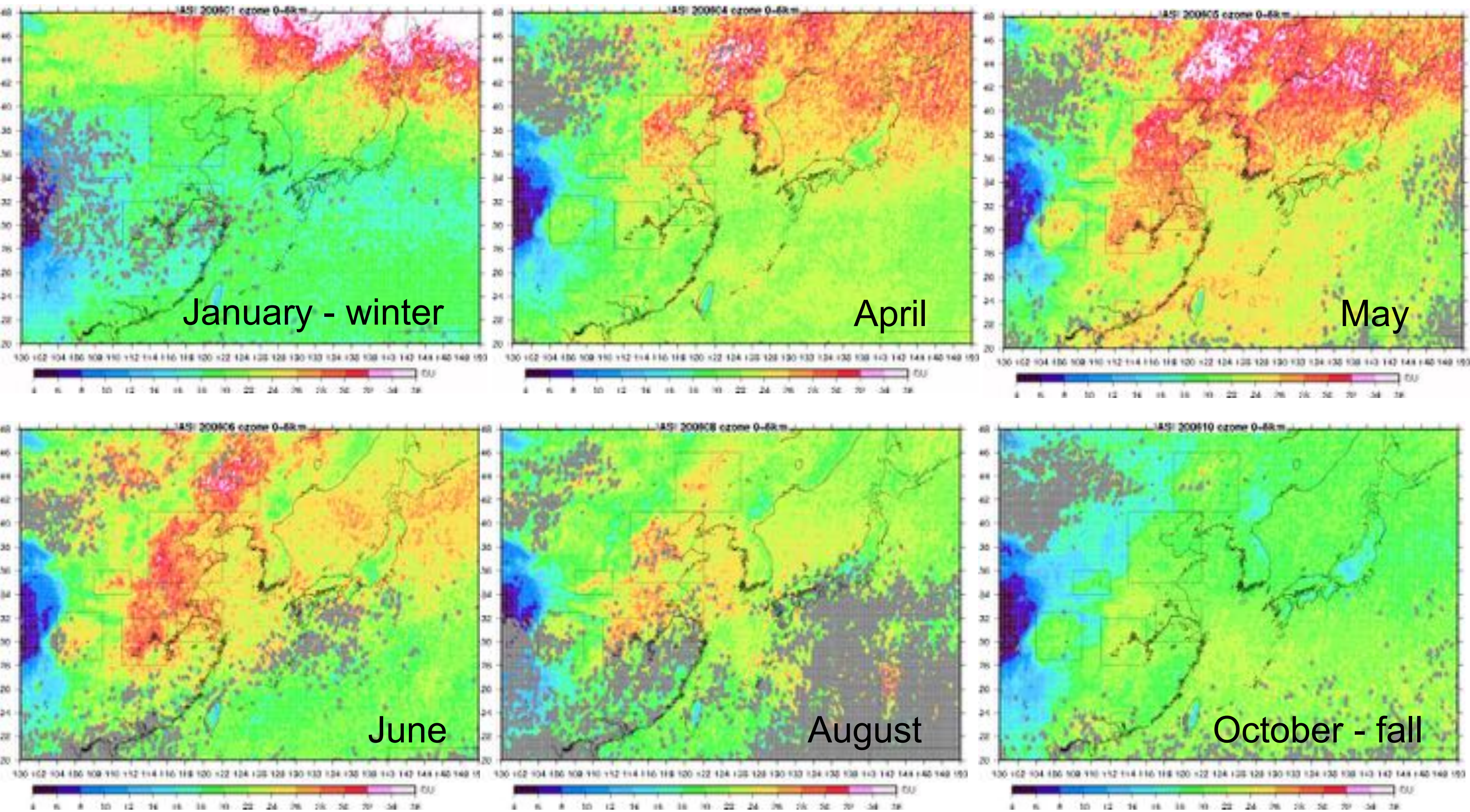
[Dufour et al., 2012]

First observations of an ozone pollution event from space



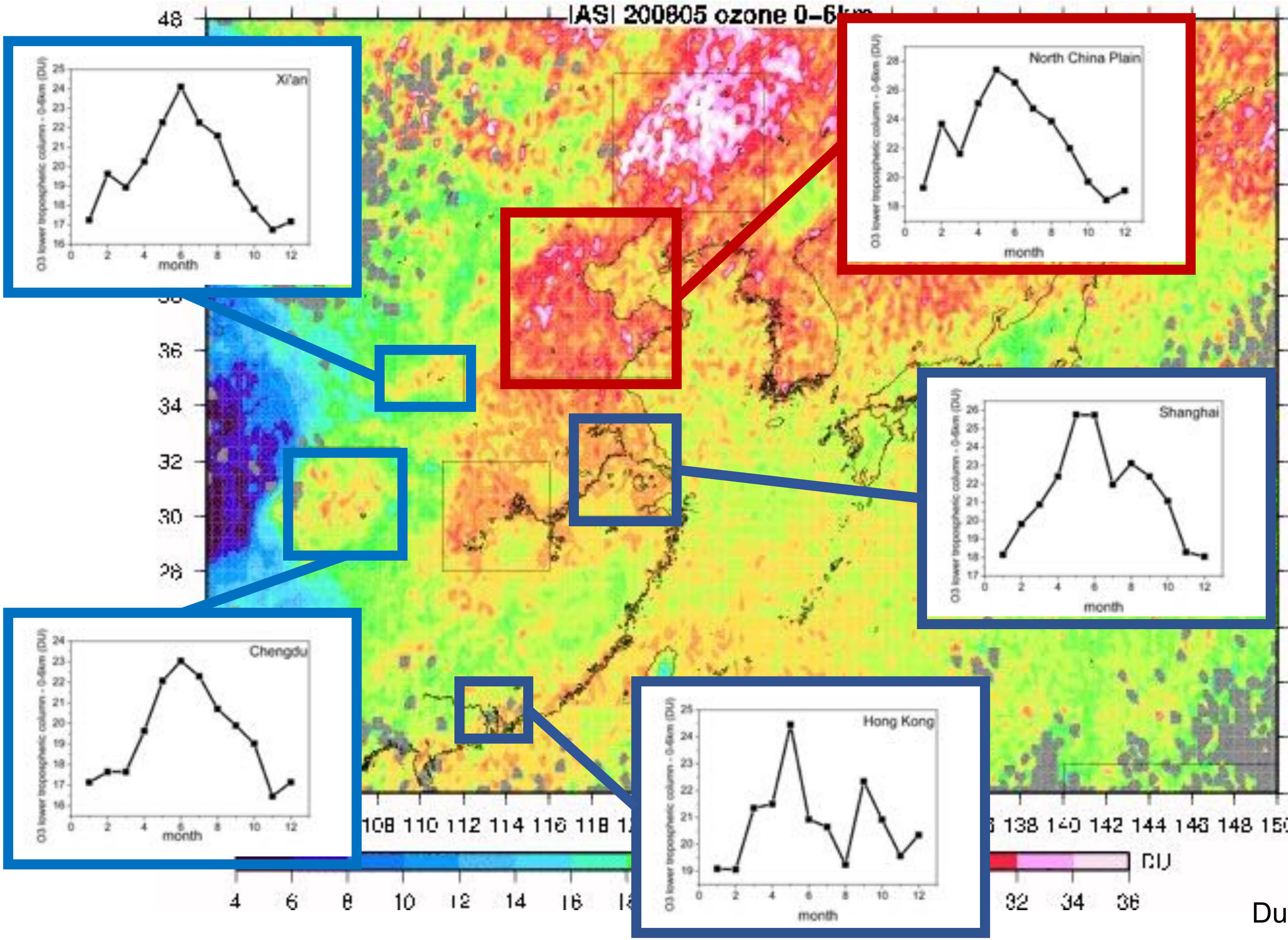
[Eremenko et al., 2008]

Monthly evolution of lower tropospheric ozone at East Asia – year 2008



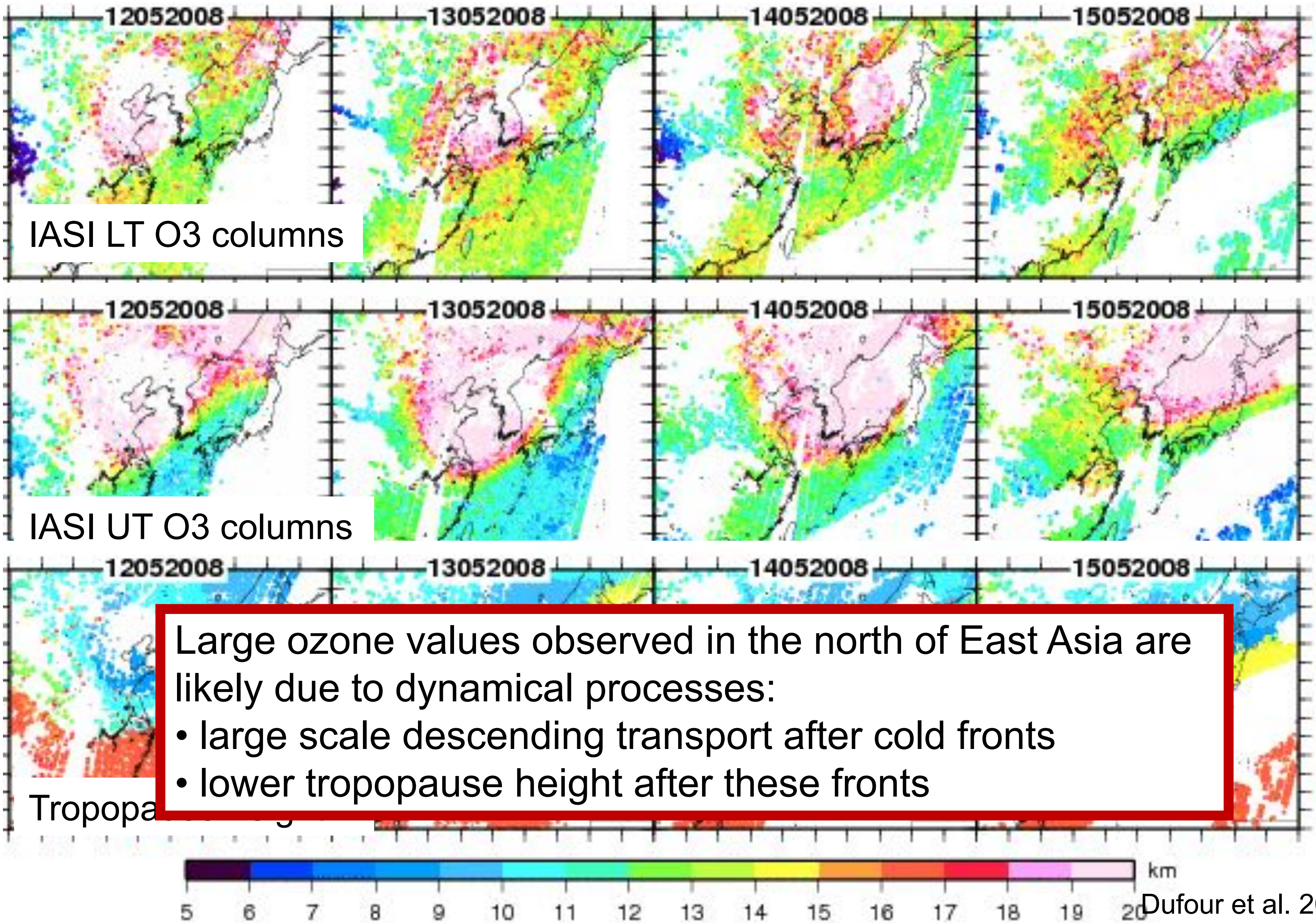
Dufour et al. 2015

Monthly evolution for selected regions



Dufour et al.

Role of stratosphere-troposphere exchanges

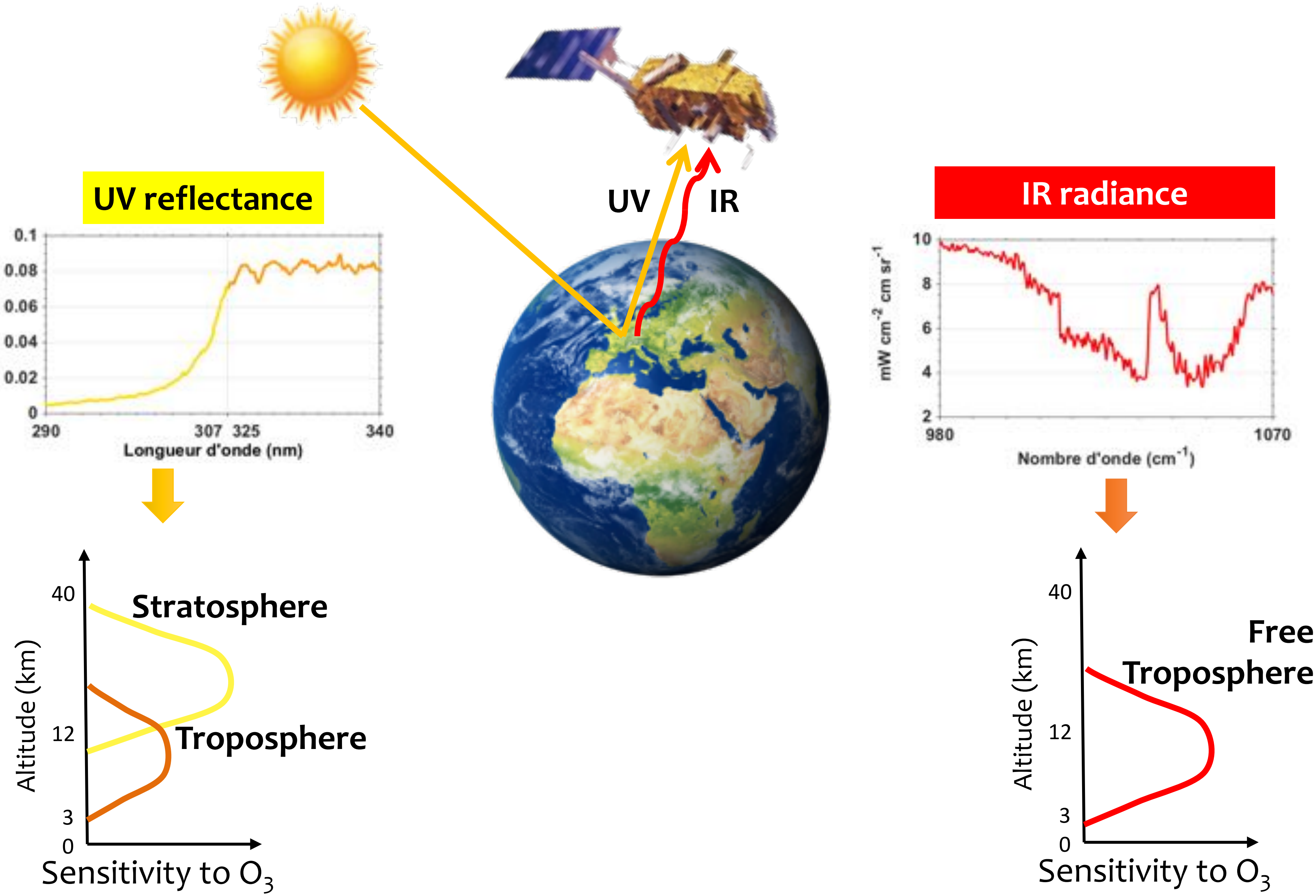


Large ozone values observed in the north of East Asia are likely due to dynamical processes:

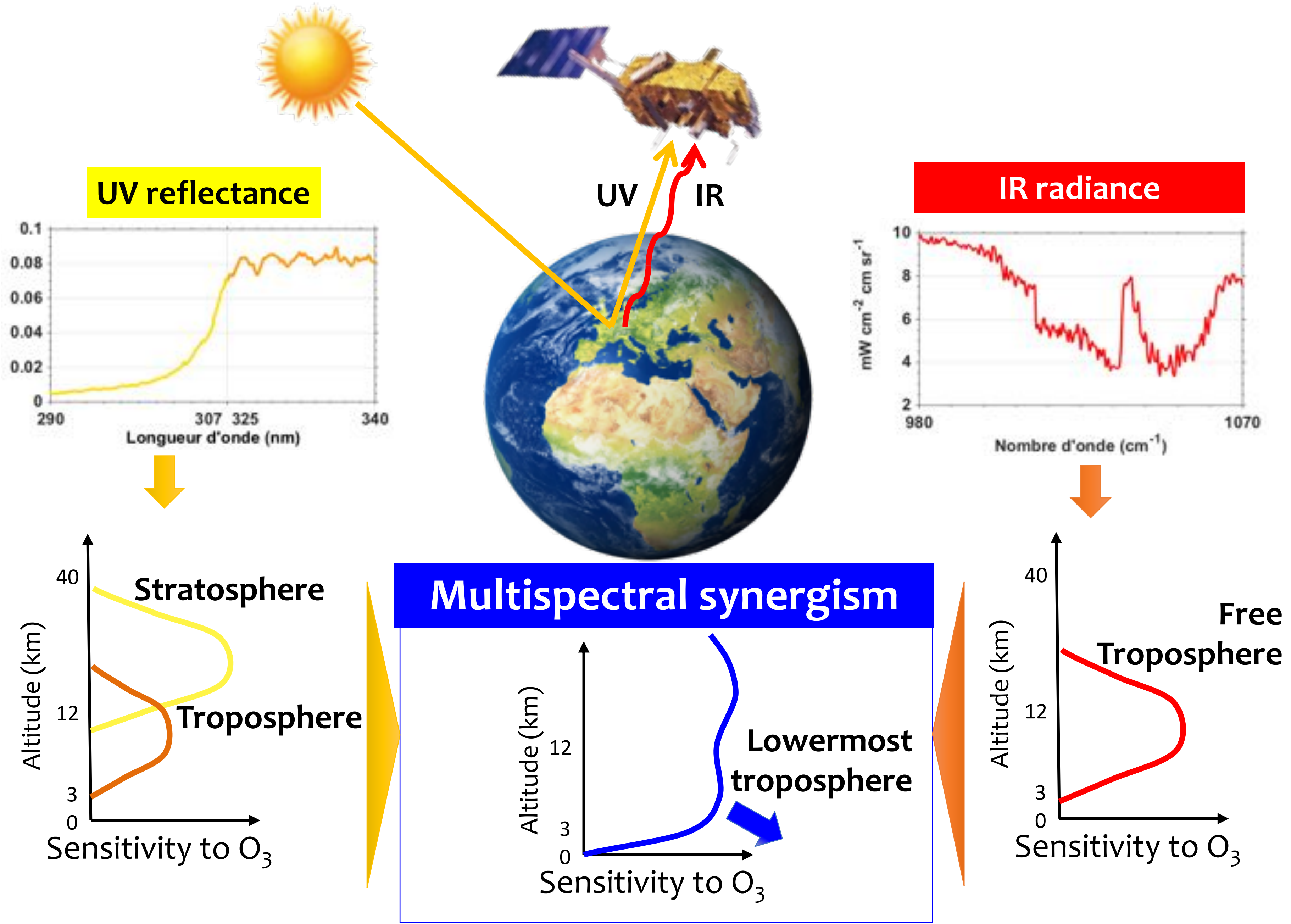
- large scale descending transport after cold fronts
- lower tropopause height after these fronts

Dufour et al. 2015

Multispectral synergism for retrieving Ozone

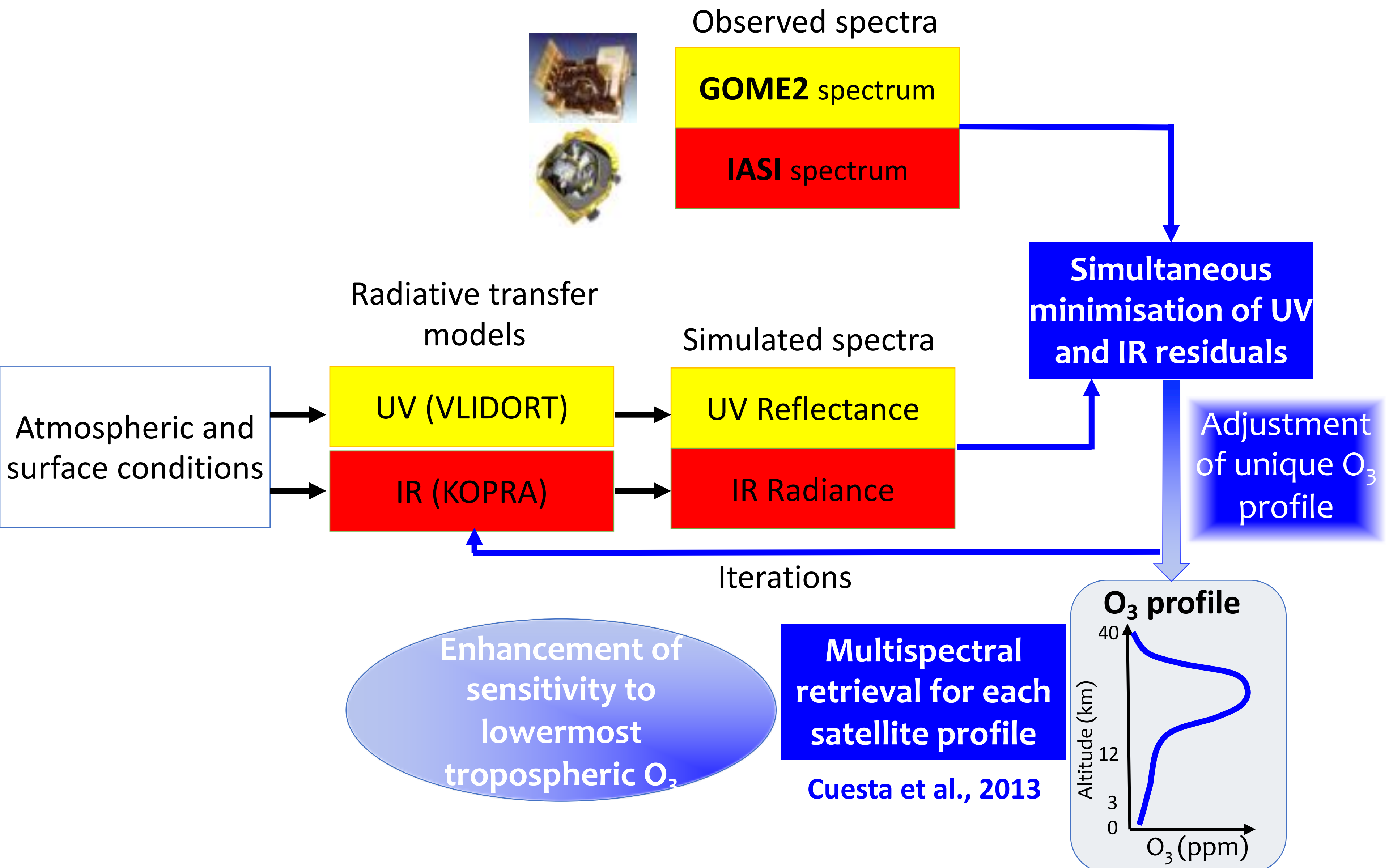


Multispectral synergism for retrieving Ozone



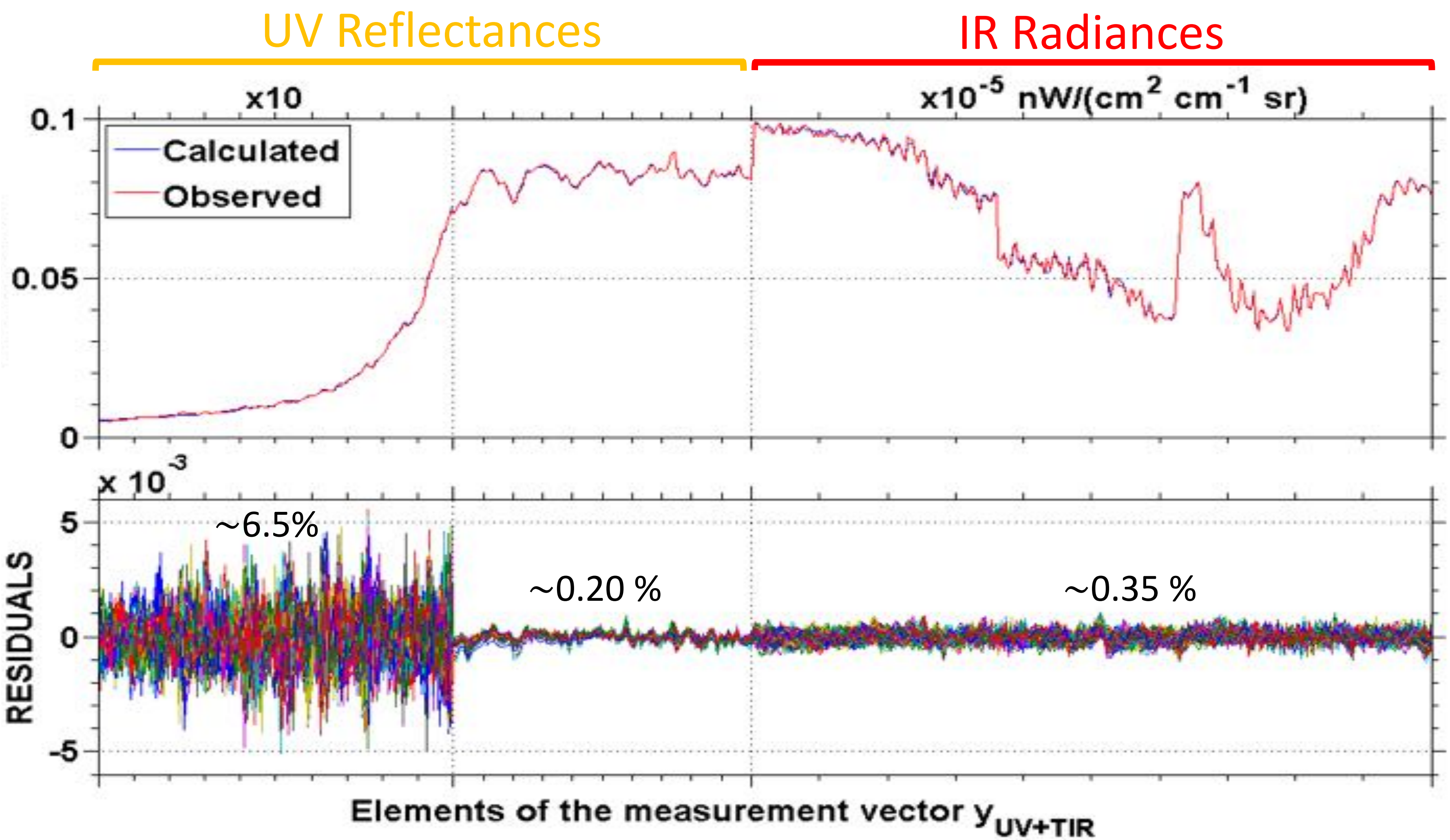
Multispectral approach IASI+GOME2

New approach of joint inversion of IR and UV co-localized spectra

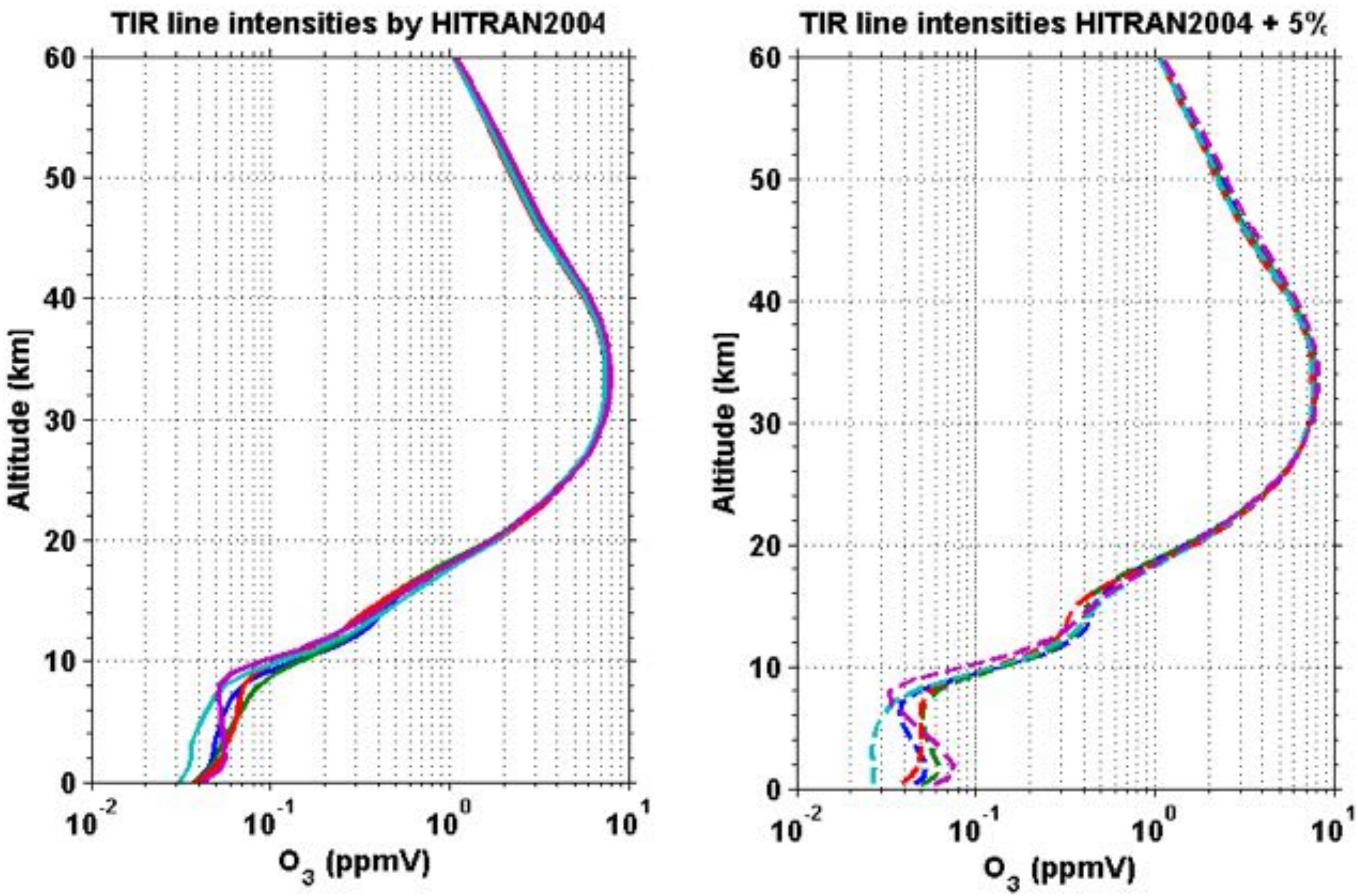


Multi-spectral fit

Simultaneous fit of IR and UV spectra → Adjusting a unique Ozone profile and instrumental parameters



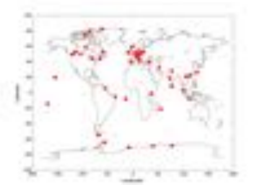
Ozone spectroscopy coherence between UV and IR?



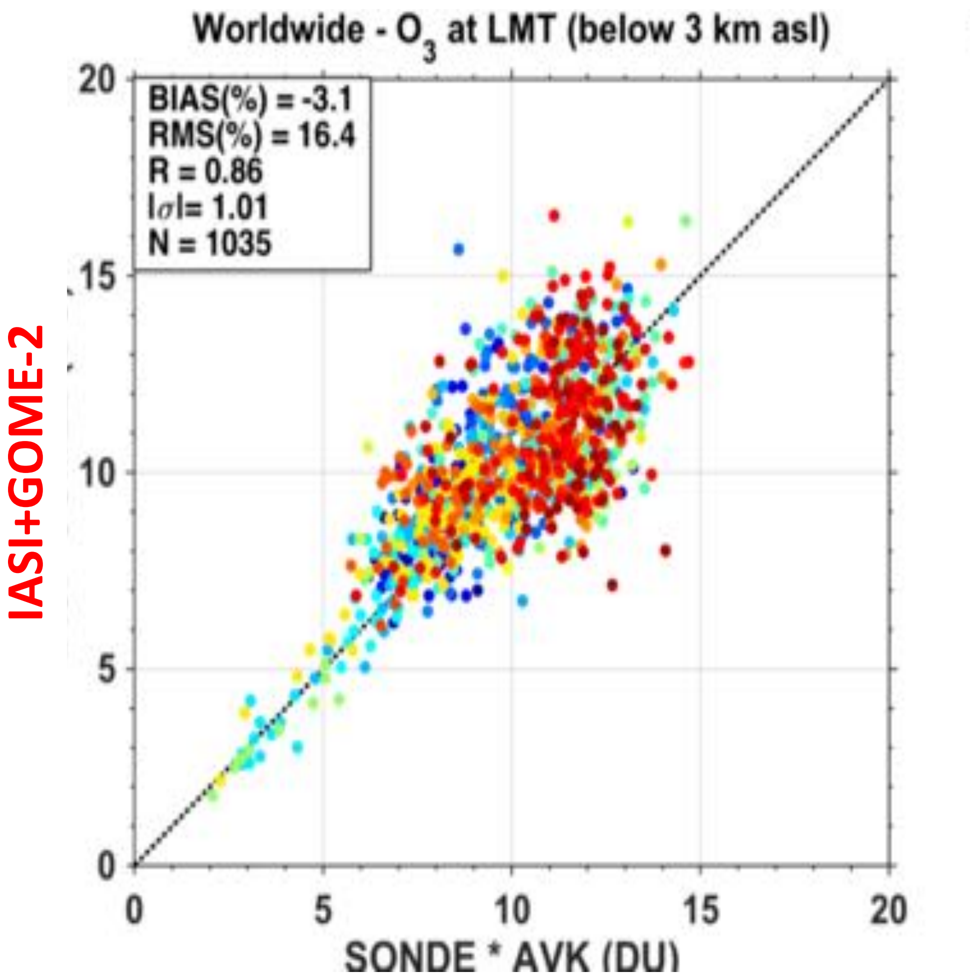
Similar results with UV cross sections -5% or HITRAN2010

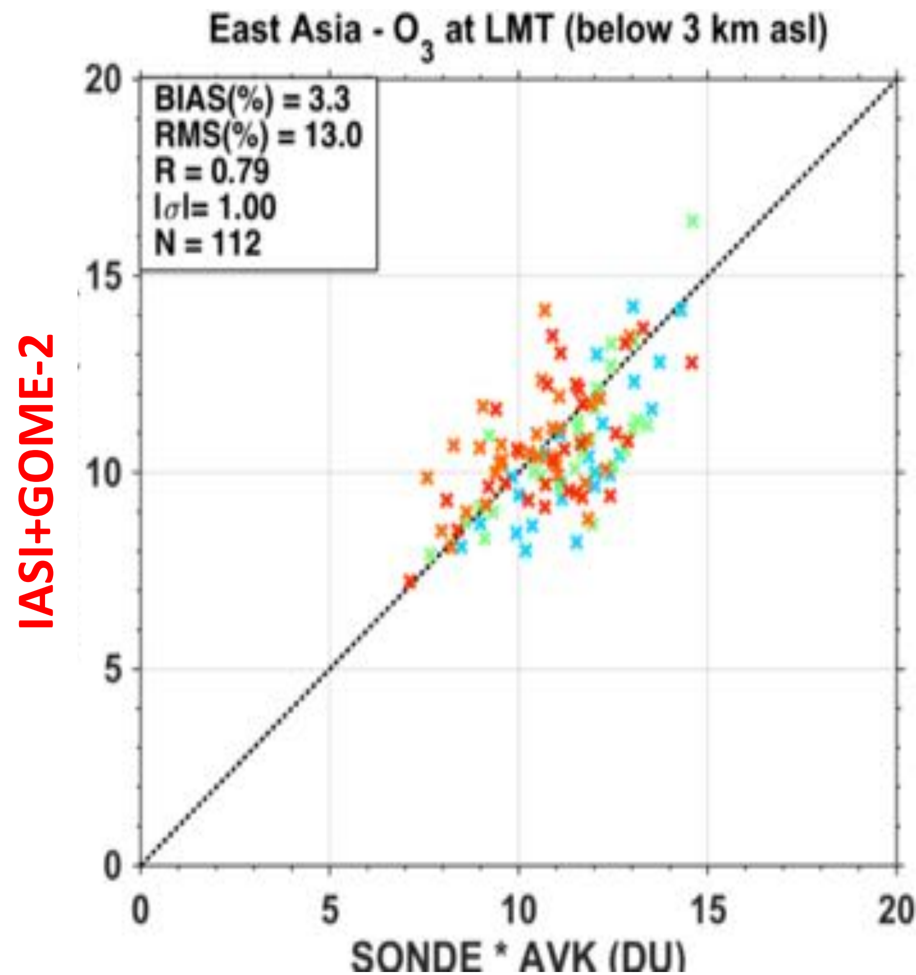
Validation of IASI+GOME2 at the Global scale

IASI+GOME2 vs O3 sondes from 44 stations in 2009 and 2010



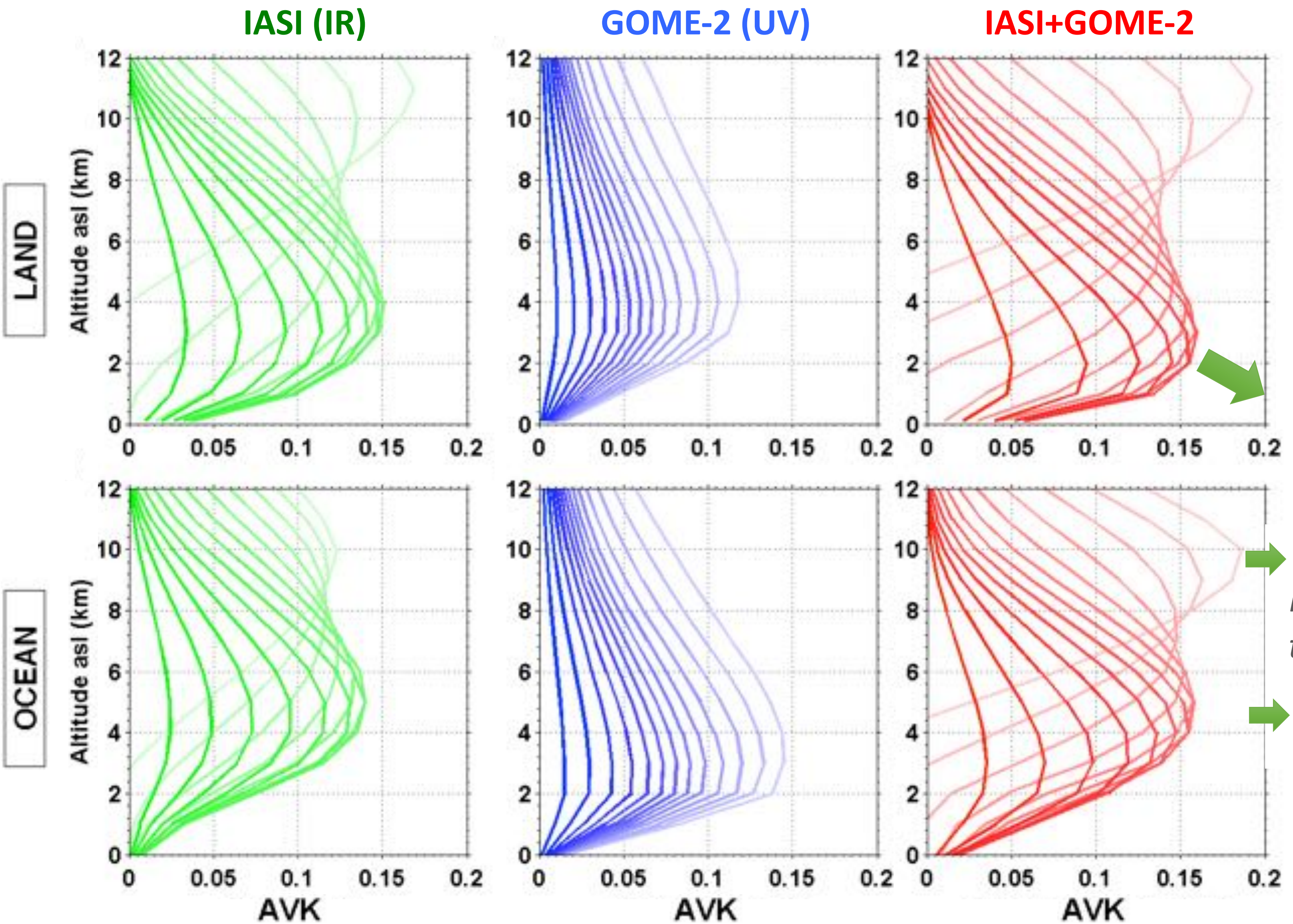
Lowermost tropospheric ozone : surface-3 km asl partial columns





Good agreement with sondes:
→Weak mean bias →Good correlation →Good variability

Sensitivity of the multispectral O3 retrieval: AVK

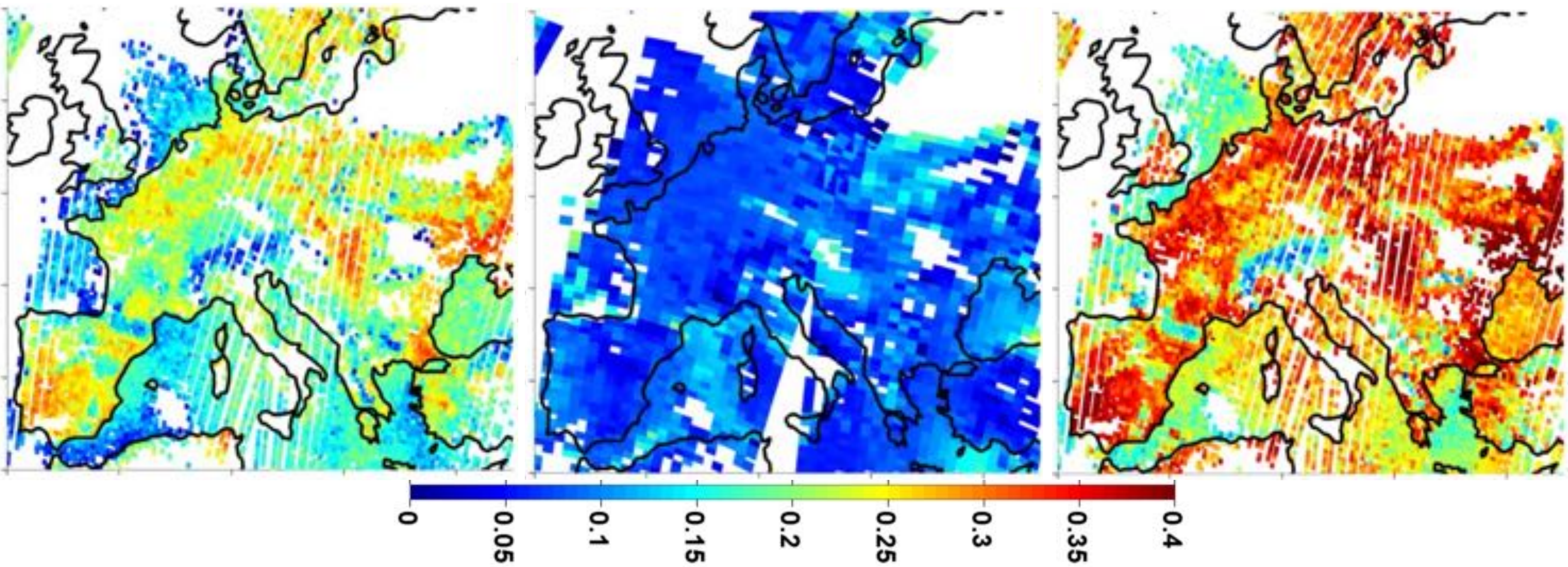


Higher sensitivity for lower layers

Two semi-independent tropospheric partial columns

Sensitivity of the multispectral O_3 retrieval: Degrees of freedom in the Lowermost Troposphere (up to 3 km asl)

IASI (IR) | **GOME-2 (UV)** | **IASI+GOME2**



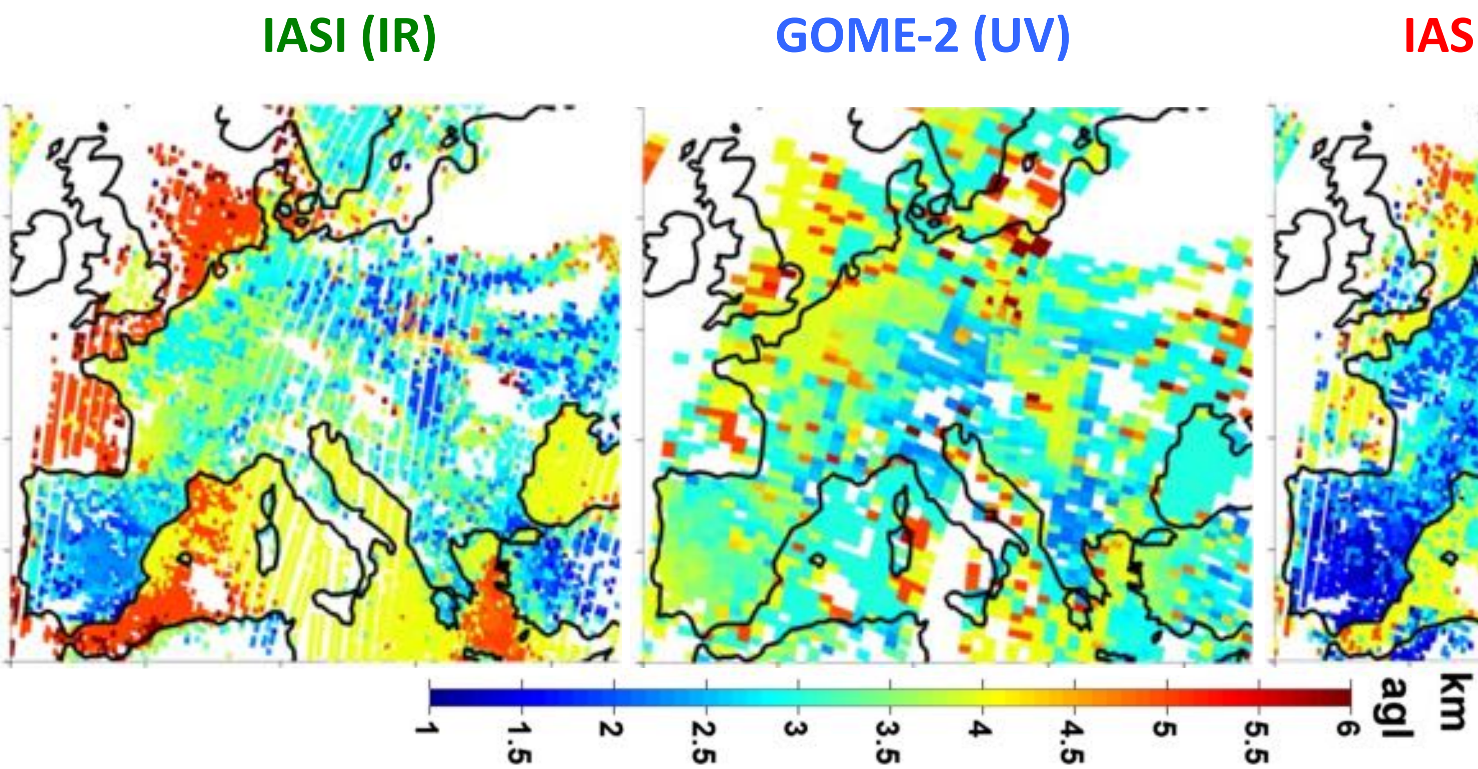
0.25 DOFs over land 0.15 DOFs over ocean

<0.10 DOFs

0.35 DOFs over land 0.25 DOFs over ocean

DOF_{IASI} + 40%

Sensitivity of the multispectral O_3 retrieval: Height of maximum sensitivity in the Lowermost Troposphere (up to 3 km asl)



3 km agl over land
4.3 km agl over ocean

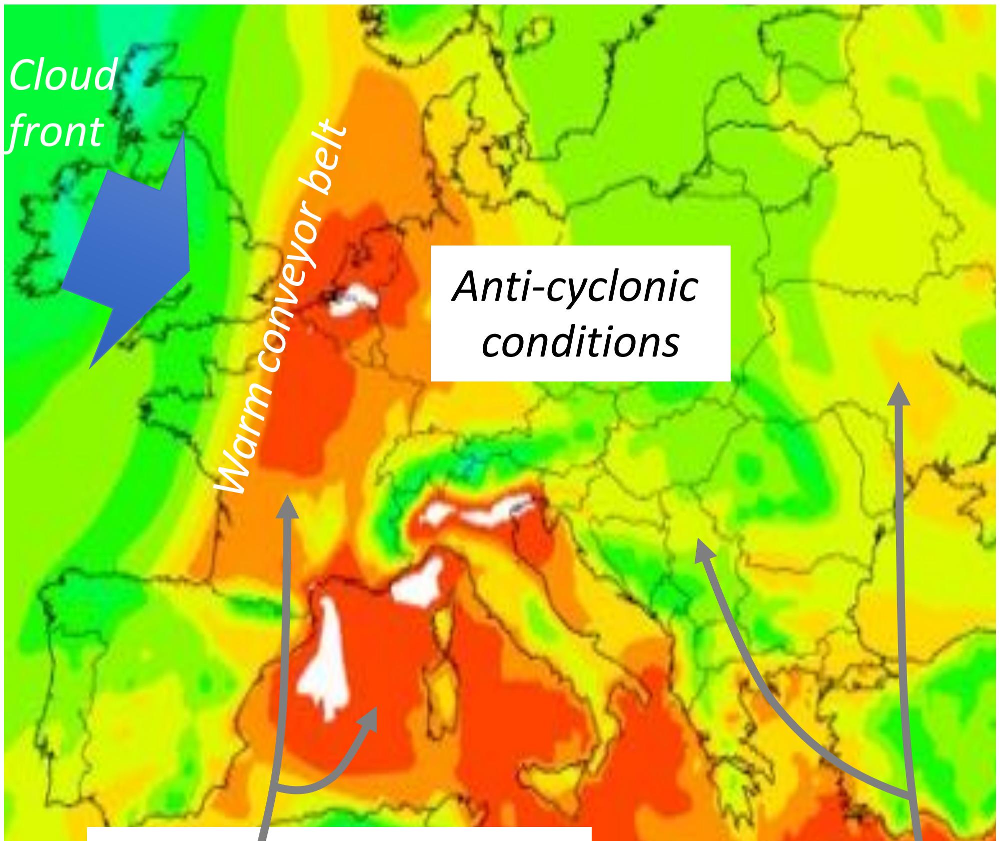
3.7 km agl

2.2 km agl over land 3.5 km agl over ocean
H_{IASI} - 800 m

A moderate O_3 pollution episode over Europe: 18 to 21 August 2009

20 August 2009 at 10 am : O_3 Surface – 6 km

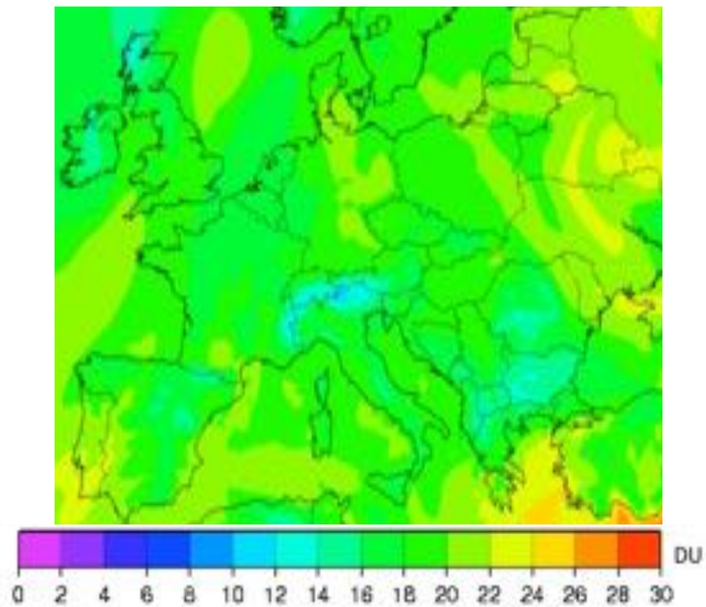
CHIMERE outputs



Western O_3 plumes → up to the lower free troposphere

Eastern O_3 plumes → below 3 km (LMT)

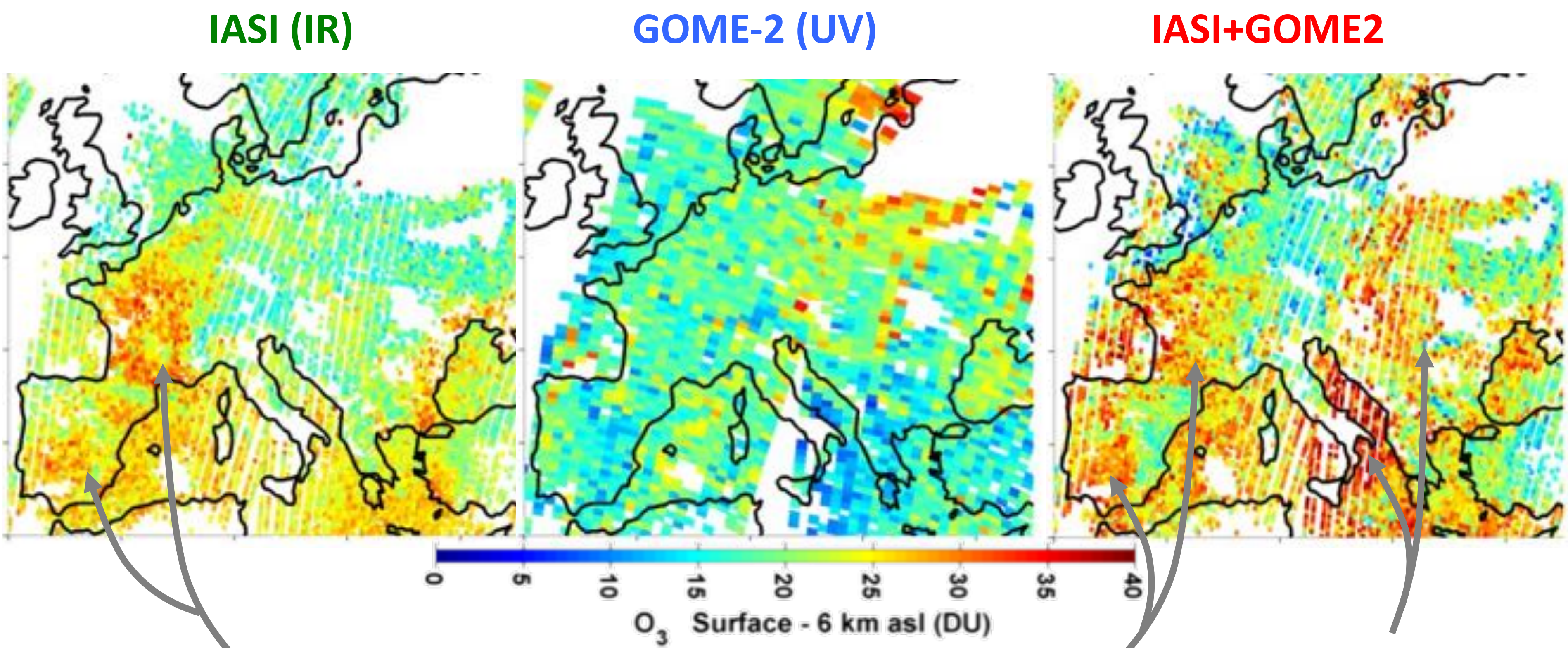
CHIMERE Switching off O_3 precursor emissions since 01/08/2009



→ Almost all O3 plumes were photo-chemically produced with emissions from Europe

Satellite observations of the O_3 pollution event : IASI+GOME2 vs. sing-band approaches

19 August 2009



Continental western O_3 plumes depicted by both IASI and IASI+GOME2 → up to 4-5 km asl

Eastern and over sea O_3 only observed by IASI+GOME2

Satellite observations of the O_3 pollution event : IASI+GOME2 vs. sing-band approaches

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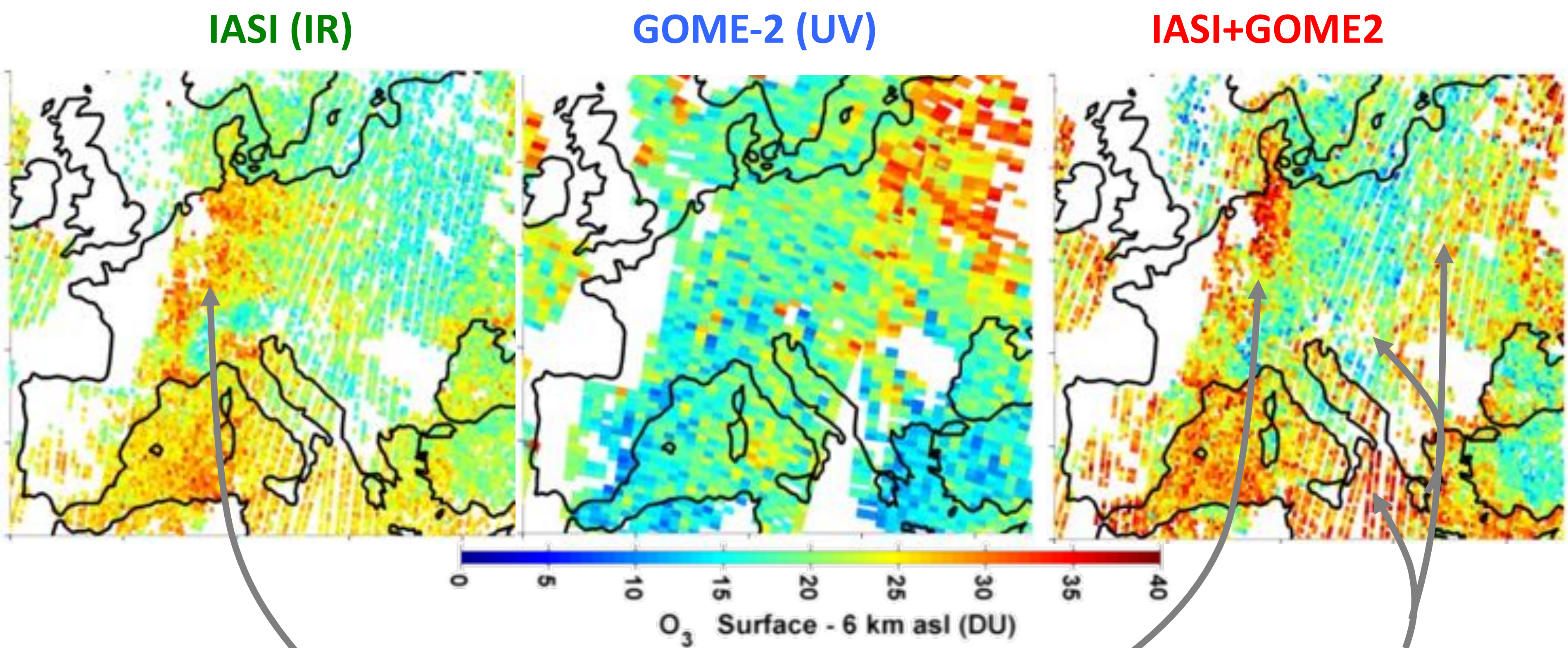
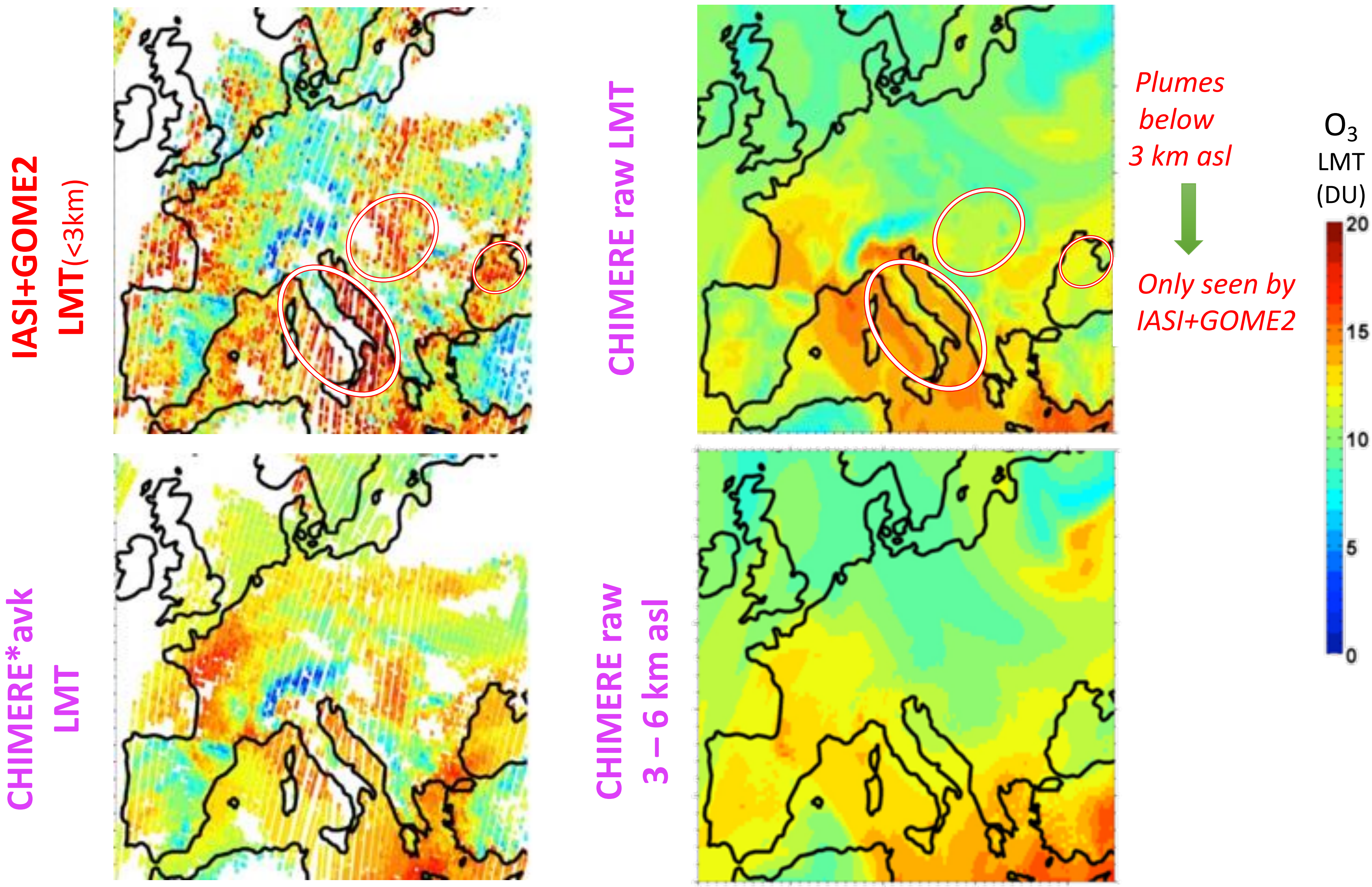


Continental western O_3 plumes depicted by both IASI and IASI+GOME2 → up to 4-5 km asl

Eastern and over sea O_3 only observed by IASI+GOME2

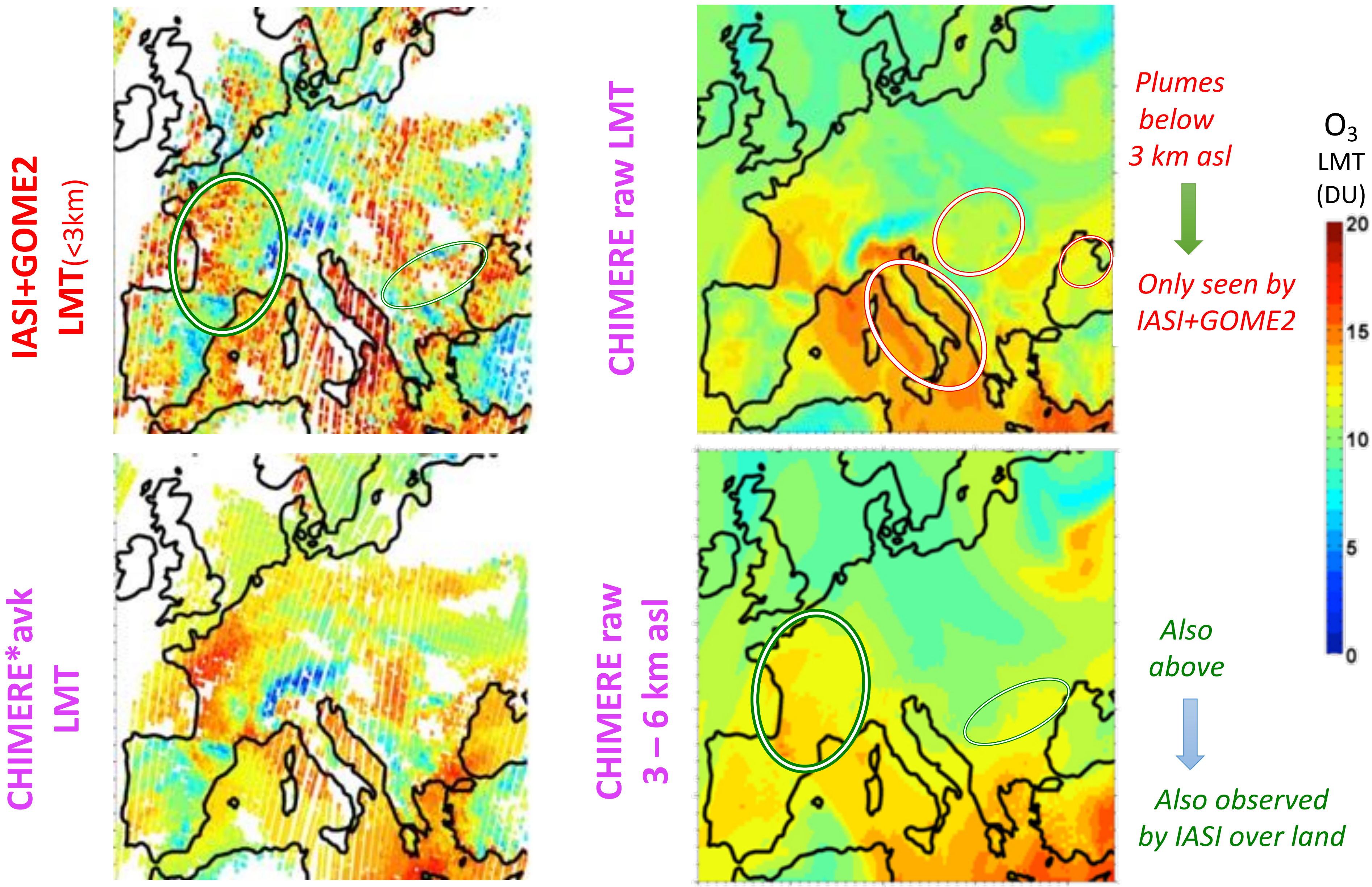
IASI+GOME2 vs. CHIMERE : LMT and above

19 August 2009



IASI+GOME2 vs. CHIMERE : LMT and above

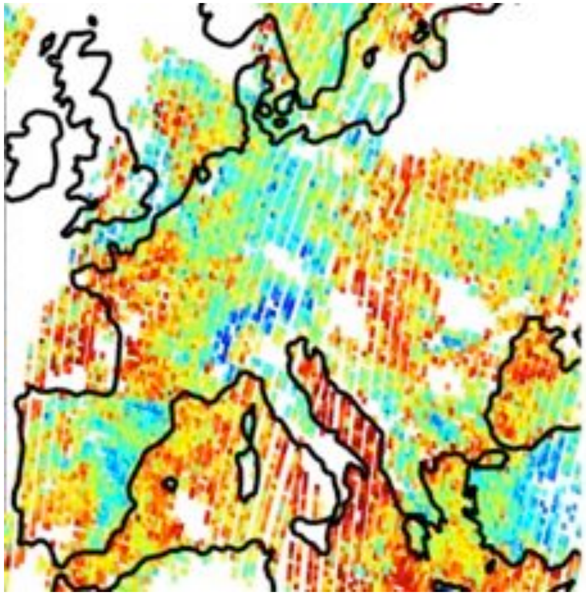
19 August 2009



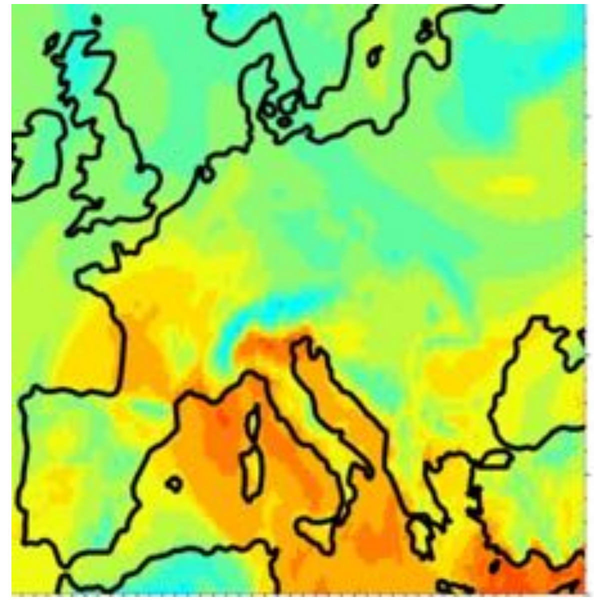
IASI+GOME2 vs. MODELS at the LMT (<3 km):

19 August 2009

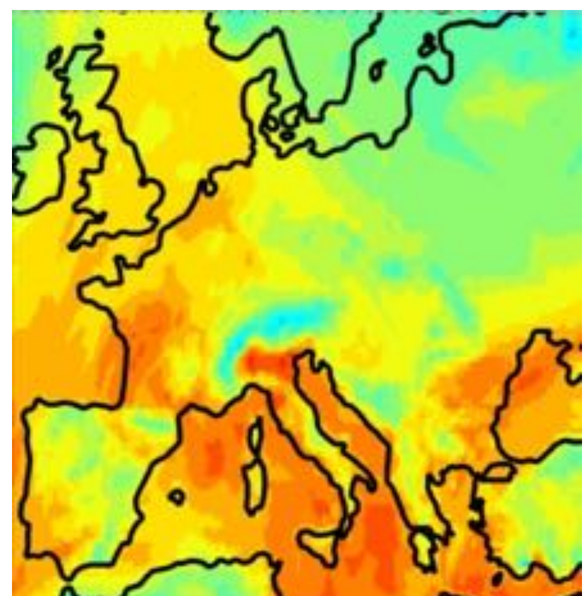
IASI+GOME2 LMT(<3km)

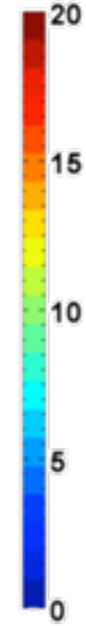


CHIMERE raw LMT



MOCAGE raw LMT



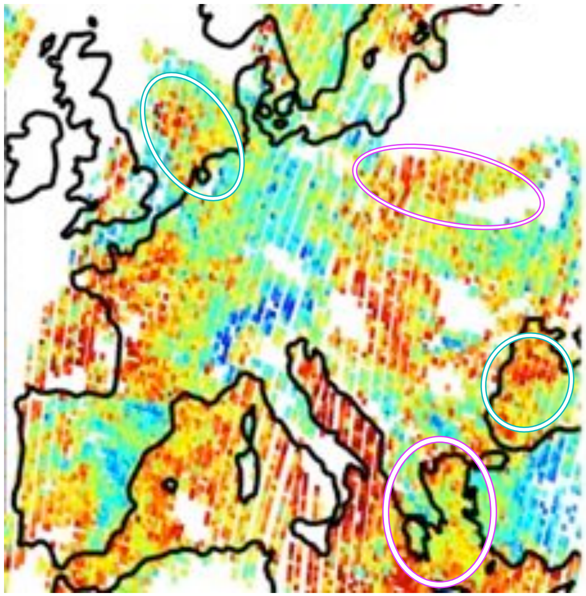


Good agreement with both models in the overall structure of O_3 plumes at the LMT

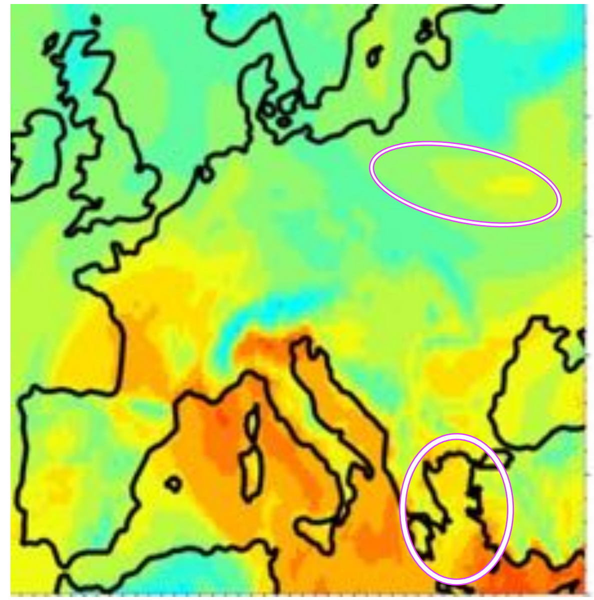
IASI+GOME2 vs. MODELS at the LMT (<3 km):

19 August 2009

IASI+GOME2 LMT(<3km)

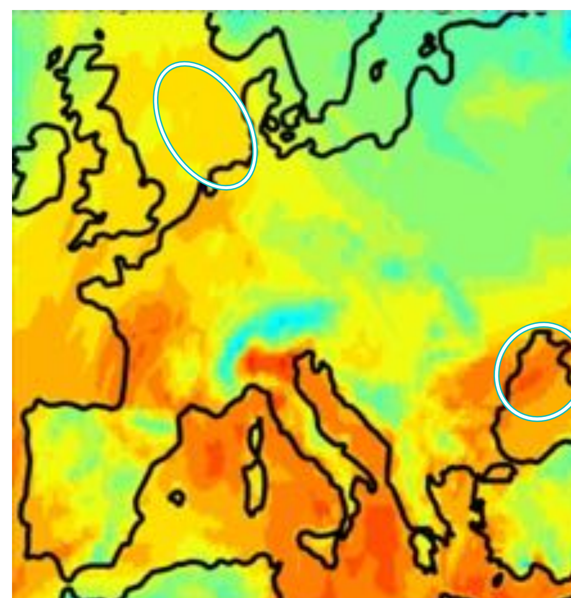


CHIMERE raw LMT

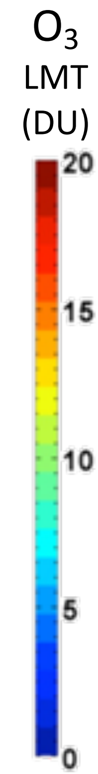


Only modelled by CHIMERE & captured by IASI+GOME2

MOCAGE raw LMT



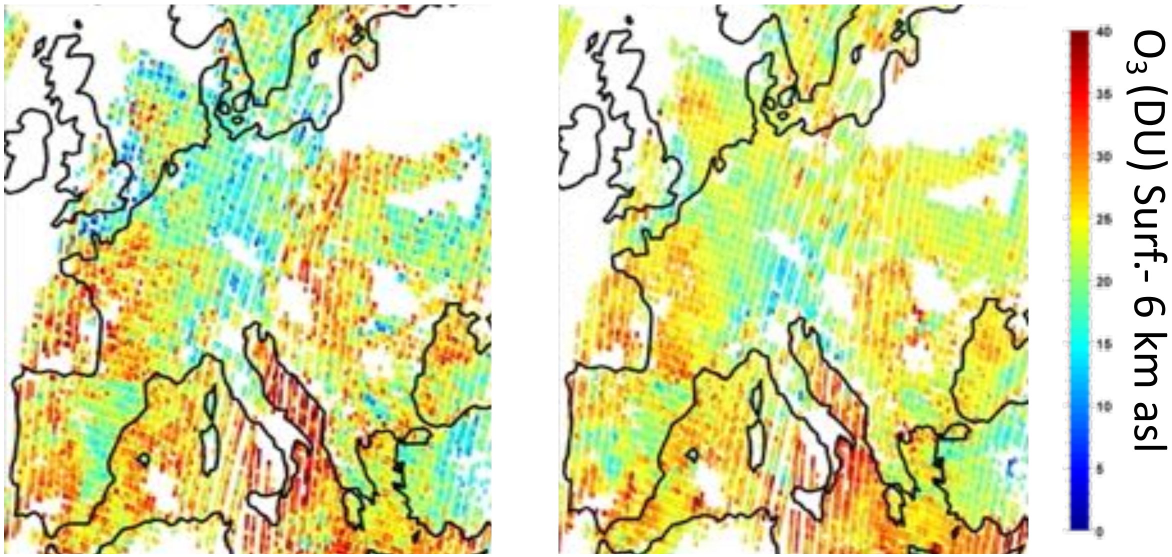
Only modelled by MOCAGE & captured by IASI+GOME2



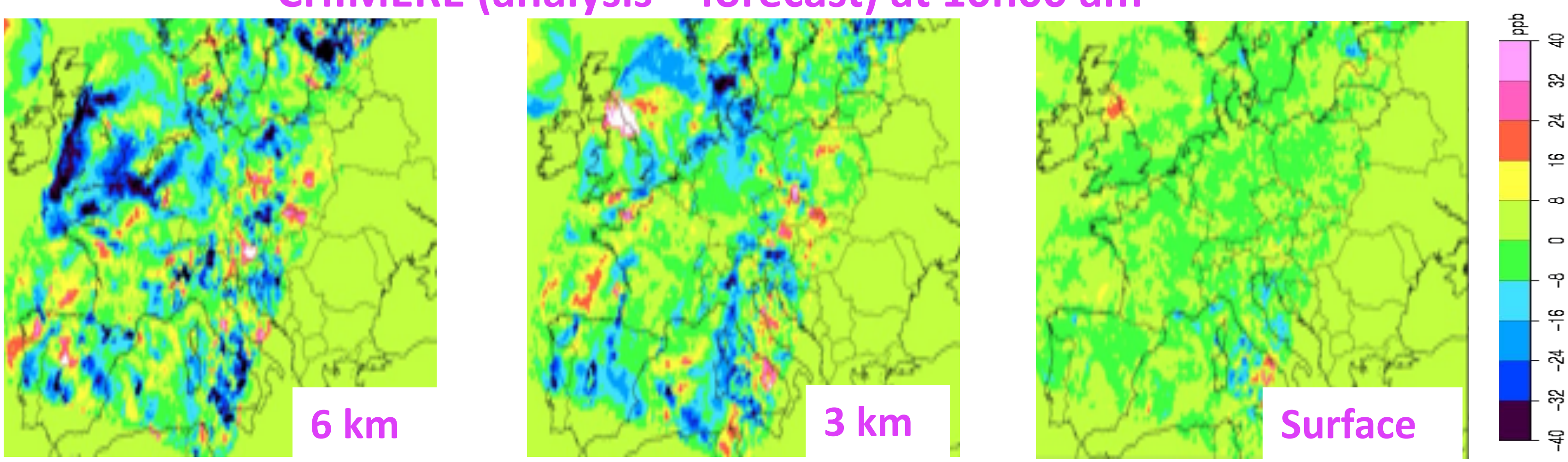
Assimilation of IASI+GOME2 LT observations into CHIMERE+EnK:

19 August 2009

IASI+GOME2 **CHIMERE analysis*AVK**



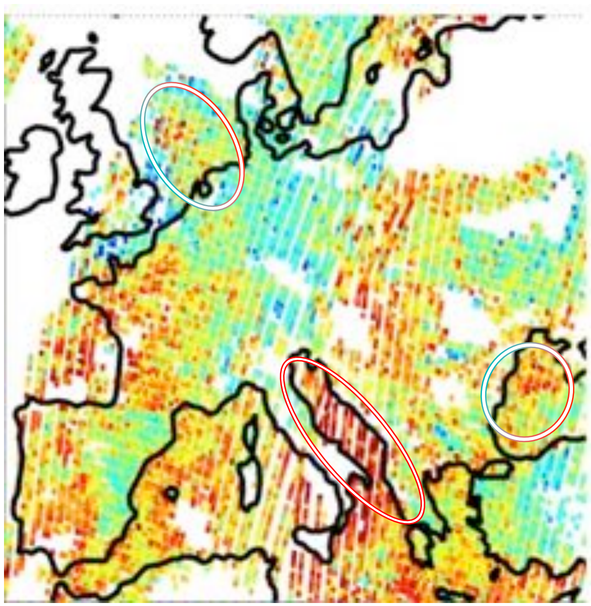
CHIMERE (analysis – forecast) at 10h00 am



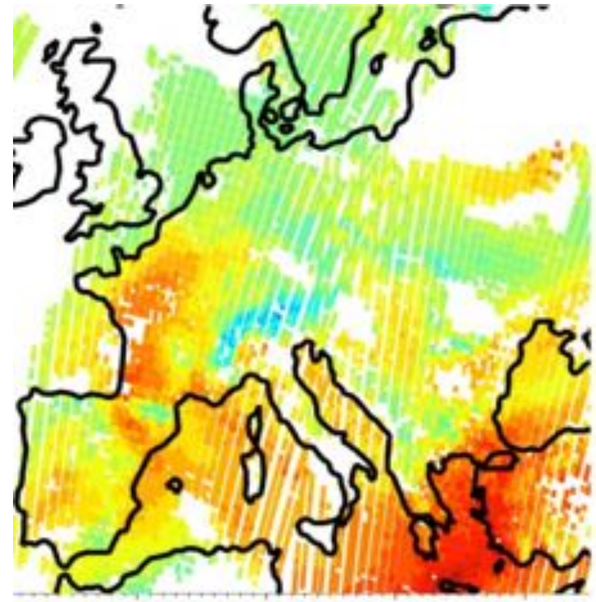
Assimilation of IASI+GOME2 into CHIMERE:

19 August 2009

IASI+GOME-2 LT(<6km)

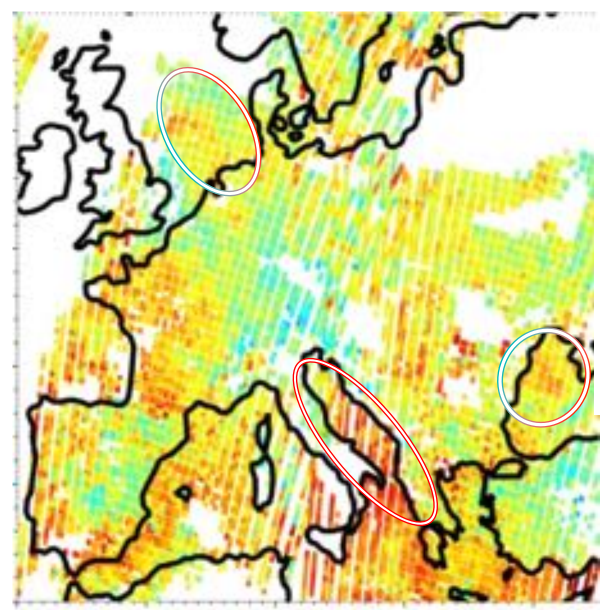


CHIMERE*AVK LT

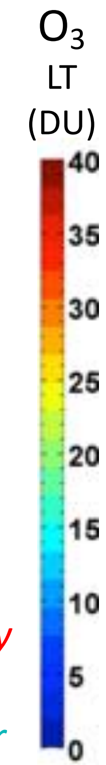


Assimilation of LT partial columns with CHIMERE+EnK

CHIMERE Analysis*AVK LT



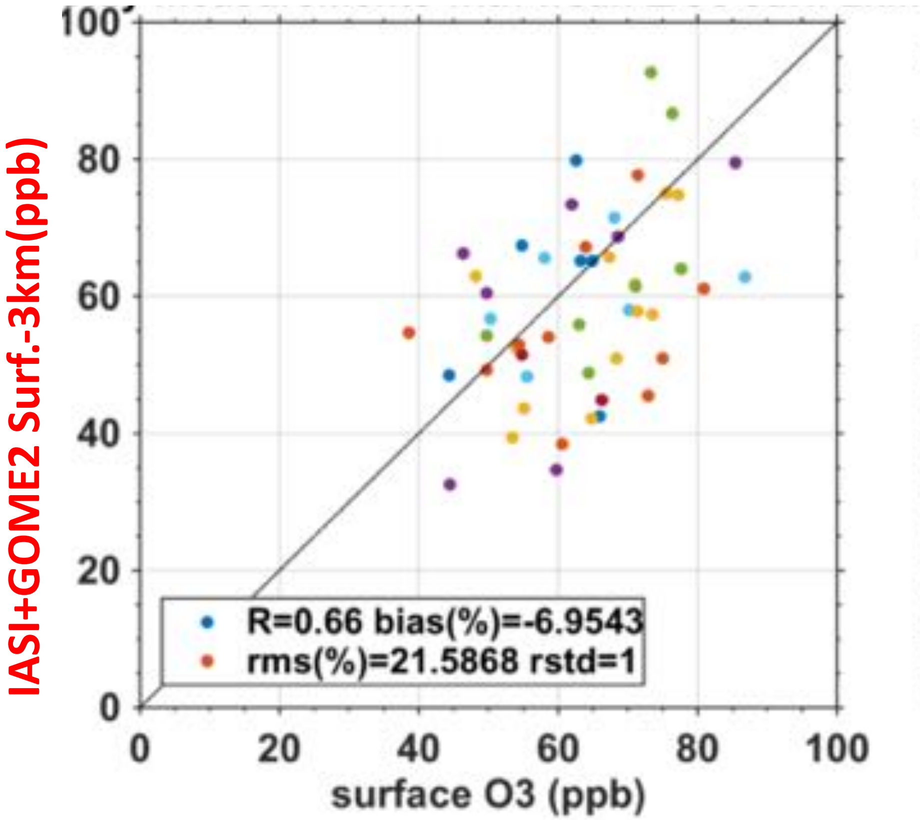
Corrections by IASI+GOME2 & also similar to MOCAGE

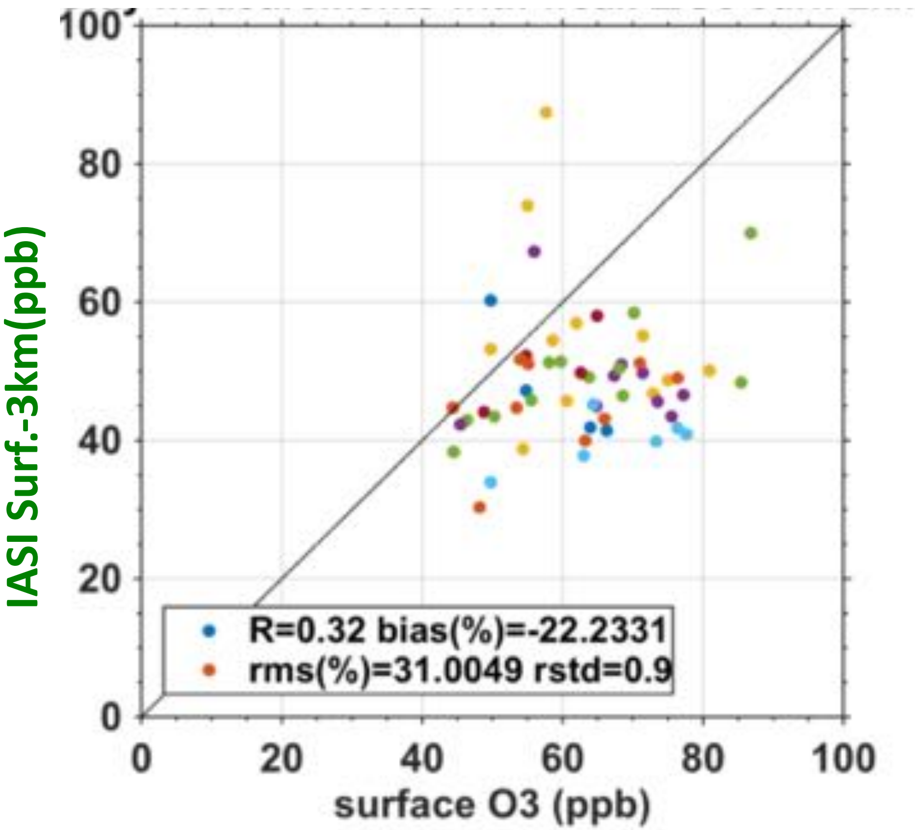


Comparison of IASI+GOME2 vs in situ measurements at the surface

2 pollution episodes: 4-9 April and 4-9 May 2009

Cases with gradient$_{surface-2\ km}$ < 20 ppb (according to CHASER)





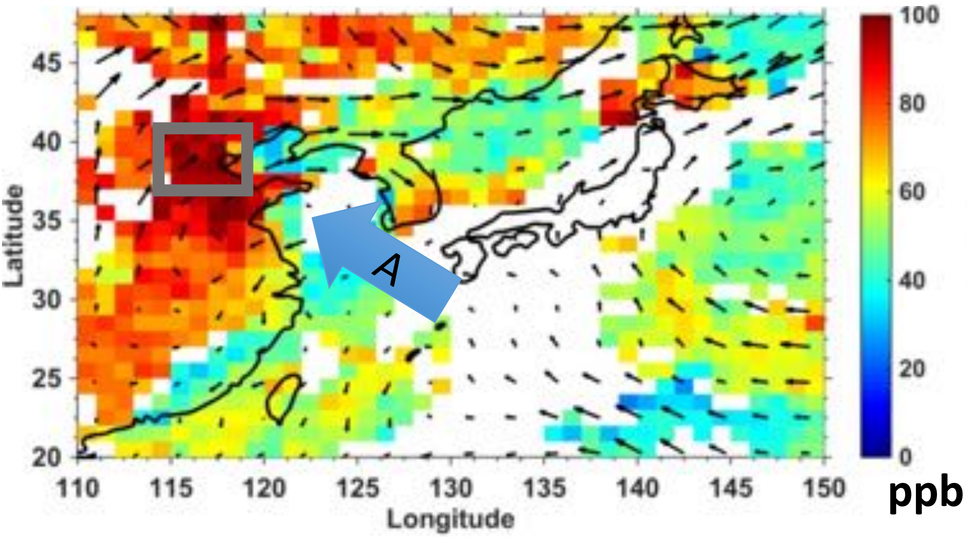
- ✓ Good correlation: **Currently unique!!!**
- ✓ Weak mean bias
- ✓ Precision near expected IASI+GOME2 errors

Surface variability of O3 is not observed by IASI only approach

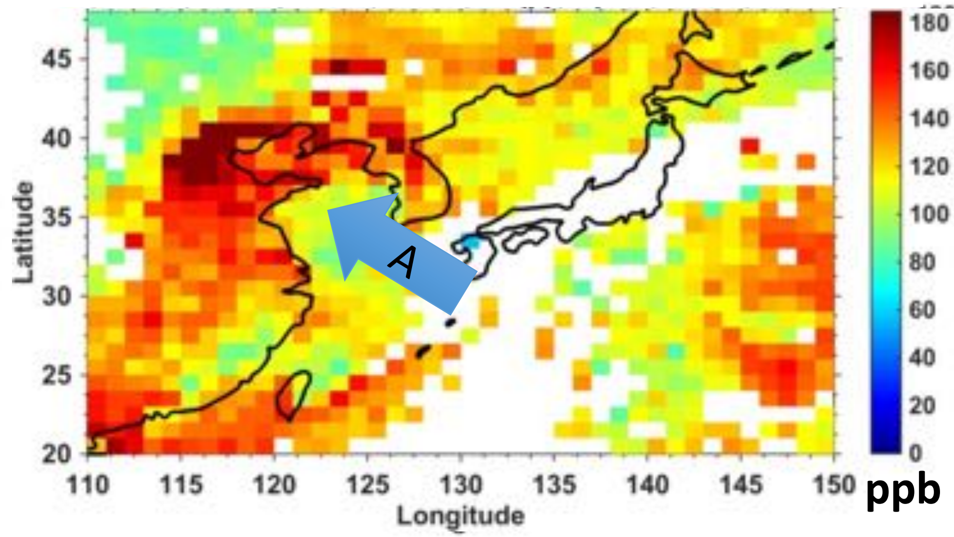
Ozone pollution over East Asia from IASI+GOME2

4 May 2009

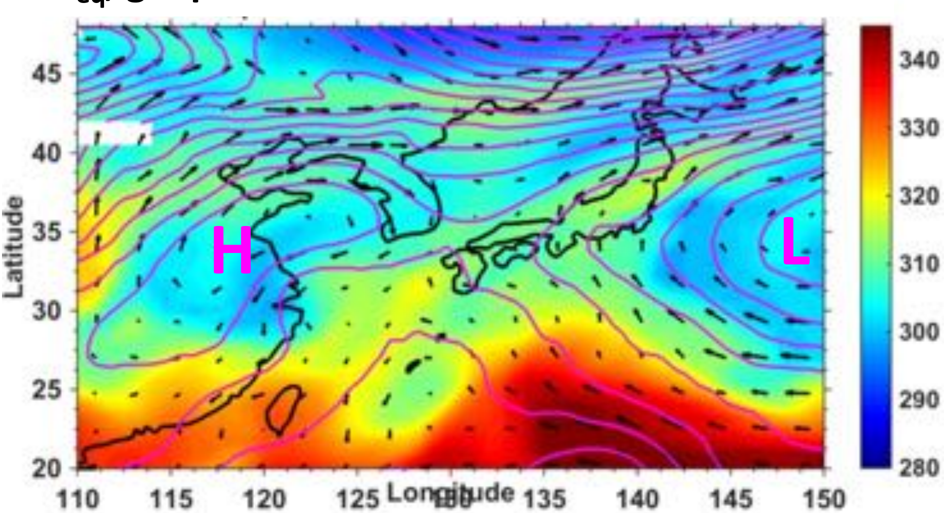
IASI+GOME2 ➔ O_3 at 2 to 3 km



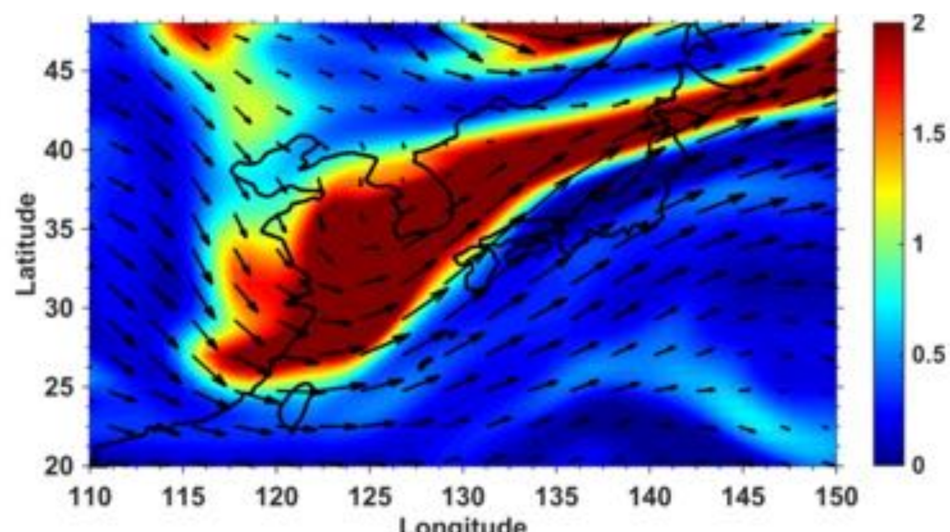
CO from IASI ➔ Anthropogenic tracer



Θ_{eq}, geopotential and winds at 850 hPa



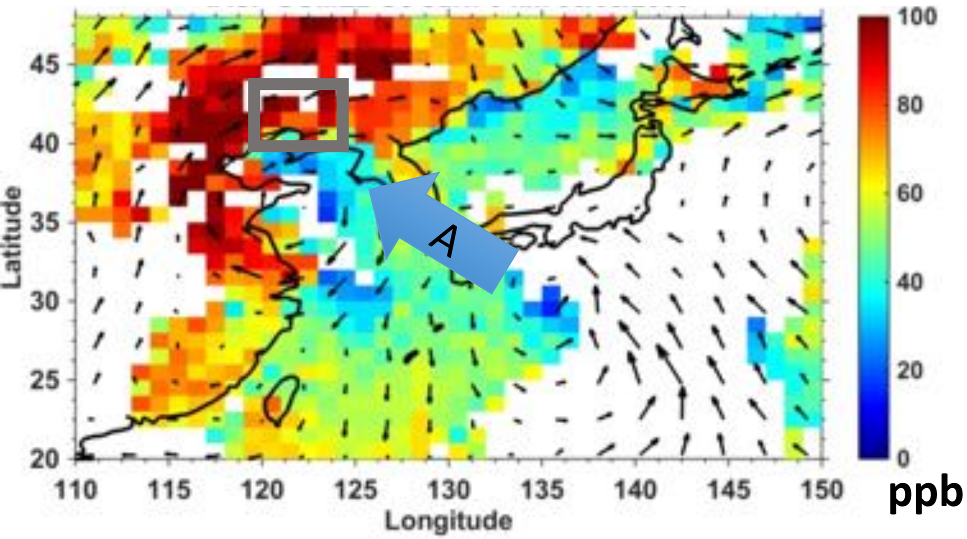
Potential vorticity at 300 hPa ➔ Stratosphere



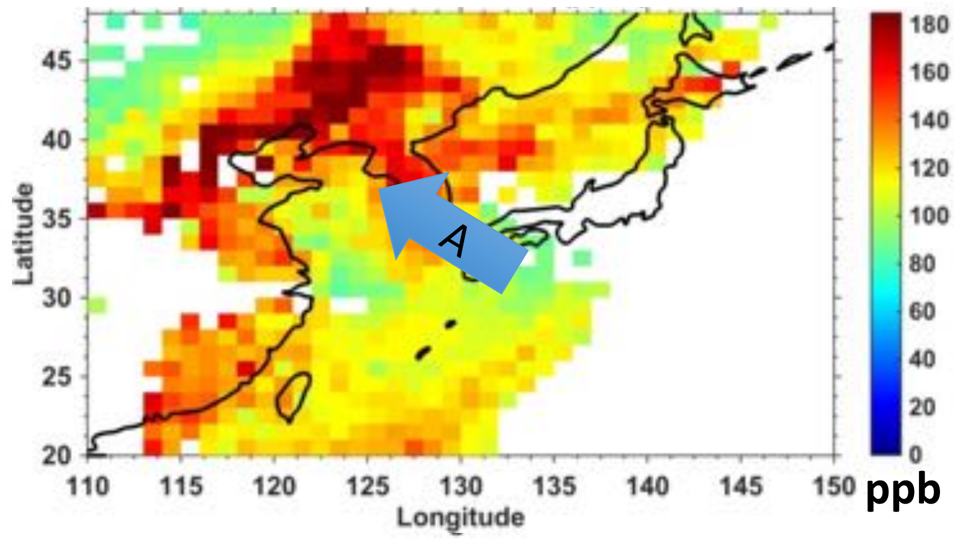
Ozone pollution over East Asia from IASI+GOME2

5 May 2009

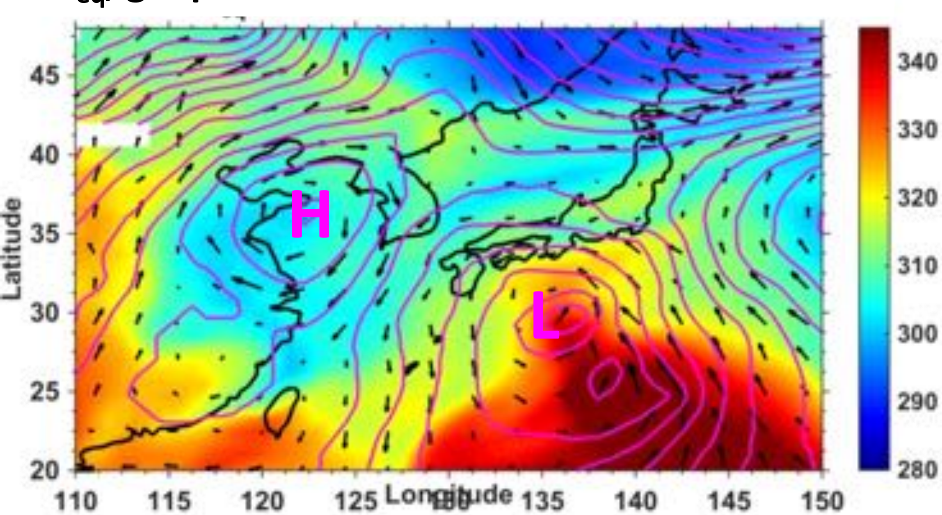
IASI+GOME2 ➔ O_3 at 2 to 3 km



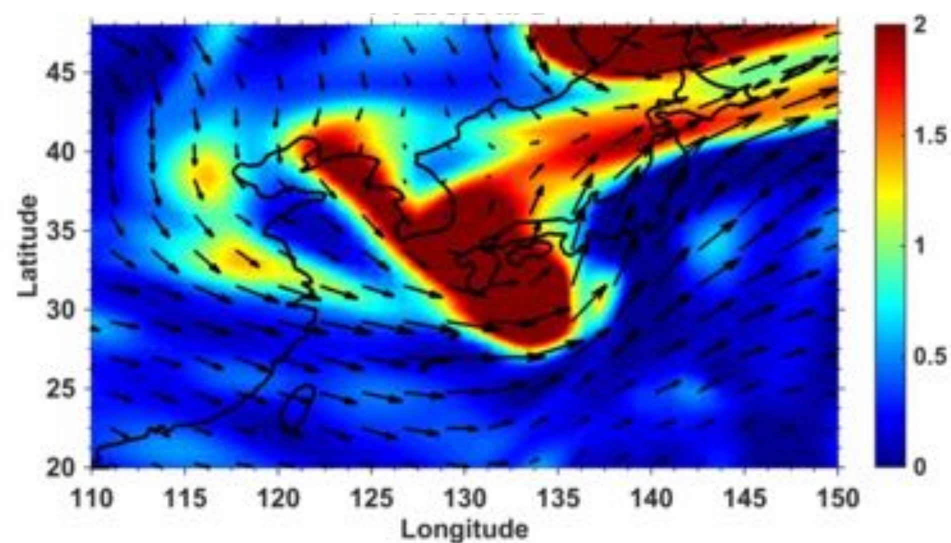
CO from IASI ➔ Anthropogenic tracer



Θ_{eq}, geopotential and winds at 850 hPa



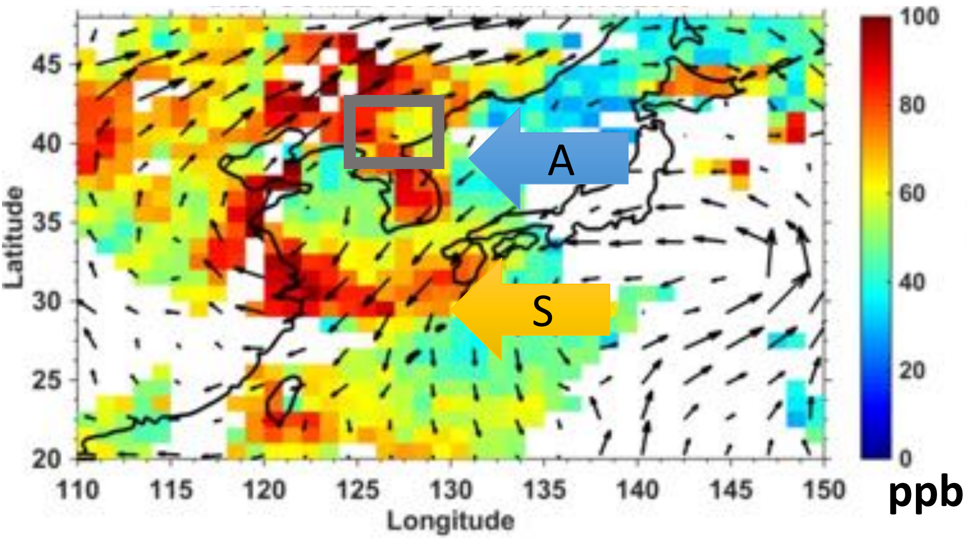
Potential vorticity at 300 hPa ➔ Stratosphere



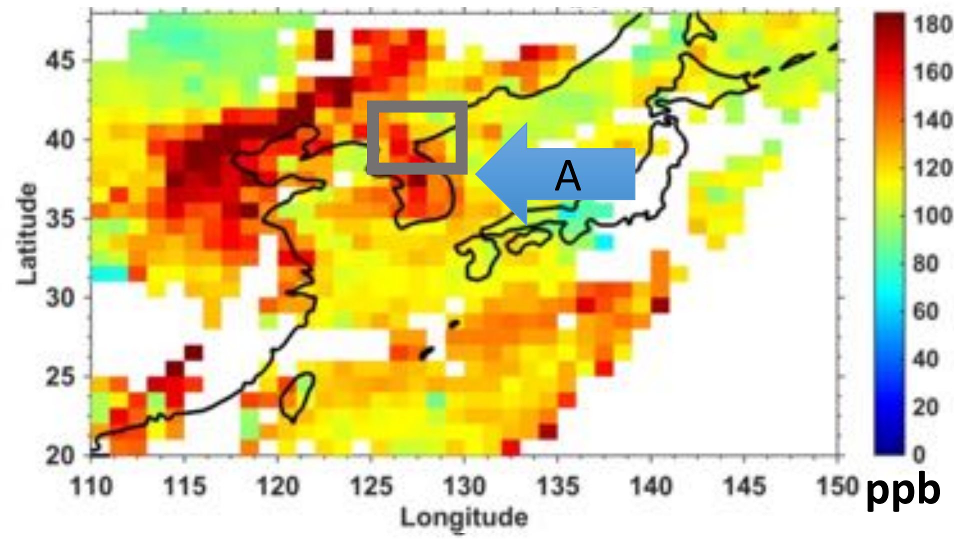
Ozone pollution over East Asia from IASI+GOME2

6 May 2009

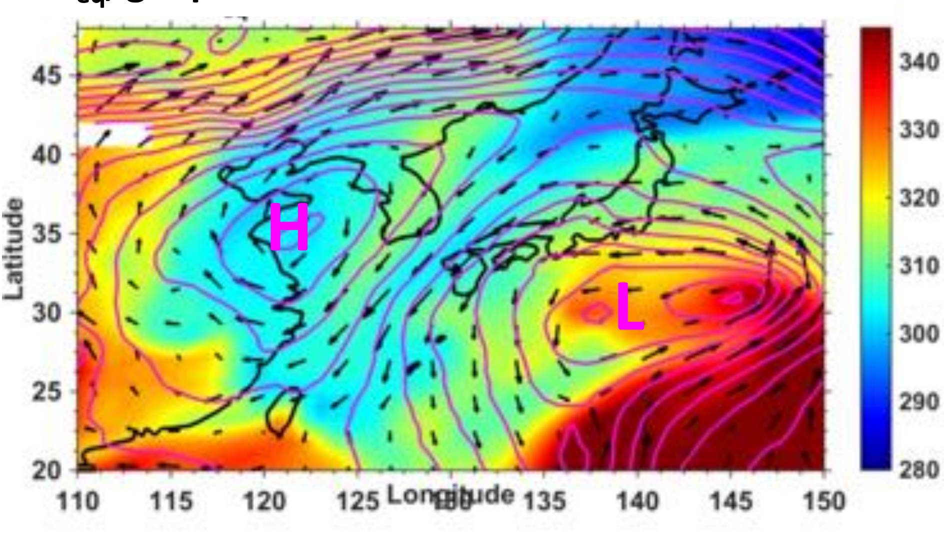
IASI+GOME2 ➔ O_3 at 2 to 3 km



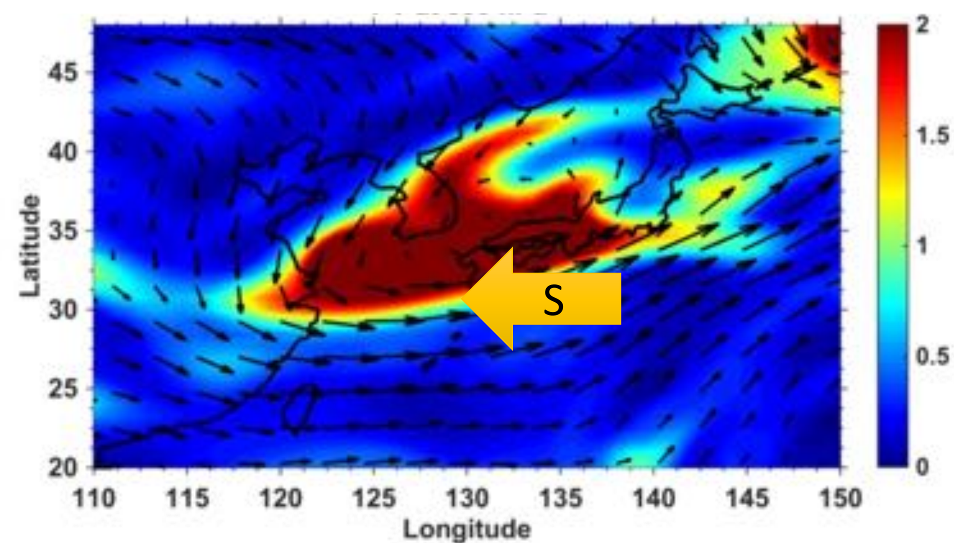
CO from IASI ➔ Anthropogenic tracer



Θ_{eq}, geopotential and winds at 850 hPa



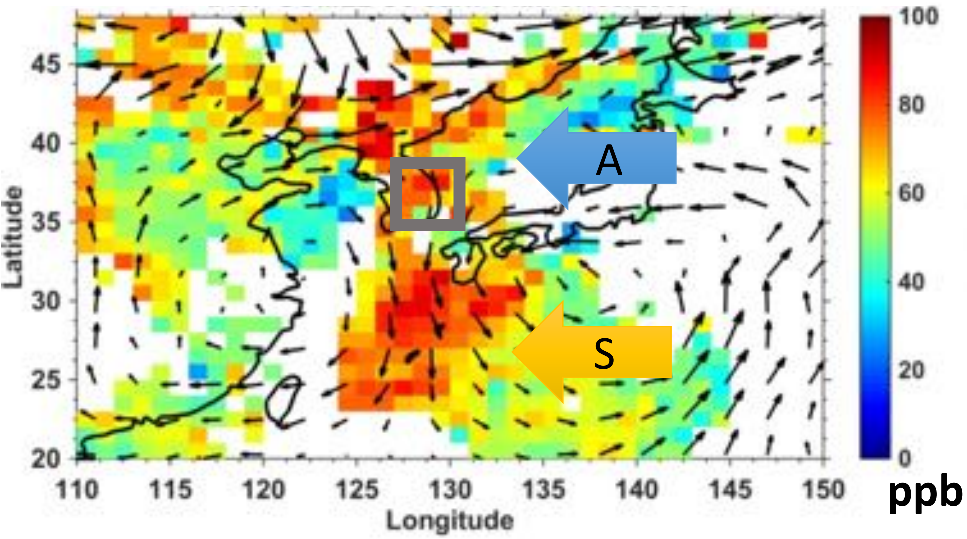
Potential vorticity at 300 hPa ➔ Stratosphere



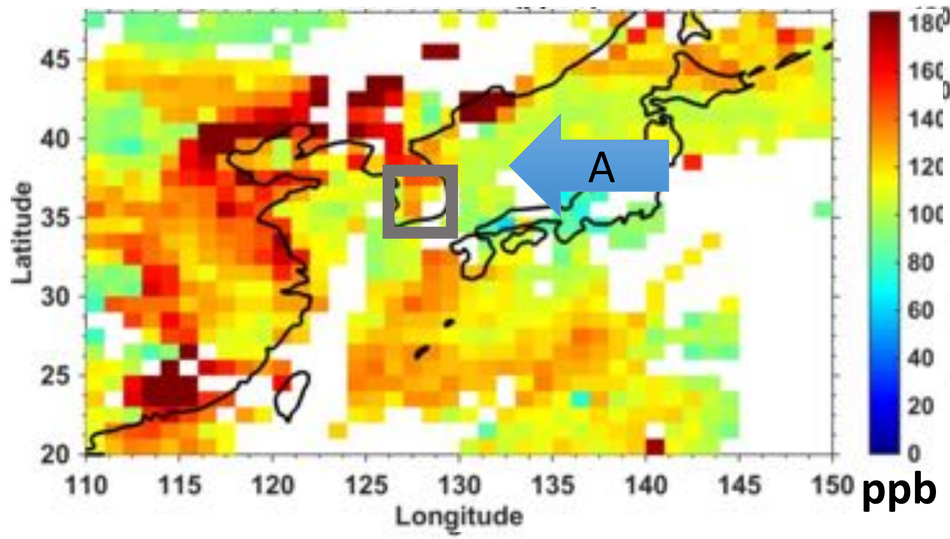
Ozone pollution over East Asia from IASI+GOME2

7 May 2009

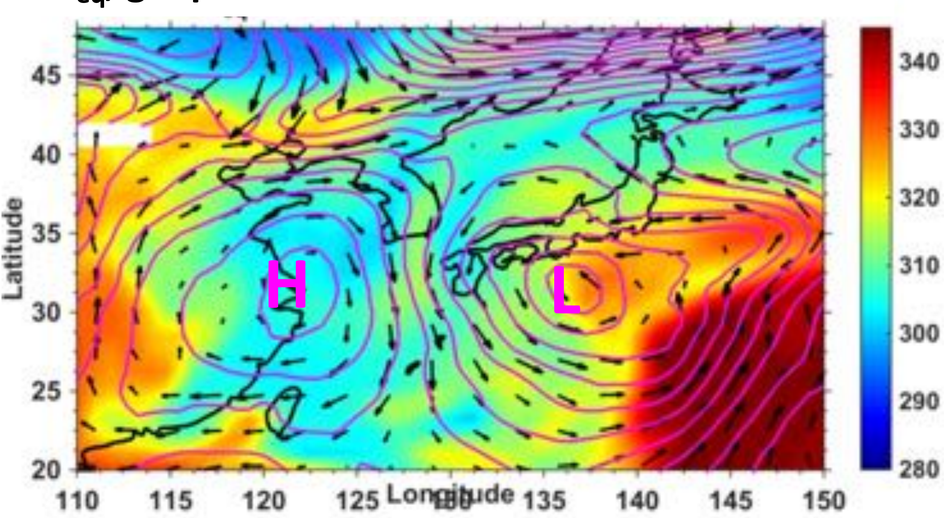
IASI+GOME2 ➔ O_3 at 2 to 3 km



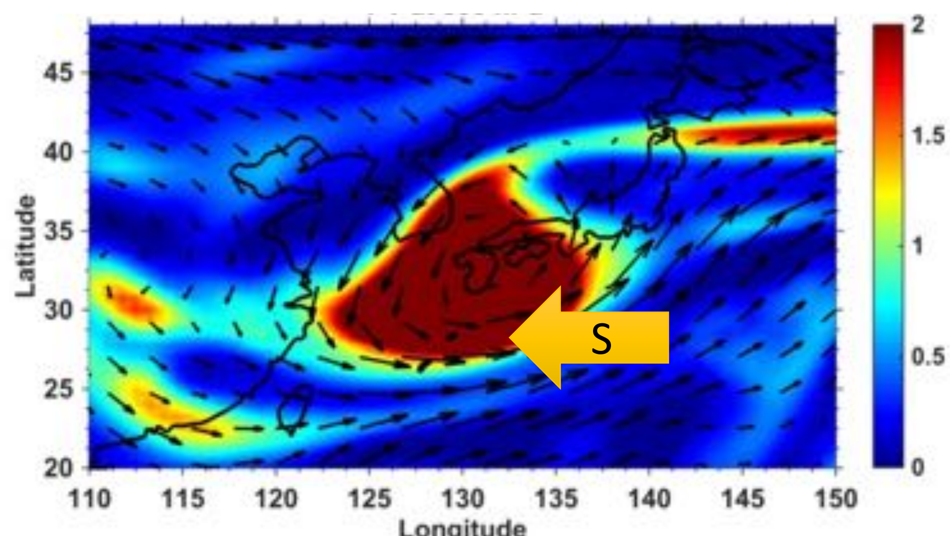
CO from IASI ➔ Anthropogenic tracer



Θ_{eq}, geopotential and winds at 850 hPa



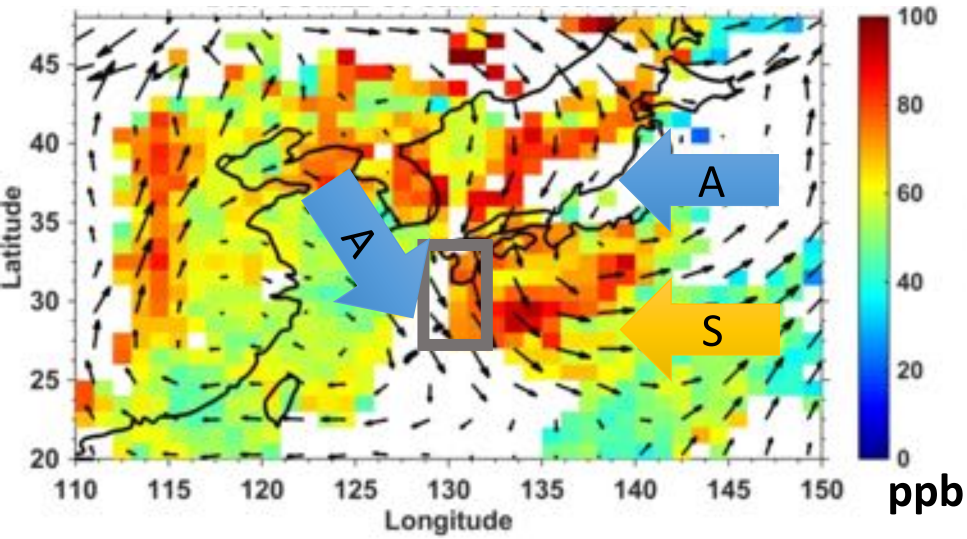
Potential vorticity at 300 hPa ➔ Stratosphere



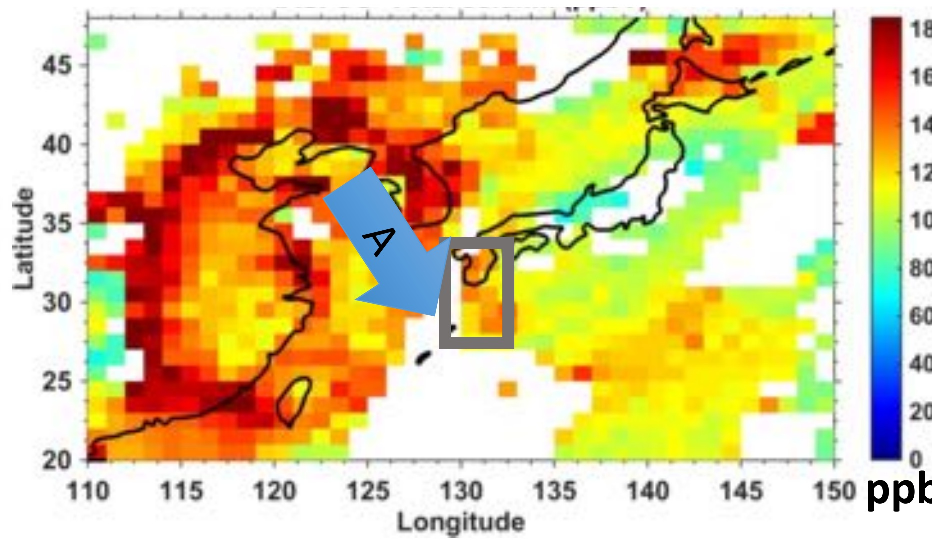
Ozone pollution over East Asia from IASI+GOME2

8 May 2009

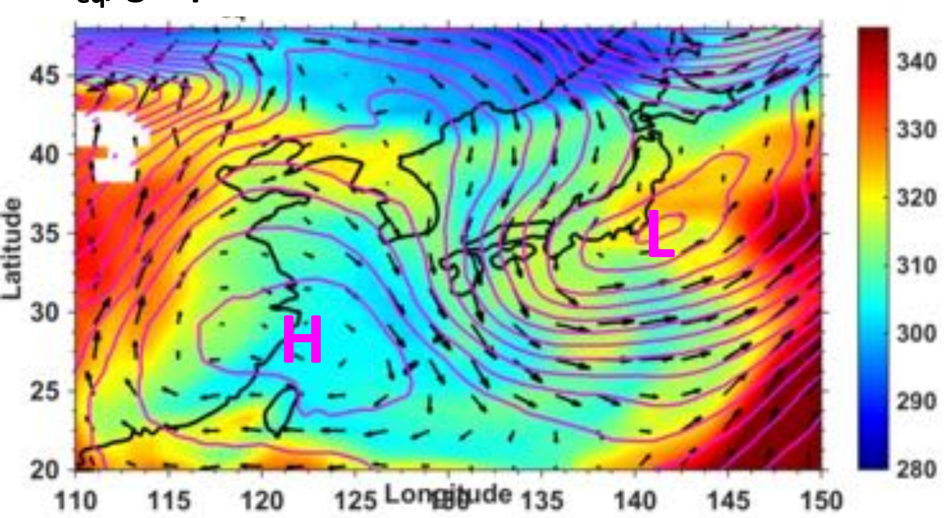
IASI+GOME2 ➔ O_3 at 2 to 3 km



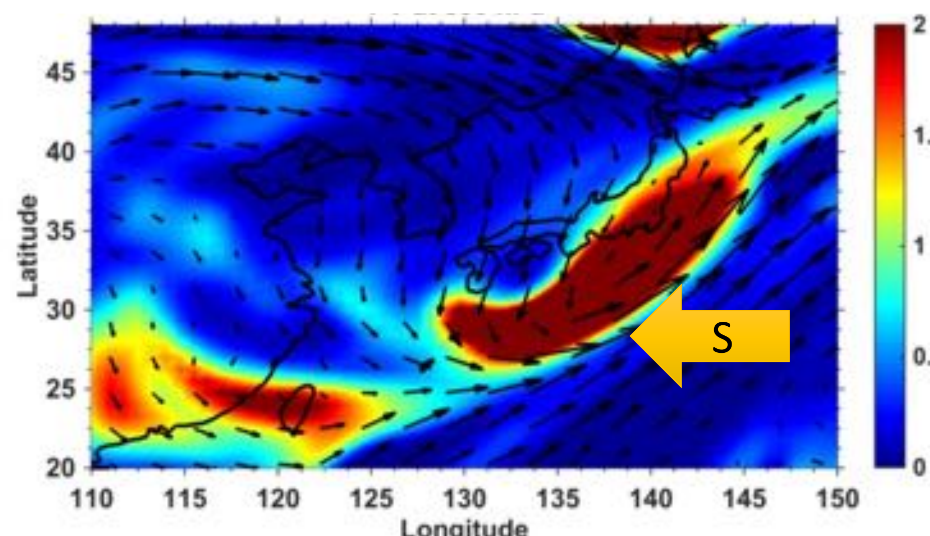
CO from IASI ➔ Anthropogenic tracer



Θ_{eq}, geopotential and winds at 850 hPa

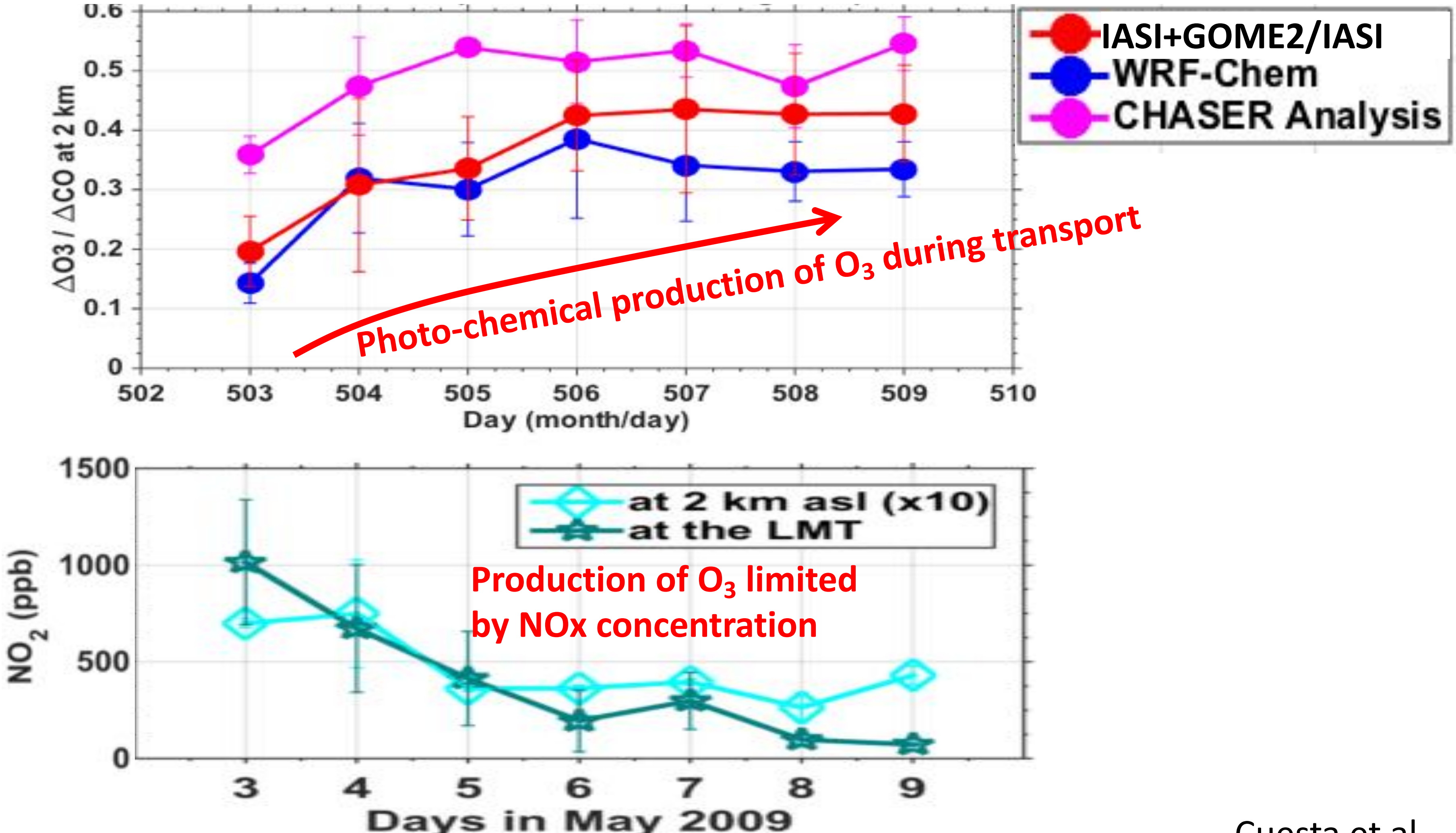


Potential vorticity at 300 hPa ➔ Stratosphere



Ozone pollution over East Asia from IASI+GOME2

ΔO_3 /ΔCO is the relative increase of O_3, accounting for air masses dispersion and considering CO as a passive tracer



Cuesta et al.

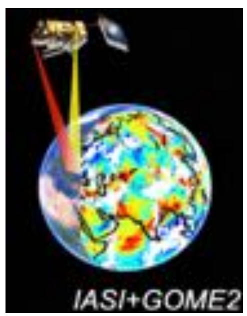
O_3 pollution over Europe during the COVID-19 lockdown of springtime 2020

[Cuesta et al. 2022 ACP]

- Quantify the impact of the COV-19 lockdown on ozone pollution over Europe
- Analyze the link with photochemical regimes : NOx-limited & VOC-limited

Which approach ?

➔Synergism of satellite observations, in-situ data and a chemistry-transport model



Chimere

The new multispectral satellite data
"**IASI+GOME2**"
➔Enhanced sensitivity to near-surface O_3

Approach to study the impact of COVID19 lockdown on ozone pollution

Complexity

➔ *Secondary pollutant with non-linear effects according to NOx-limited and VOC-limited regimes*

Observations → Satellite / In-situ

2020 vs 2019

Ambiguity on differences in meteorological conditions

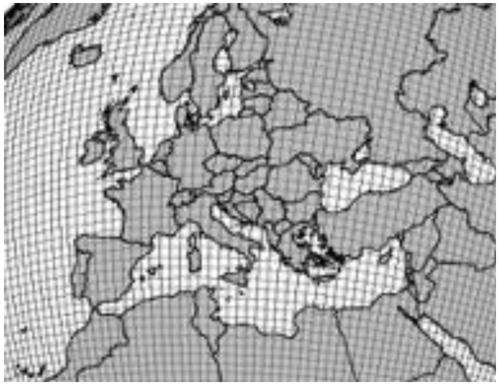
↕ Comparison & Adjustment for differences meteorological conditions

Chemistry-transport model

2020 (with reduced emissions COVID) vs 2020 (standard emissions)

Ambiguity on emissions during COVID lockdown

The chemistry-transport transport model **CHIMERE**



CHIMERE v2017 (Menut et al., 2020)

20 x 20 km^2 - 9 vertical levels

Anthropogenic emissions from HTAP v2.2

Meteorological fields from the BOLAM model

MEGAN biological emissions

COVID run :

↓ road traffic, ↓ industry, ↓ airplane & ship traffic (% from CAMS covid inventory)

April 2020 (COVID emissions), April 2020 (reference emissions) & April 2019

Model-derived COVID lockdown effect

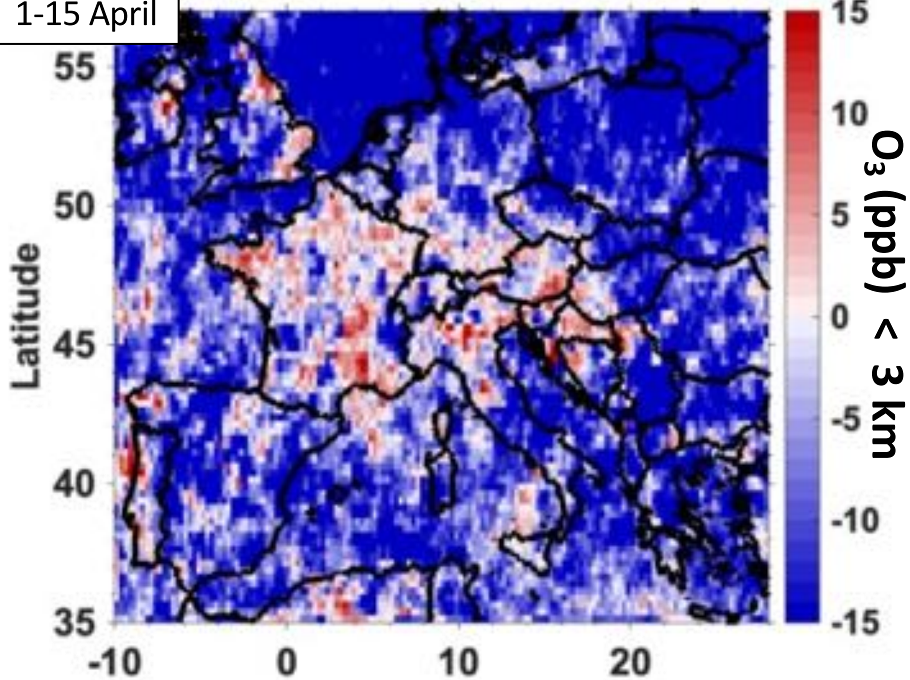
Δ Meteorology correction for observations

Satellite IASI+GOME2 vs Surface In situ

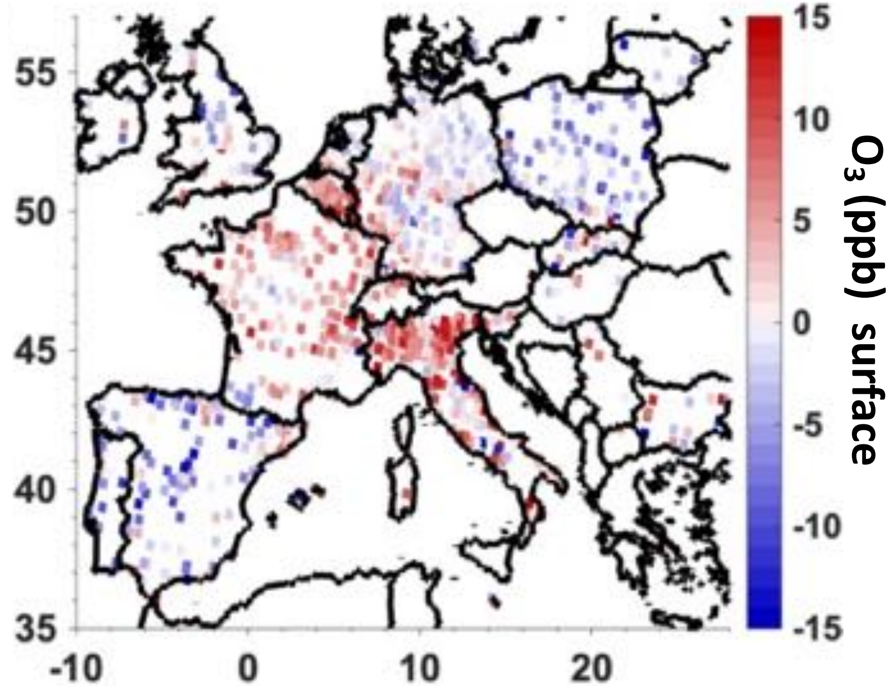
O_3 (2020) – O_3 (2019) ➔ Lockdown effect + ΔMeteorology

IASI+GOME2 satellite observation

1-15 April



In situ measurements at the surface



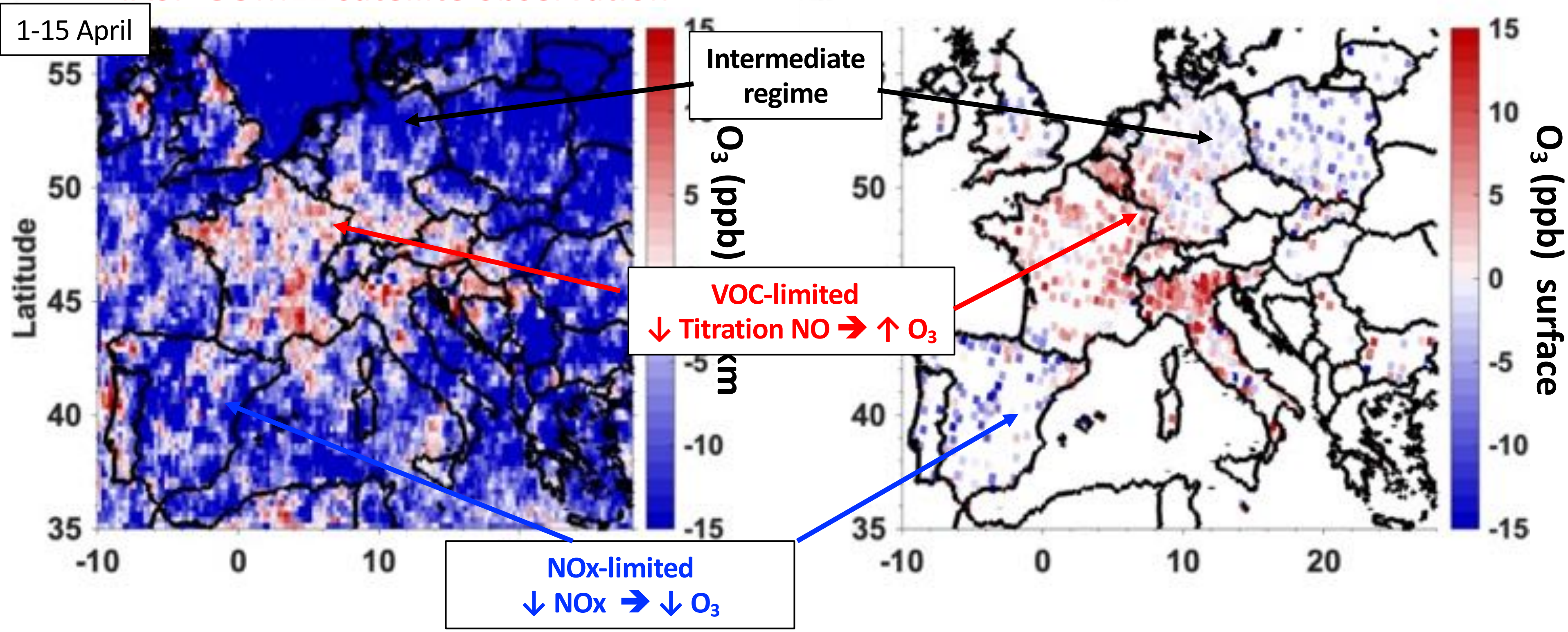
Agreement with regimes from Beekmann and Vautard, 2010

Good satellite/in situ agreement on spatial distribution and concentrations in absolute value!

Satellite IASI+GOME2 vs Surface In situ

O_3 (2020) – O_3 (2019) ➔ Lockdown effect + ΔMeteorology

IASI+GOME2 satellite observation | **In situ measurements at the surface**

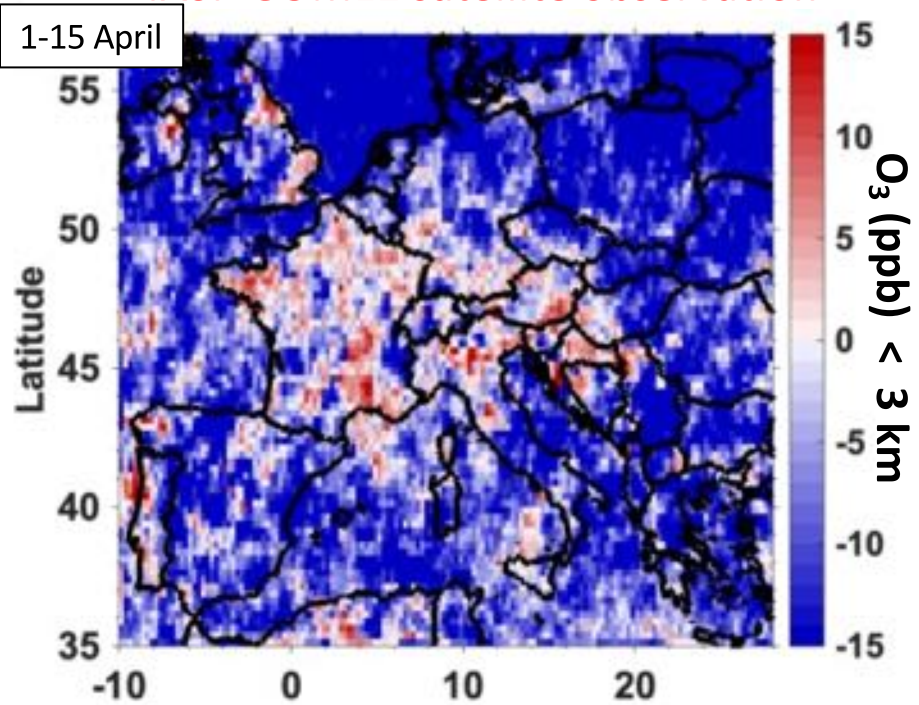


Clear signatures from VOC-limited & NOx-limited regimes from Beekmann and Vautard, 2010

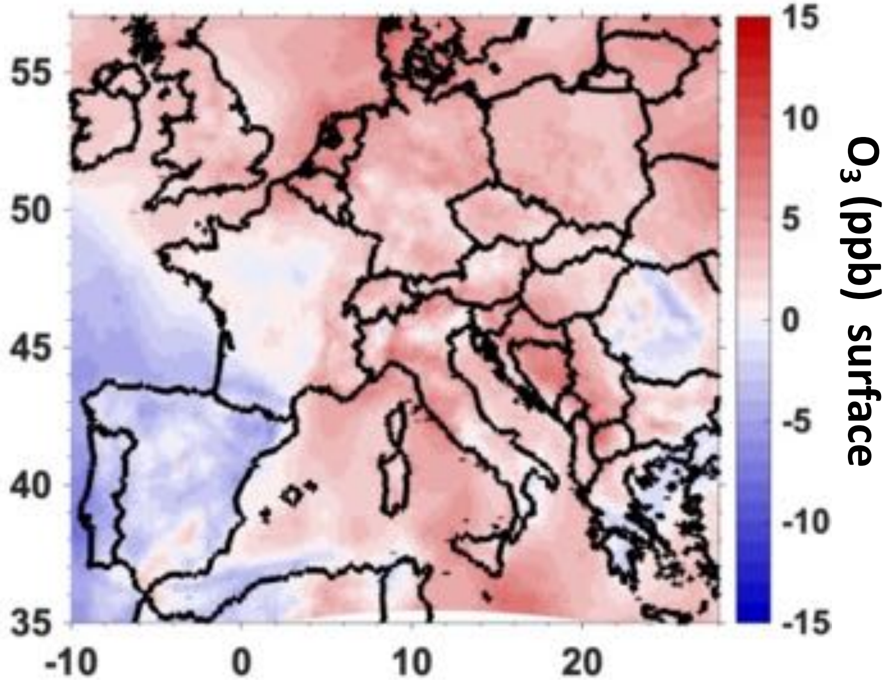
Satellite IASI+GOME2 vs CHIMERE model

O_3 (2020) – O_3 (2019) ➔ Lockdown effect + ΔMeteorology

IASI+GOME2 satellite observation



CHIMERE simulations



Not very clear signatures from VOC-limited & NOx-limited regimes

Estimation of the impact of the COVID-19 lockdown from models and observations

From the **CHIMERE model**

$$\Delta O_{3\,mod}^{\,covid} = O_{3\,mod_{COVID}}^{\,2020} - O_{3\,mod_{STD}}^{\,2020}$$

From **surface** & **satellite observations**

"business as usual" inventory

$$\Delta O_{3\,obs}^{\,covid} \approx O_{3\,obs}^{\,2020} - O_{3\,obs}^{\,2019} - \left(O_{3\,mod_{STD}}^{\,2020} - O_{3\,mod_{STD}}^{\,2019}\right)$$

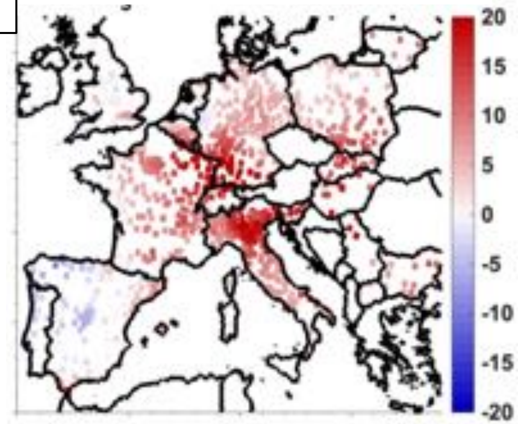
➔Adjustment for changes in meteorological conditions between 2020 and 2019 using model simulations

Impact of COVID-19 lockdown for Surface MDA8 O_3

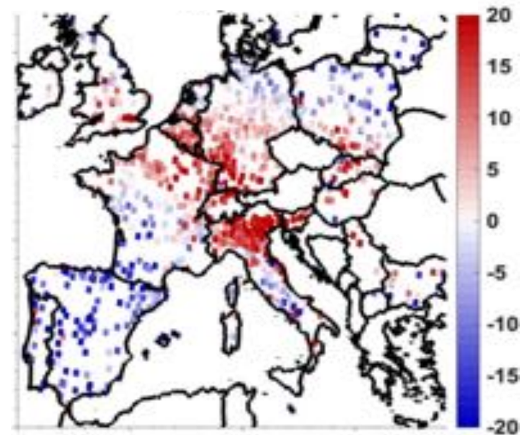
1-30 April

Our approach

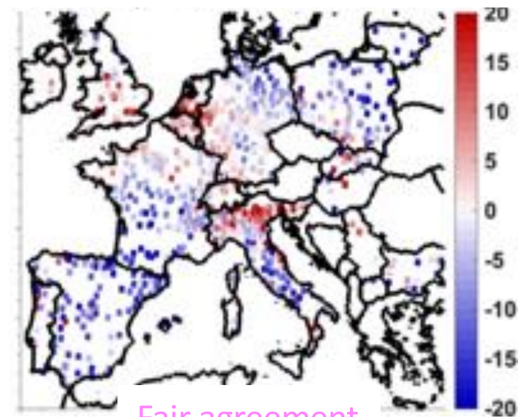
CHIMERE STD $\Delta O3^{2020\text{-}2019}$



In situ $\Delta O3^{2020\text{-}2019}$

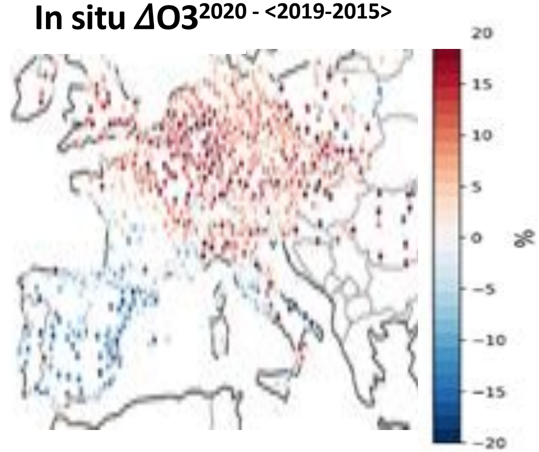


In situ $\Delta O3^{COVID}$ (meteo adjusted)

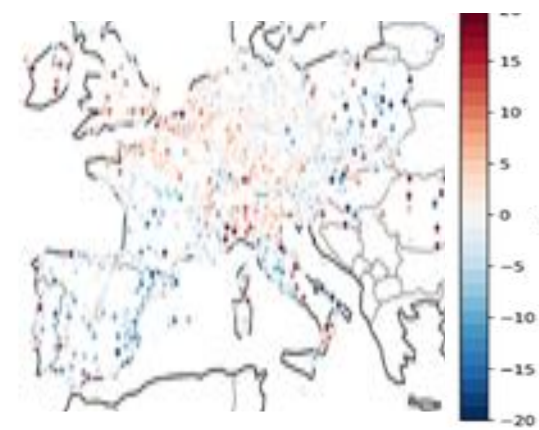


Fair agreement

In situ $\Delta O3^{2020\text{ - }<2019\text{-}2015>}$



In situ $\Delta O3^{COVID}$ (meteo adjusted)

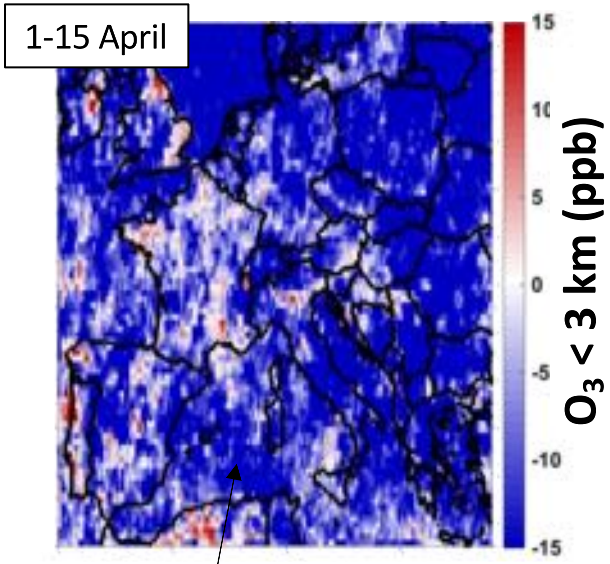


From Ordoñez et al., 2020
In situ surface
& statistical predictive model

COVID-19 lockdown impact on O_3 pollution

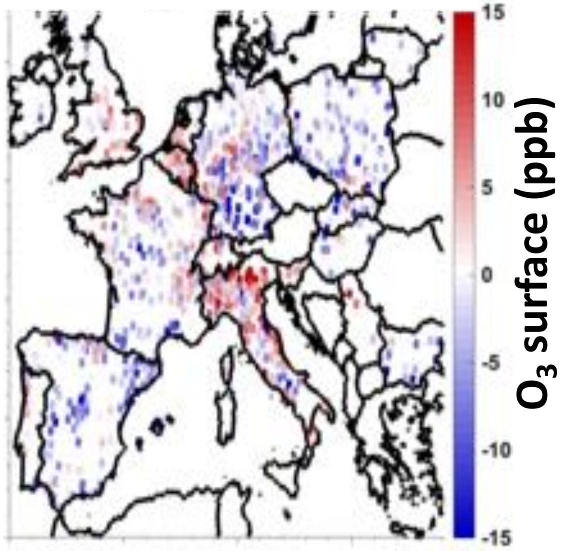
Satellite IASI+GOME2

Meteo-adjusted



In situ surface

Meteo-adjusted



Satellite/in situ fair agreement

NOx-limited

↓ NOx ➔ ↓ O_3

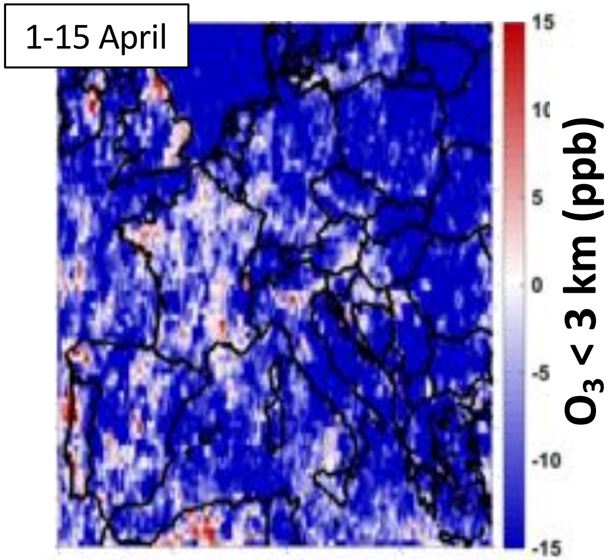
VOC-limited

↓ Titration NO ➔ ↑ O_3

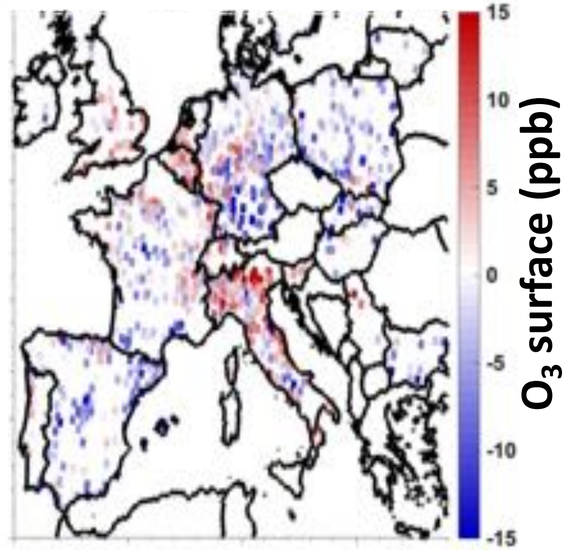
Large-scale reduction seen by ozone sondes & lidars in the free troposphere (Steinbrech et al., 2021)

COVID-19 lockdown impact on O_3 pollution

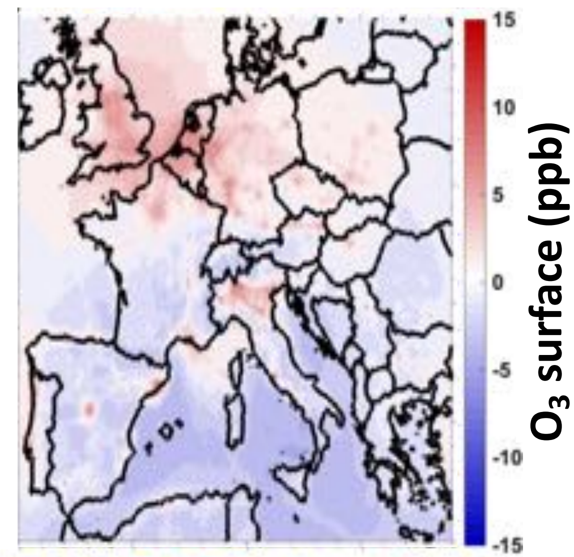
Satellite IASI+GOME2
Meteo-adjusted



In situ surface
Meteo-adjusted



CHIMERE model
COVID-STD

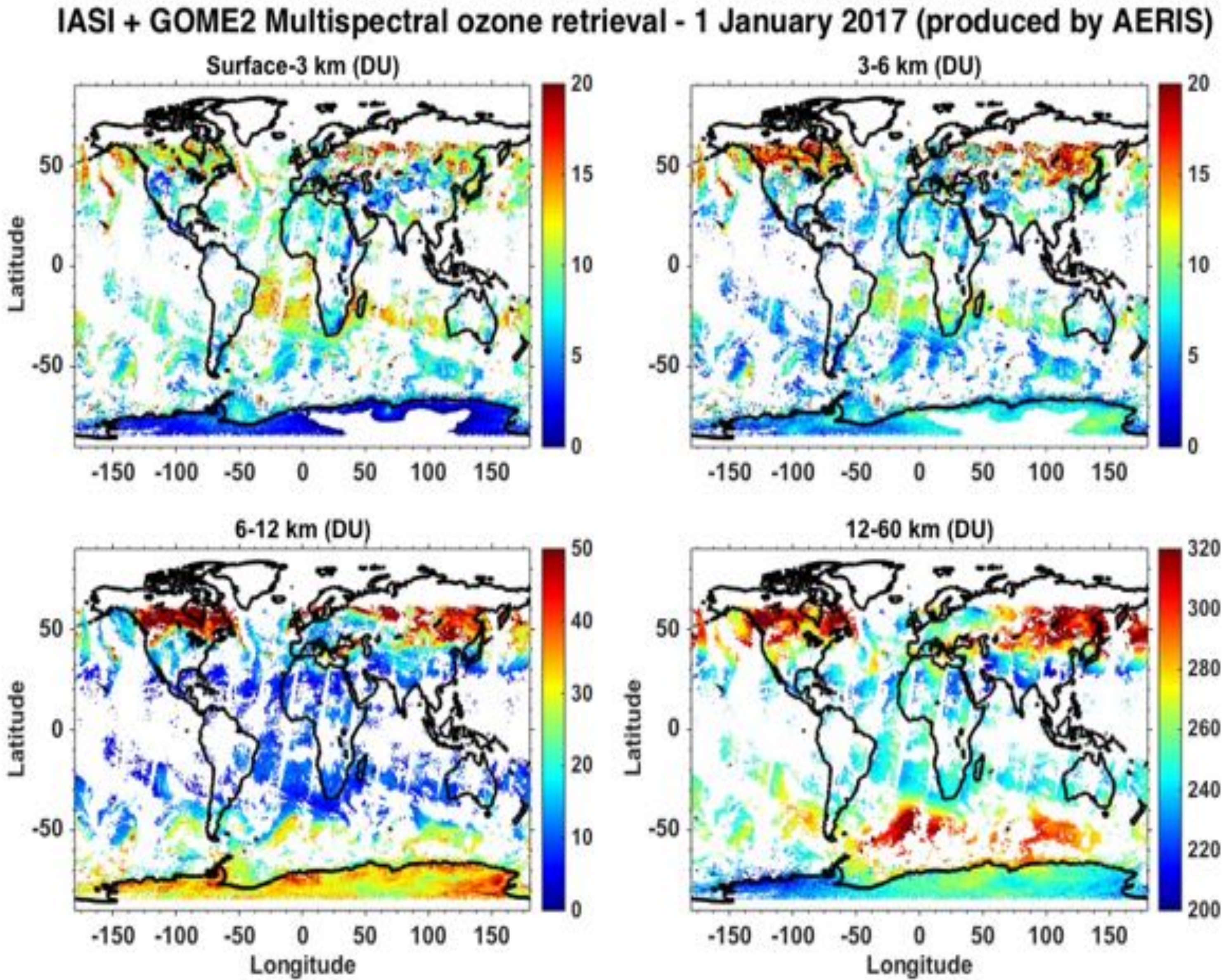


NOx-limited
↓ NOx ➔ ↓ O_3

VOC-limited
↓ Titration NO ➔ ↑ O_3

Agreement over France, Benelux and Italy.
The ***model :*** ***➔ underestimates the accumulation of O_3 over the Po Valley***
➔ overestimates that over Germany and Poland
➔ Misses the large-scale reduction

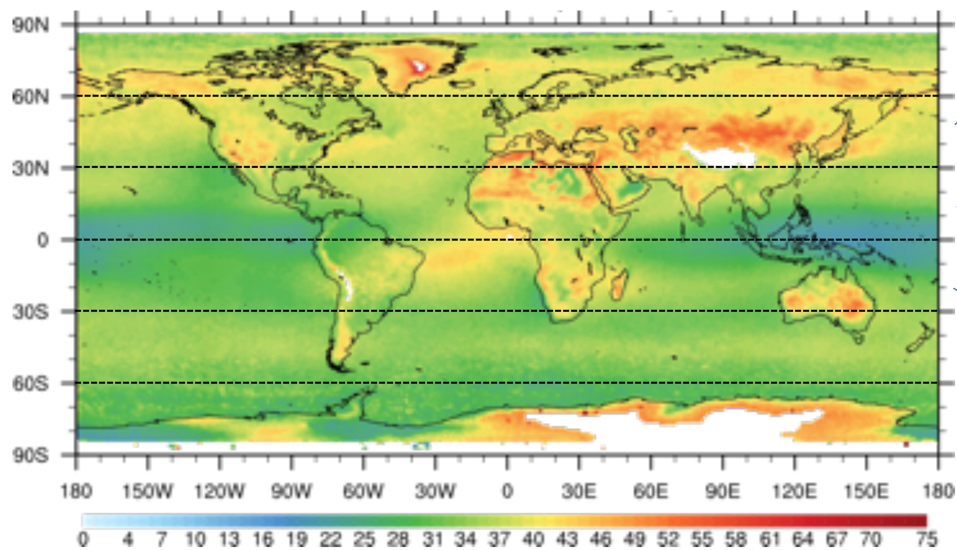
Global production and distribution of IASI+GOME2 multispectral satellite observations starting in 2017
http://www.aeris-data.fr



Multi-annuel evolution of O_3 pollution at global scale

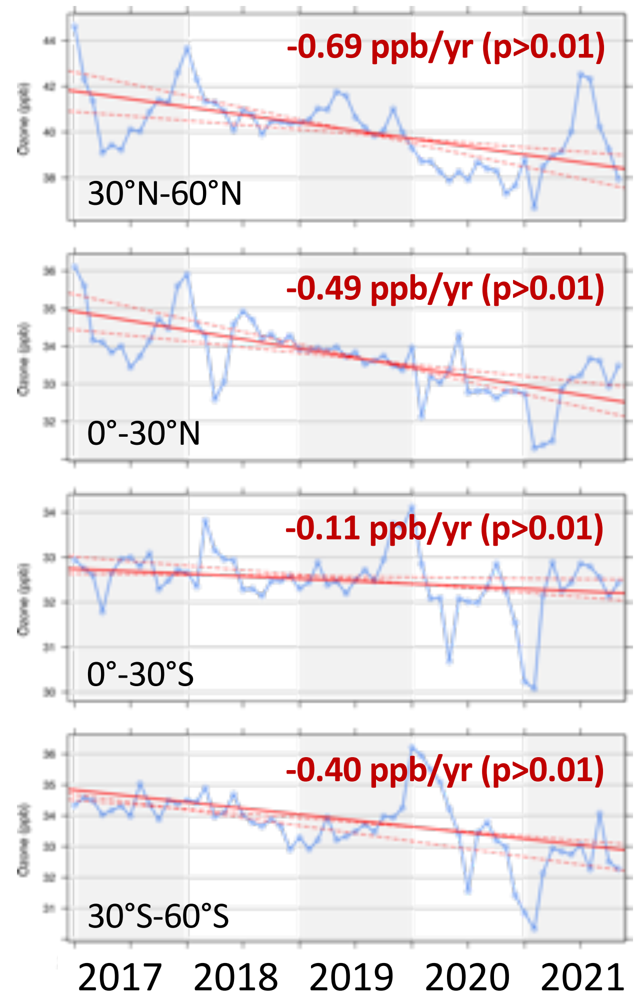
➔ **5 years** of global IASI+GOME2 data at AERIS

IASI+GOME2 Ozone from surface to 3 km a.s.l. (2017-2021)



Global decreasing trend, especially at middle latitude in Northern Hemisphere

Trend of Zonal Mean Ozone



Currently in production at TGCC/CEA … 2014 2015 2016

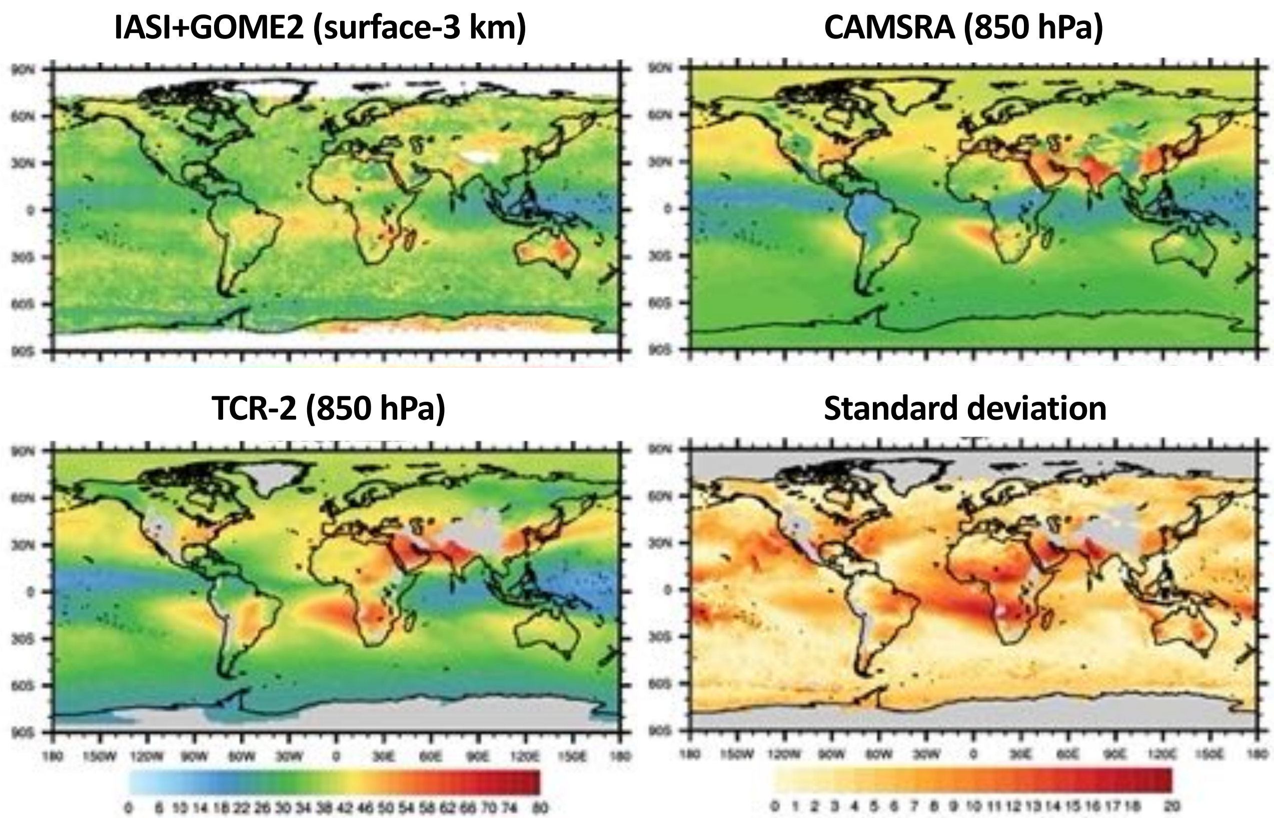
Global comparison : IASI+GOME2 vs Chemical reanalysis

<u>Chemical reanalysis</u>

- CAMSRA (Innes et al., 2019)
- TCR-2 (Miyazaki et al., 2020)

Global distribution is roughly similar but we can see some large standard deviation regions

September-October-November 2017

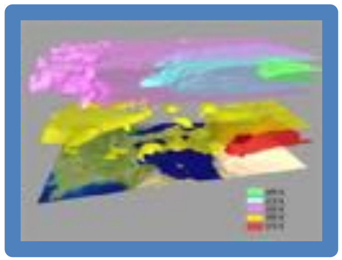


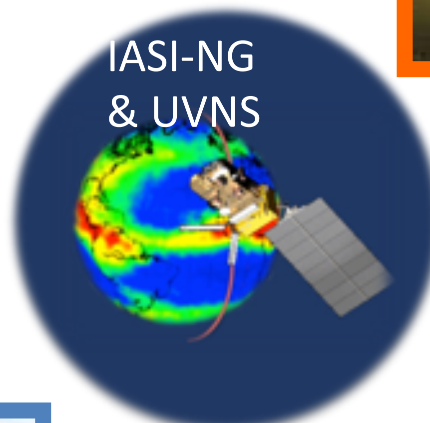
S.D. is calculated from the seasonal values of the three datasets

The future

- Upcoming satellite missions with better performances ➔ ESP-SG & MTG

Atmospheric profiling





Improvement on pollution forecast
3 EU controlled pollutants (CO, O_3 and NH_3)

Better tracking of long range pollution (e.g. fire emissions)

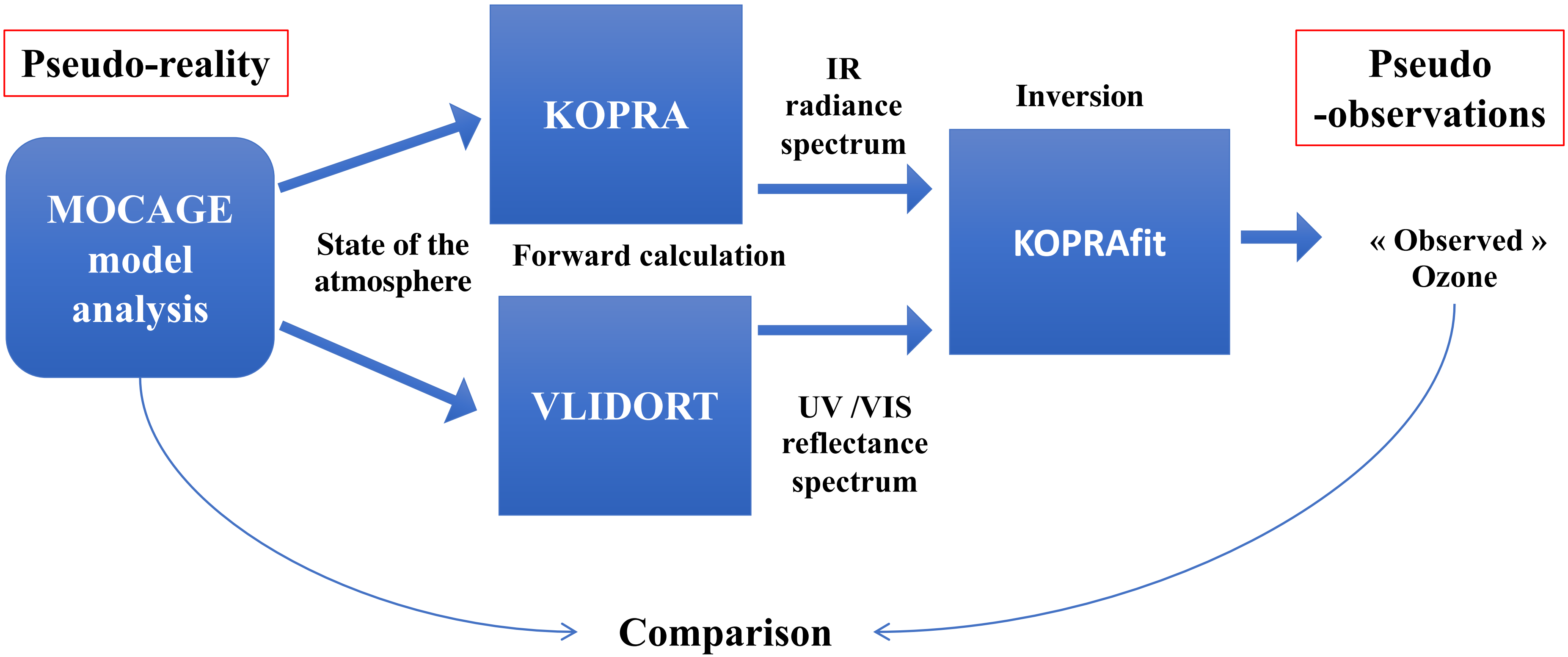
Essential Climate Variables monitoring and understanding
Clouds, GHG, aerosols

Improved volcanoe alerts
Early alerts possible + SO_2 and ash tracking

For T, WV, O_3, CO, CO_2, etc : more information on the vertical.
For weak absorbers : improved detection limit + more species measured instead of detected

Pseudo-observation simulator

→ For quantifying the added values of future satellite observations



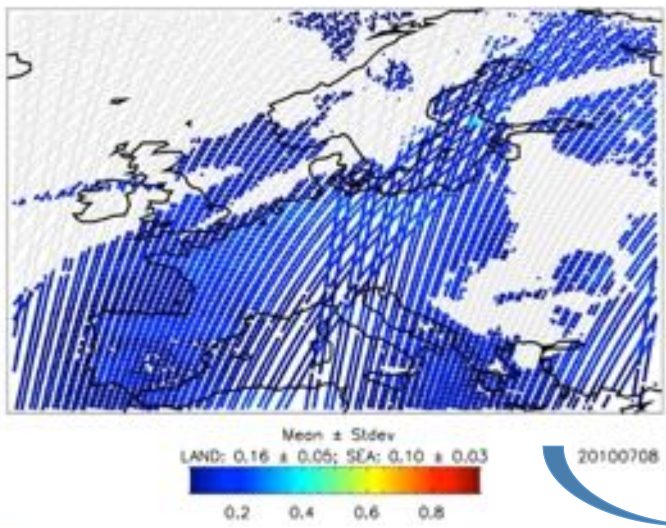
Sensitivity enhancement with IASI-NG+UVNS

IASI-NG ➔ ½ radiometric noise and ½ spectral resolution wrt IASI

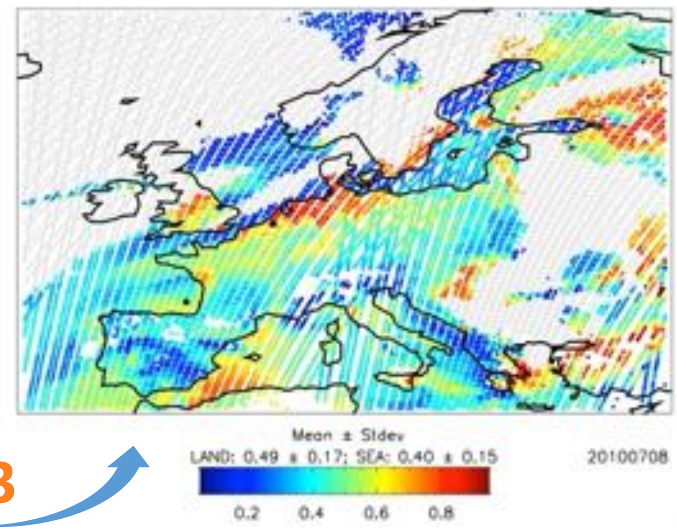
UVNS ➔ 1/3 radiometric noise and 2 x spectral resoluiton wrt GOME-2

IASI+GOME2 | IASI-NG+UVNS

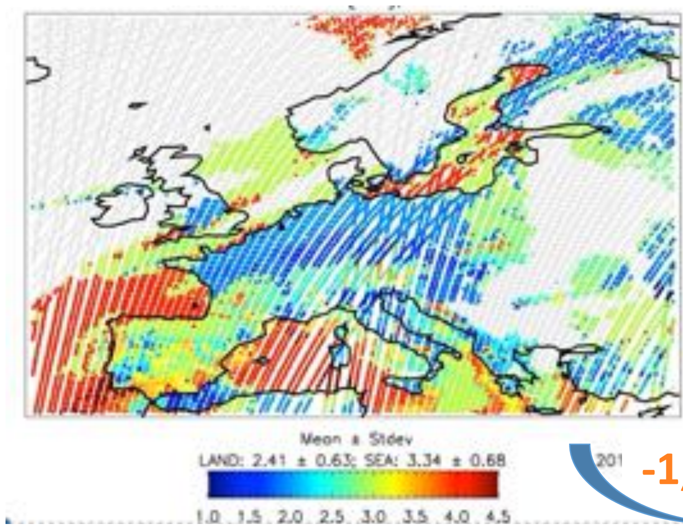
Degrees of freedom
DOF (surf.-2 km)



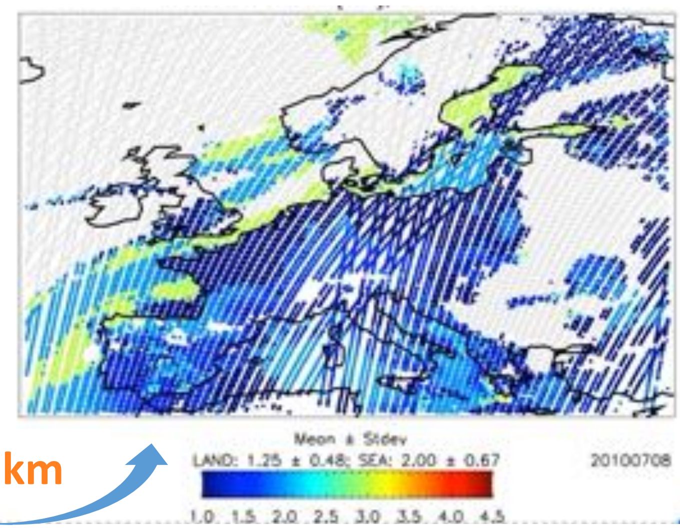
x3



Max. Sensitivity height
H^{max} (surf.-2 km)

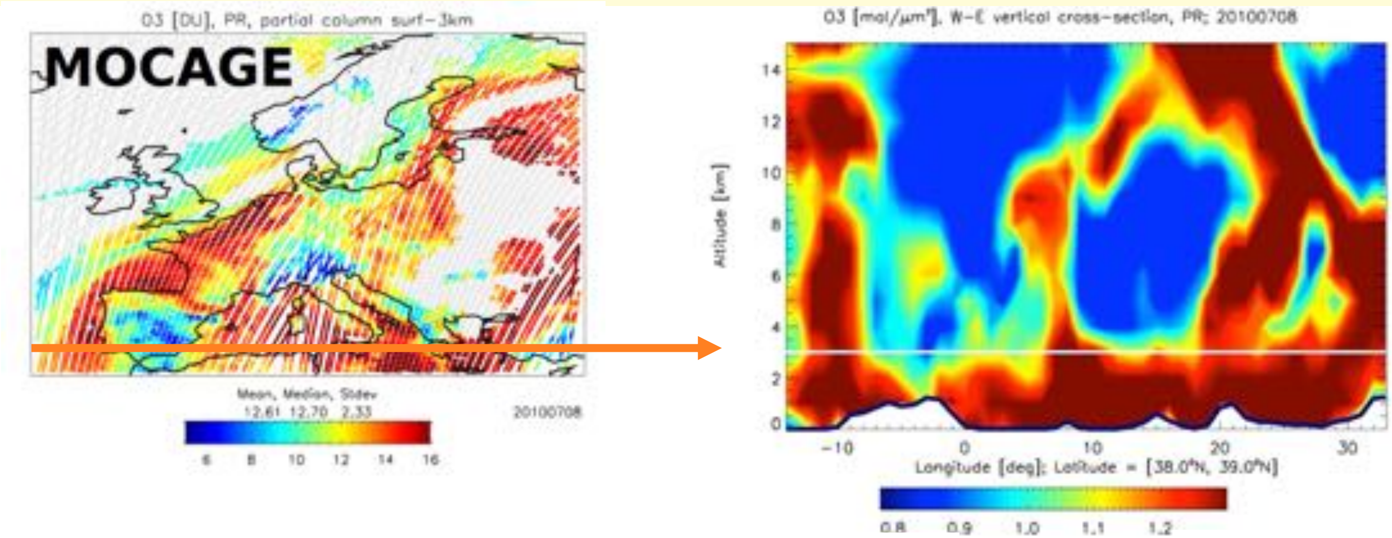


-1,2 km

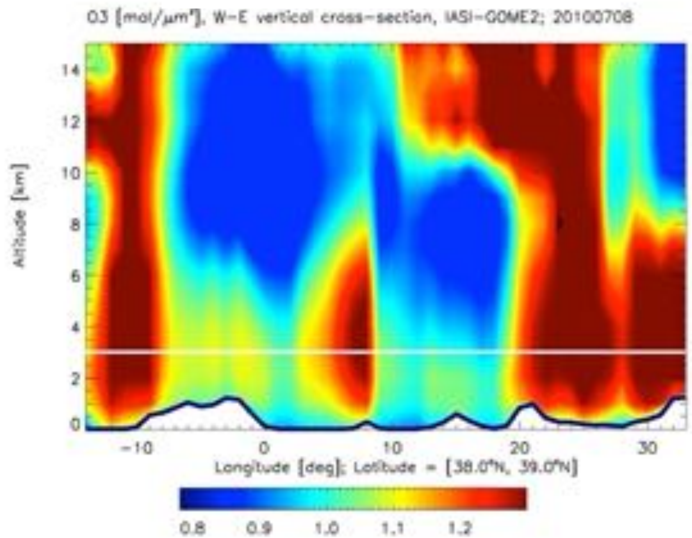


H^{max}_{land} = 1,25 km agl ➔ Air Quality !!

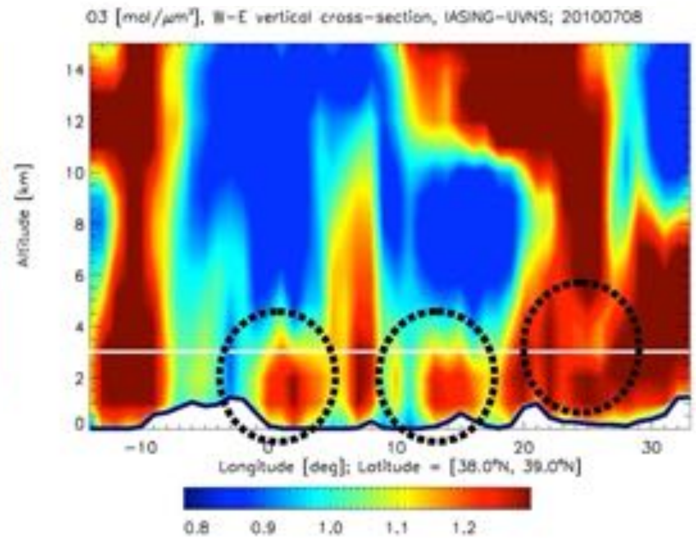
Observation of O3 pollution with IASI-NG+UVNS



IASI+GOME2



IASI-NG+UVNS



- O_3 plumes below 2 km of altitude
- Better vertical resolution

Some conclusions

- Spectrally-resolved satellite observation are widely used to study atmospheric chemistry and air pollution
- Retrieval approaches are designed for extracting the information on the 3D distribution of atmospheric constituents from spectra measured in the UV, Visible, IR and Microwaves
- The performance for deriving the atmospheric composition relies on:
  - ✓ The quality of the atmospheric measurements (calibration, resolution, knowledge of errors, etc.)
  - ✓ The quality of the "direct" model (**spectroscopy** databases, **physical representation of the atmosphere and surface**) → particularly for multispectral approaches
  - ✓ Appropriate constraints of the retrievals
- **Multispectral approaches** are promising tools for observing air pollution (sensitivity for lowest layers, 3D distributions, etc.)

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AERIS

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