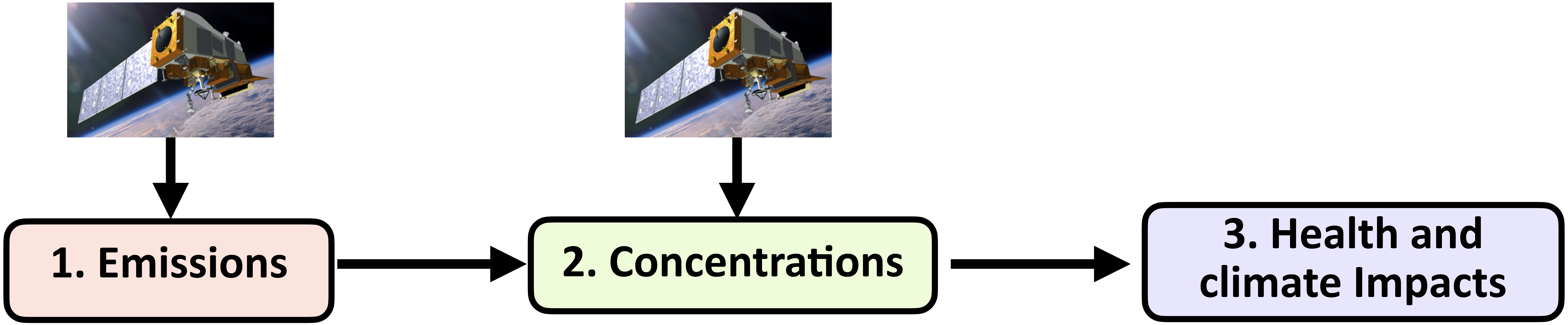
Jet Propulsion Laboratory
California Institute of Technology

Data assimilation applications of sounder composition products



Kazuyuki Miyazaki, Kevin Bowman, Vivienne Payne,
Jet Propulsion Laboratory, California Institute of Technology

What is the impact of IR soundings in regional and global models?

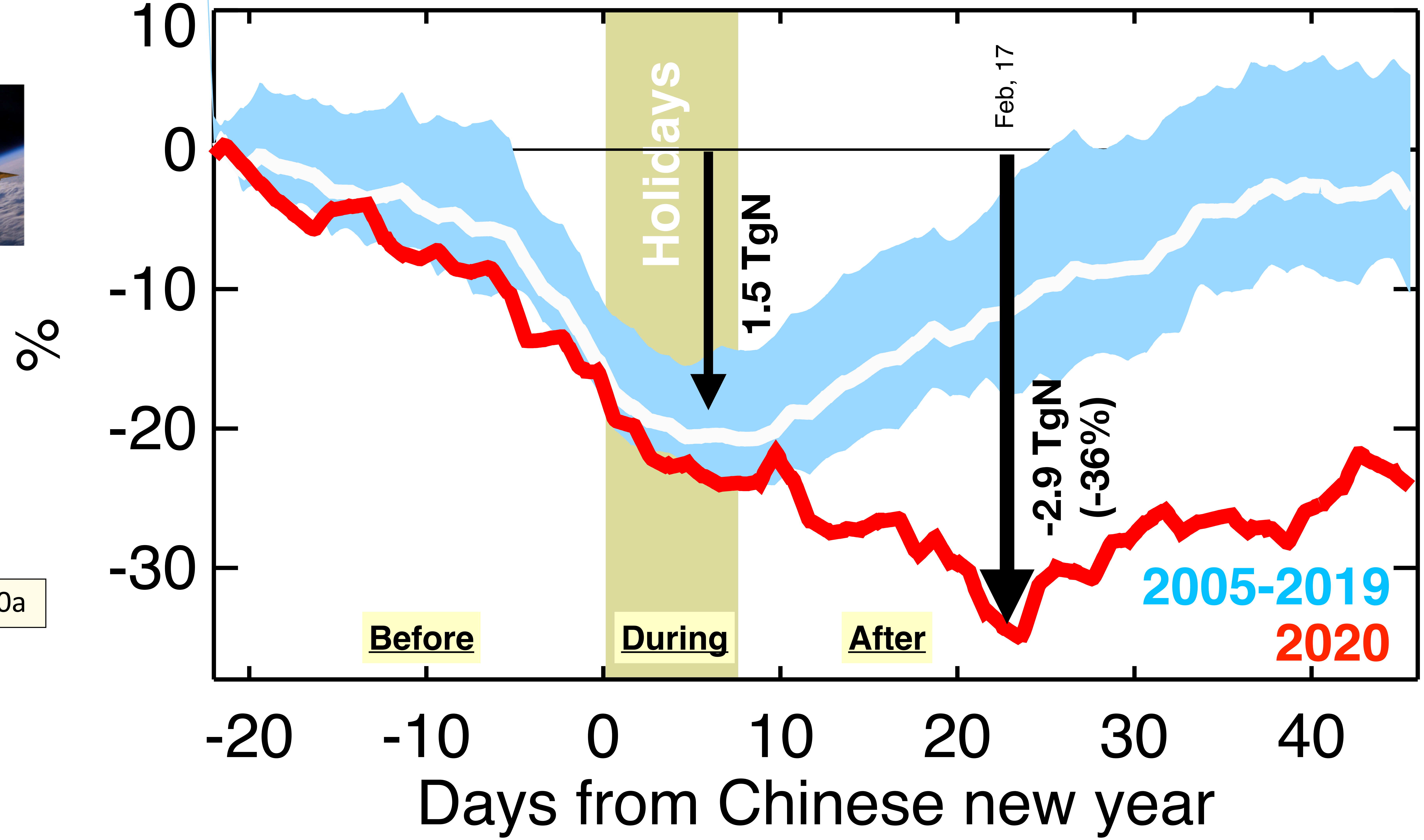
What is the optimum latency for regional and global models?

Impact of IR sounders on reanalysis for climate studies

Do you use IR soundings for both retrievals as well as direct assimilation in operations? How are retrievals used?

1. Emissions

Chinese NOx emissions

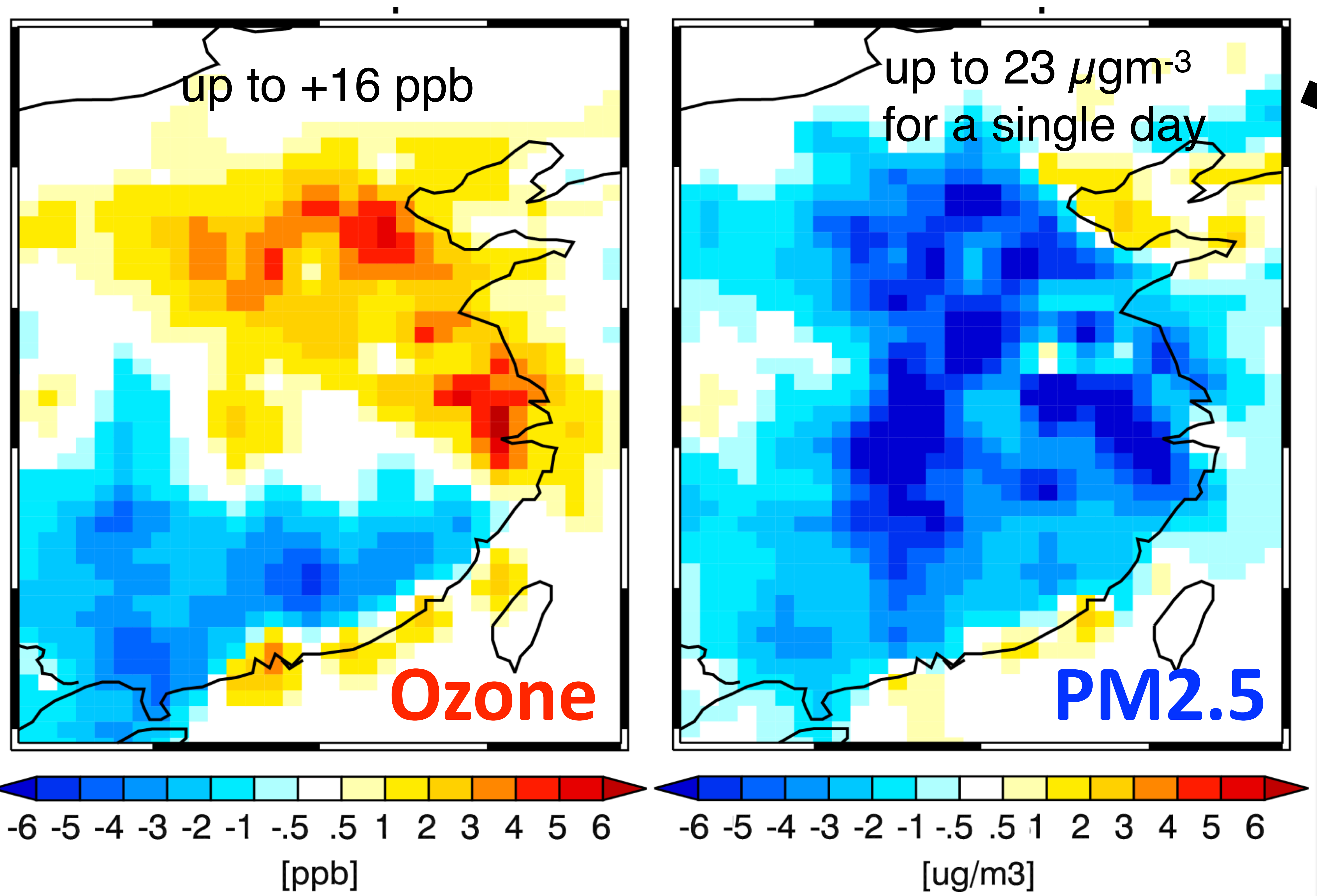


Miyazaki et al., 2020a

-3 TgN/yr = 10% of global total emissions

∼ Europe (4.1 TgN/yr), US (4.2 TgN/yr), India (3.4 TgN/yr)

MDA8 ozone and PM2.5 response to the COVID emission anomaly

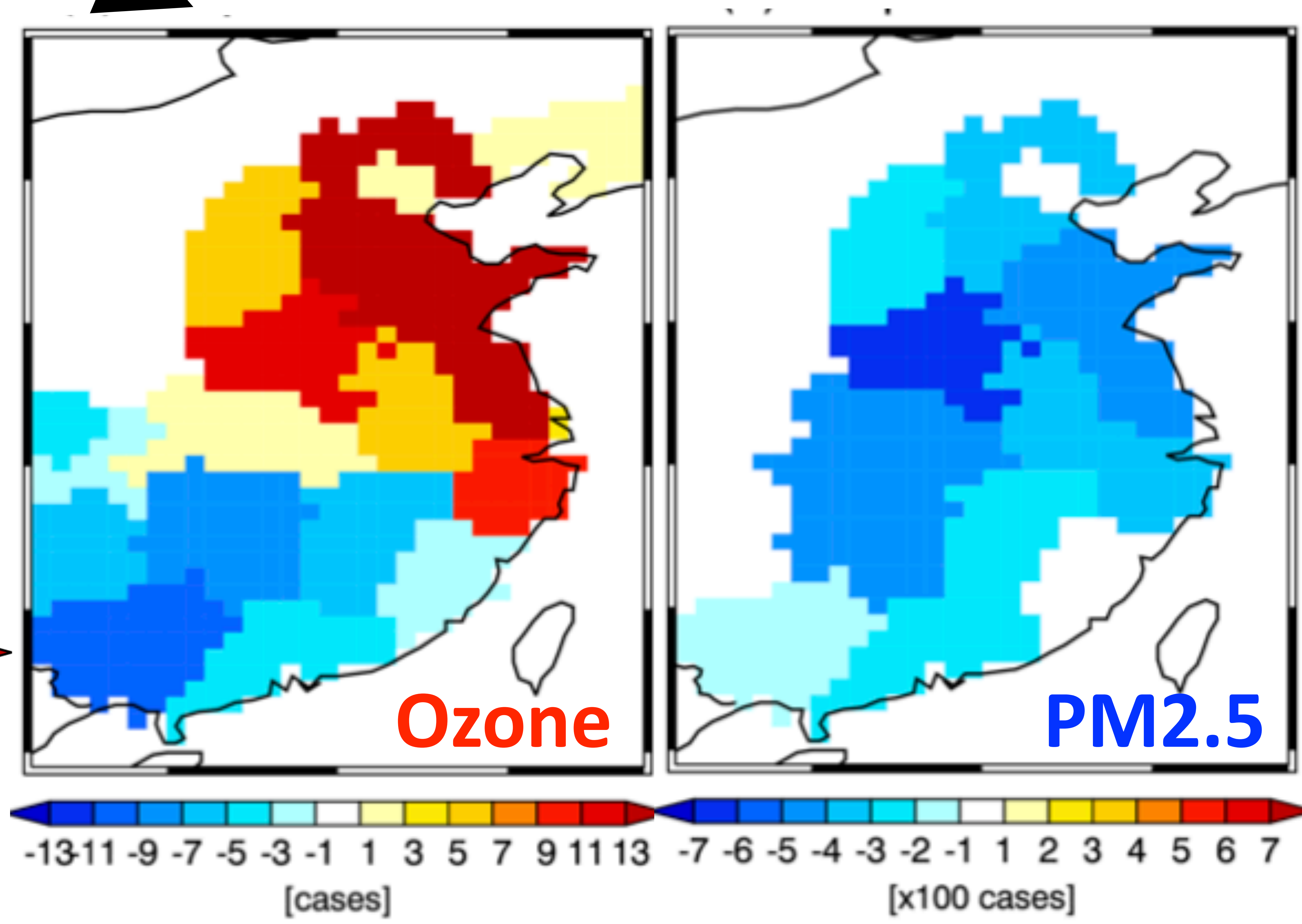


(Feb 15-25, 2020)

2. Concentrations

Miyazaki et al., 2020a

3. Health Impacts



- 2,100 more ozone-related and at least 60,000 fewer PM2.5-related morbidity incidences,
- Augmented efforts to reduce hospital admissions

MOMO-Chem (Multi-mOdel Multi-cOnstituent Chemical) Data Assimilation System

MLS

TES

OMI

MOPITT

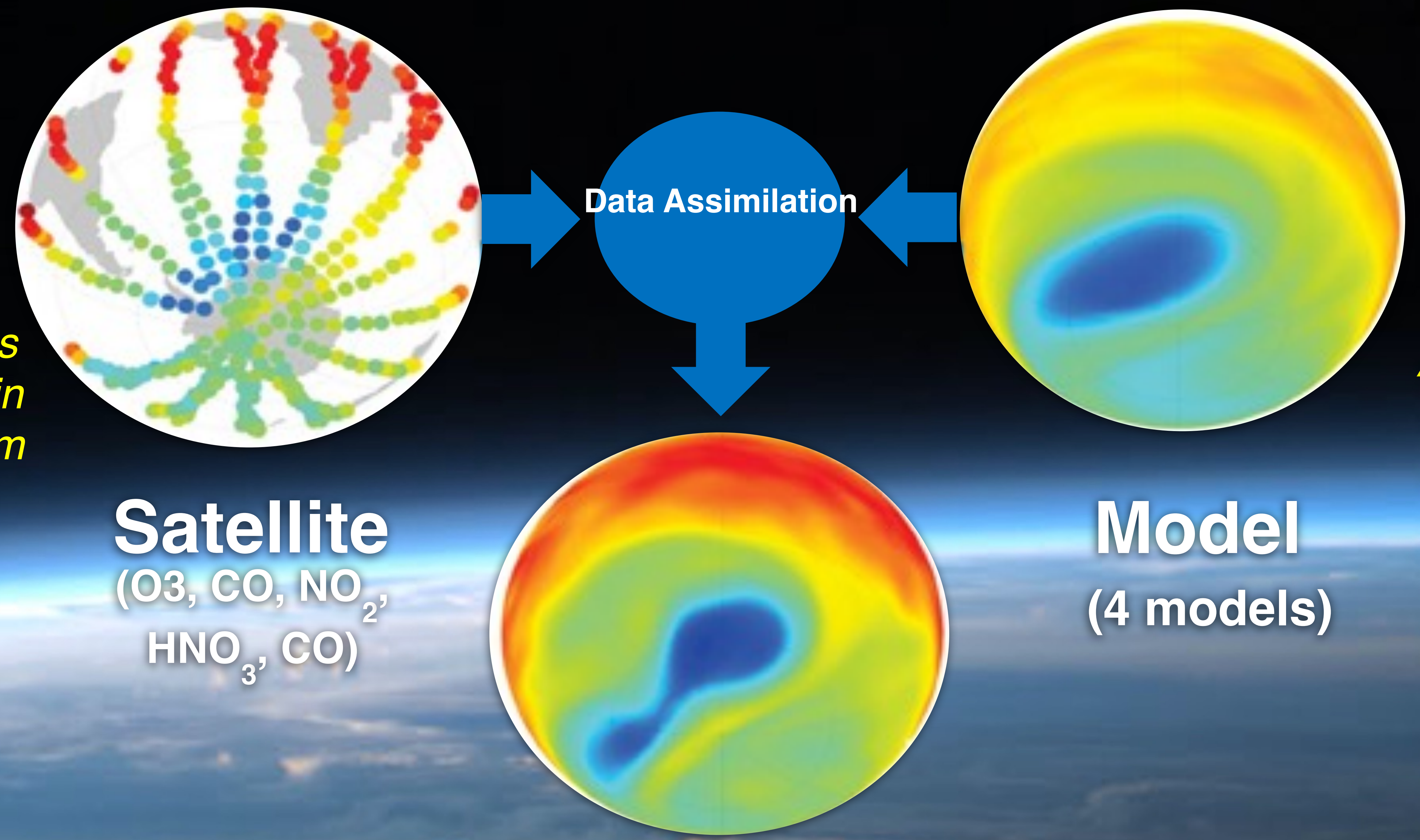
AIRS

SCIAMACHY

GOME-2

TROPOMI

Satellite Observations Assimilated in MOMO-Chem



Models Used for Assimilation

CHASER Chemistry Climate Model

MIROC-ESM

TCR

GEOS-Chem

Validation against in-situ & aircraft measurements

DISCOVER-AQ

KORUS-AQ

SEAC4RS

INTEX-B

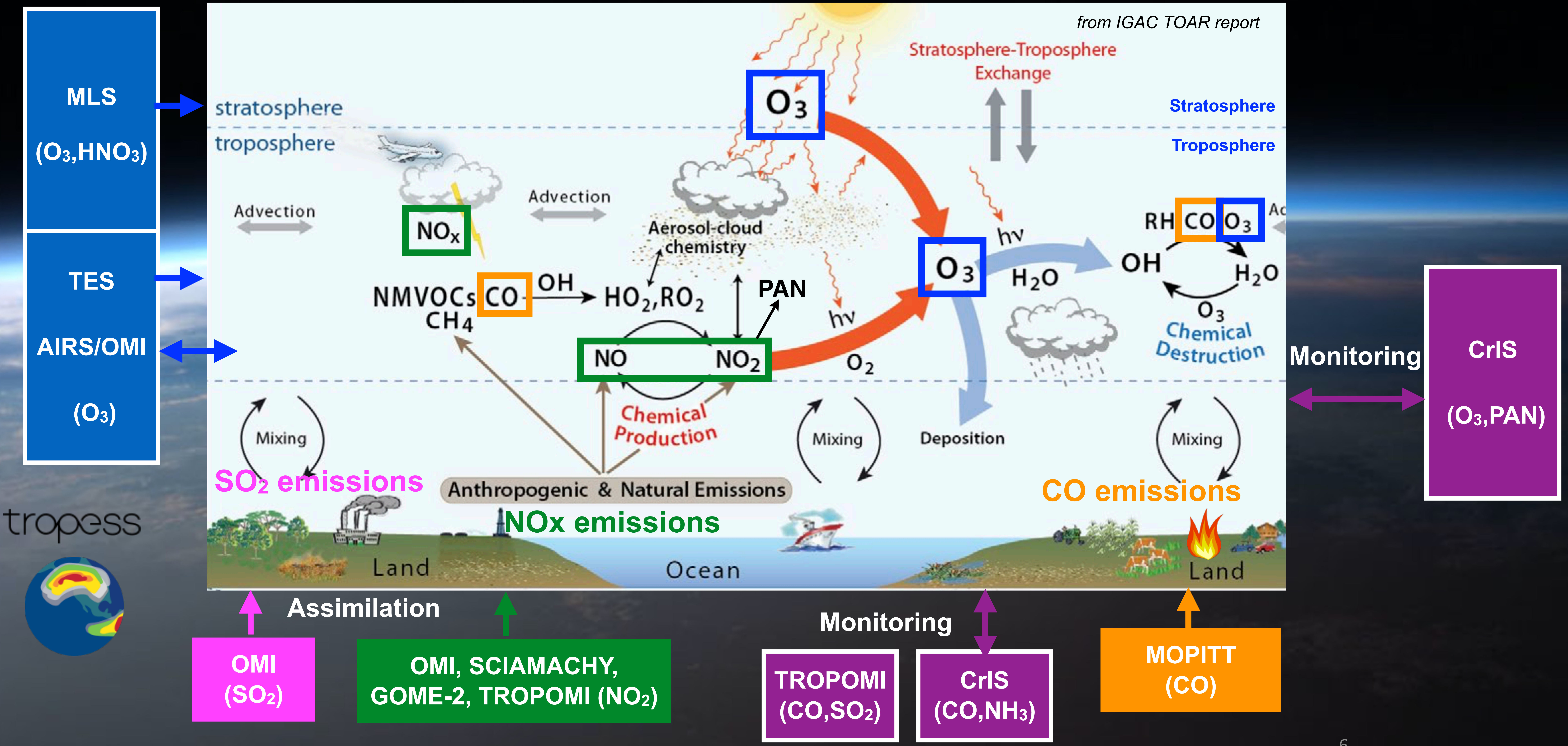
SHADOZ

ATom

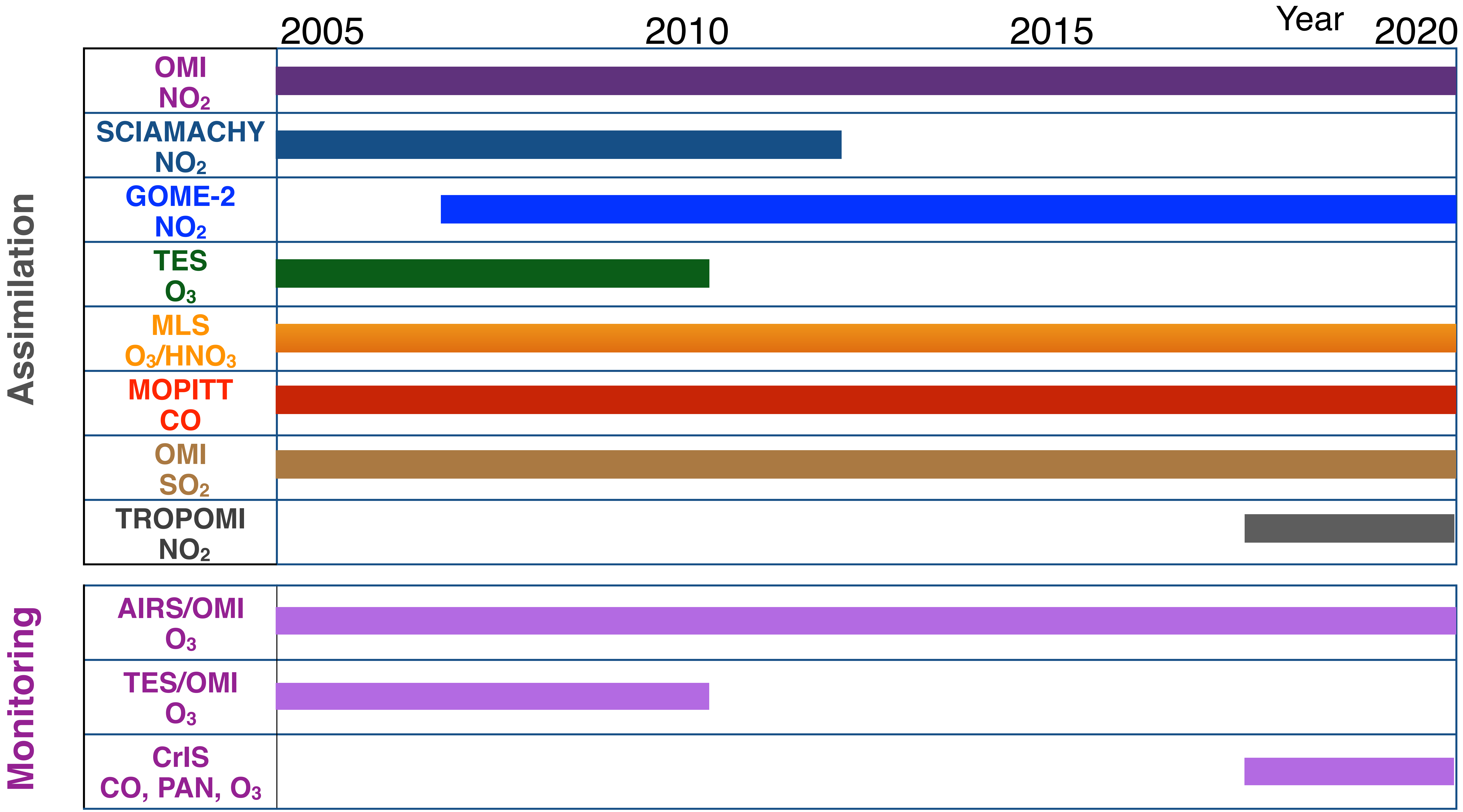
Tropospheric Chemical Reanalysis

- 16 years (2005-present), two-hourly, global, surface to lower stratosphere chemical concentrations of 35 species, including O_3, NOx, OH, SO_2, VOCs
- Anthropogenic, biogenic, biomass burning, and lightning emissions (NOx, CO, SO_2)
- Used in various science applications, including validation of NASA satellite products
- Able to support OSSE activities in support of mission formulation

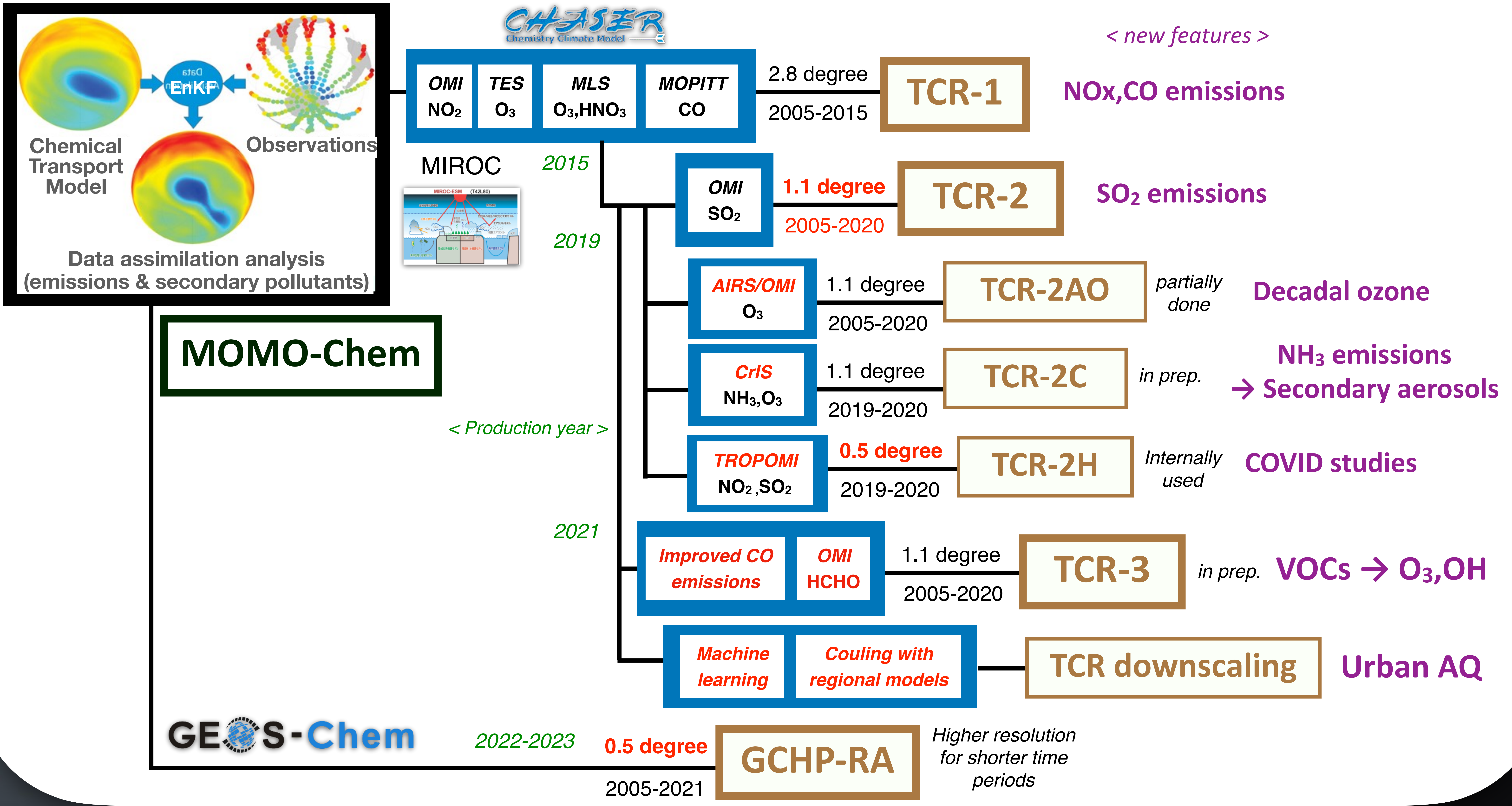
Multi-constituent multi-satellite chemical data assimilation



Decadal tropospheric chemistry reanalysis: TCR-2



JPL MOMO-Chem (Multi-mOdel Multi-cOnstituent Chemical) Data Assimilation



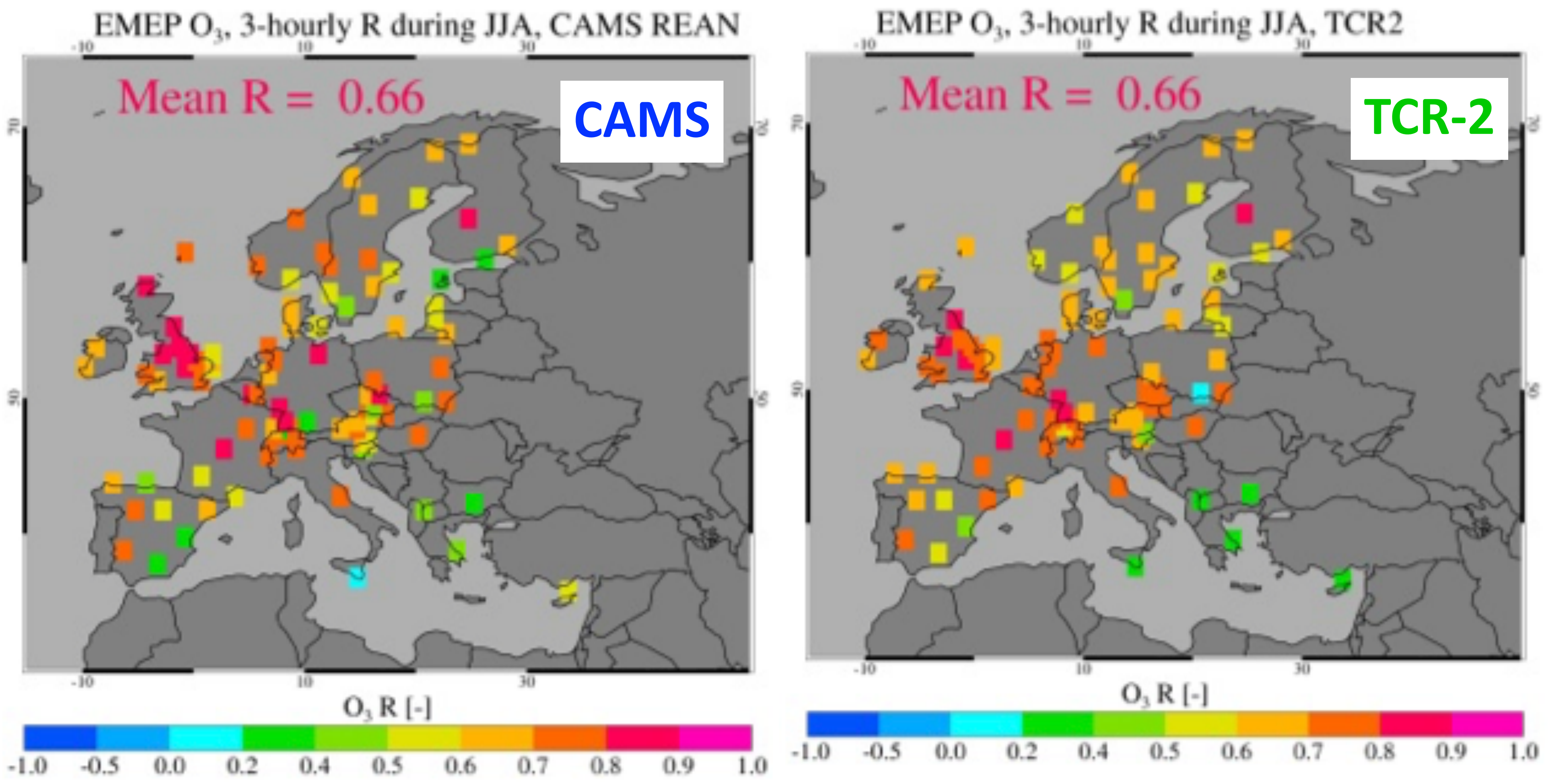
IGAC TOAR-II chemical reanalysis Focus Working Group

Kazuyuki Miyazaki, *WG co-lead, Jet Propulsion Laboratory*
Dylan Jones, *WG co-lead, Univ. of Toronto, Canada*
Helen Worden, *TOAR-II SC, NCAR, USA*

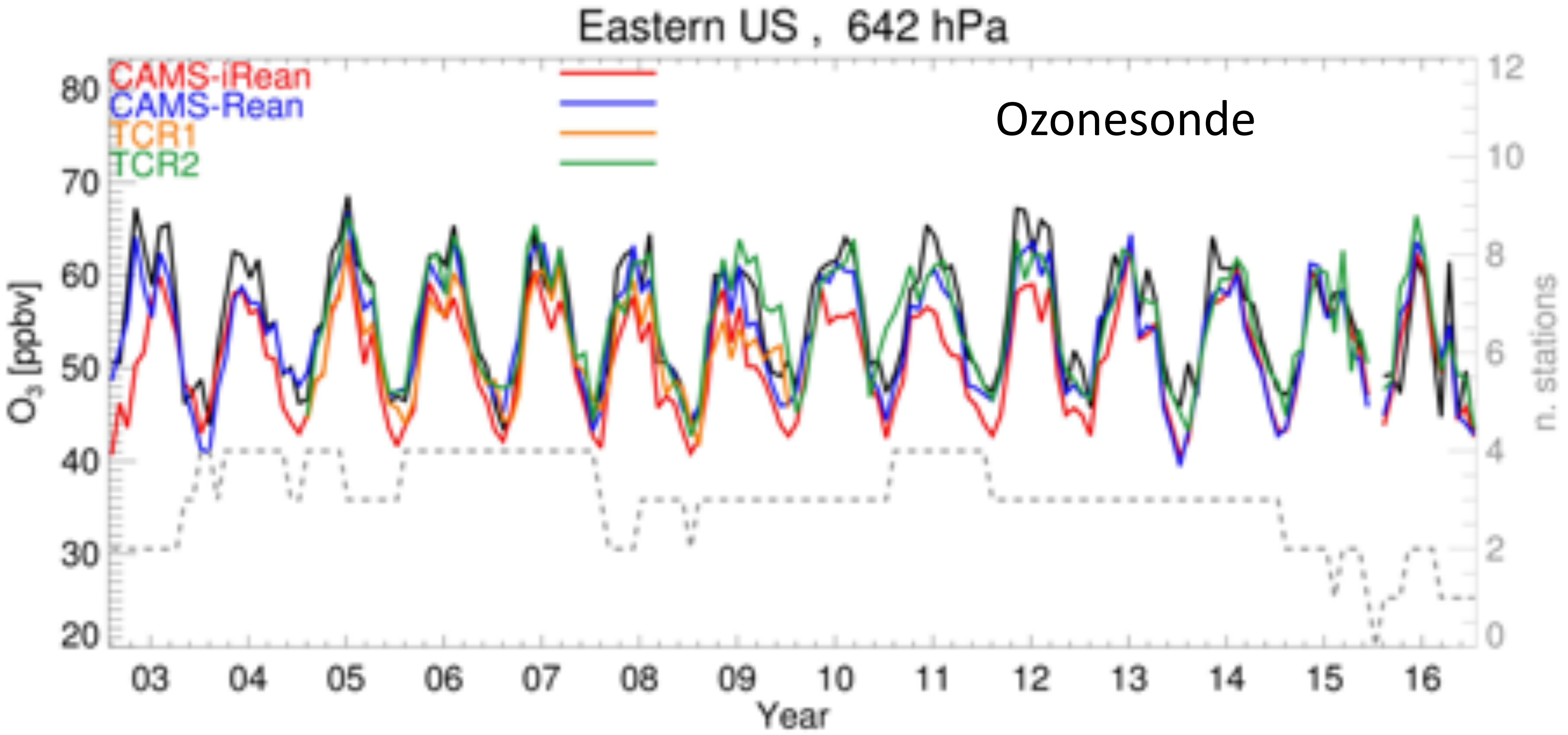
Overview and Goals in support of TOAR-II

- Evaluation of chemical reanalyses with TOAR-II observations will assess the potential of using reanalysis data for studying spatial gradients at both regional and global scales and trends in areas with sparse in-situ observations.
- Assess the relative importance of individual observations to improve surface ozone analyses and help to design observing systems that better capture the distribution and regional trends in tropospheric ozone.
- Inter-comparisons of top-down precursor emissions from reanalyses, and their impacts on surface/tropospheric ozone and subsequent radiative effects will facilitate evaluation of emission scenarios and environmental policy in realistic conditions
- Improve the TOAR-II observation quality control processes and representativeness

Ozone reanalysis inter-comparisons



Products	Model	DA	Period
CAMS-iRA	IFS (CB05) T159 (1.1)	4D-VAR	2003-2018
CAMS-RA	IFS(CB05)+Aerosol T255 (0.7)	4D-VAR	2003-present
TCR-1	CHASER-EnKF T42 (2.8)	EnKF	2005-2016
TCR-2	MIROC-Chem-EnKF T106 (1.1)	EnKF	2005-2018

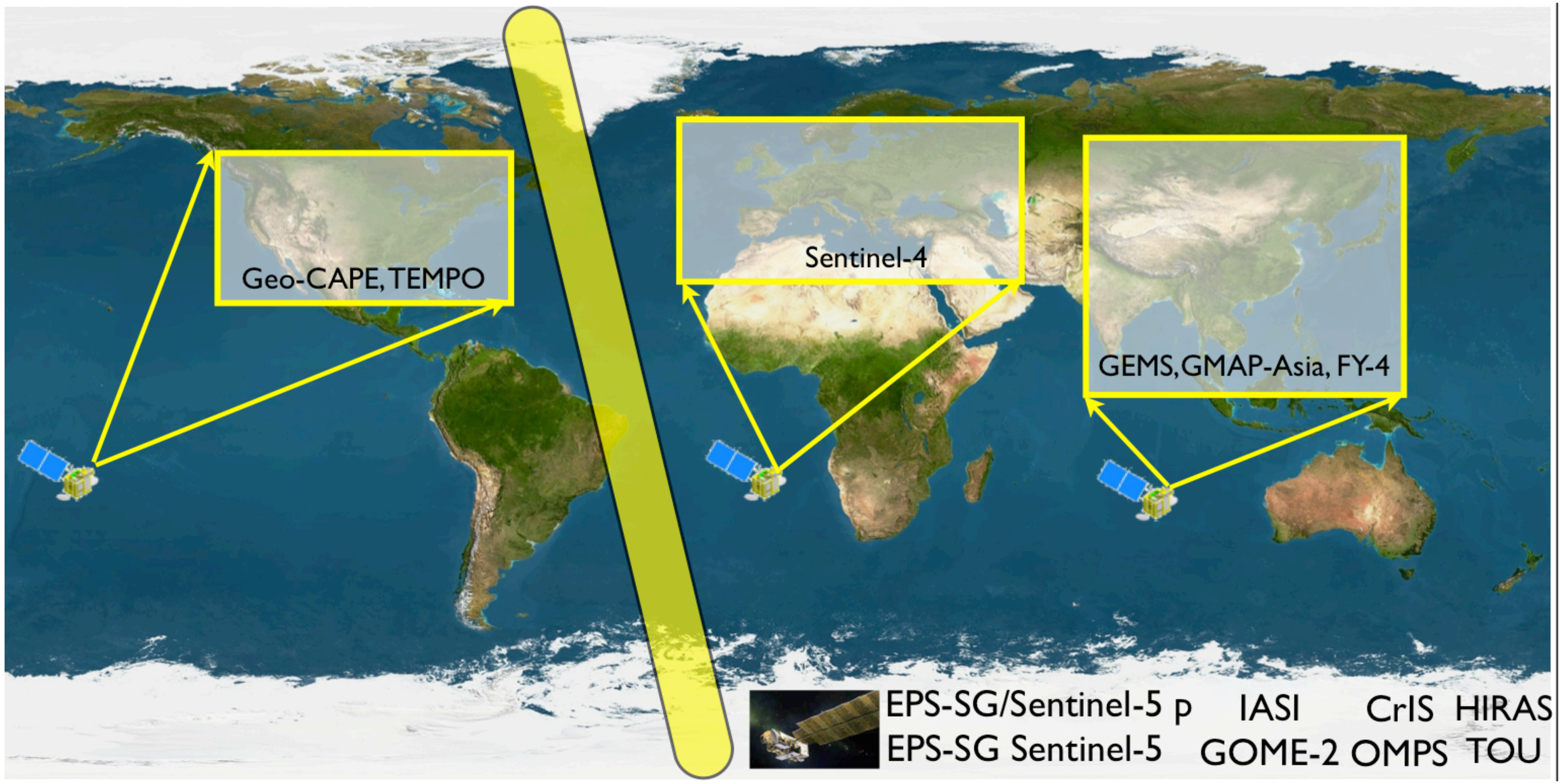


RMSE (ppbv)

CAMS-iRA	4.9
CAMS-RA	3.2
TCR-1	5.0
TCR-2	3.4

Huijnen et al., 2020

Towards an Air Quality Constellation



How does the constellation improve knowledge of global air quality?

- GEO sounders (GEO-CAPE, TEMPO, Sentinel-4, GEMS) will provide an unprecedented number of composition observations at high spatial resolution.
- LEO sounders (IASI, CrIS, S5p) provide the global picture and thread the GEO observations together.

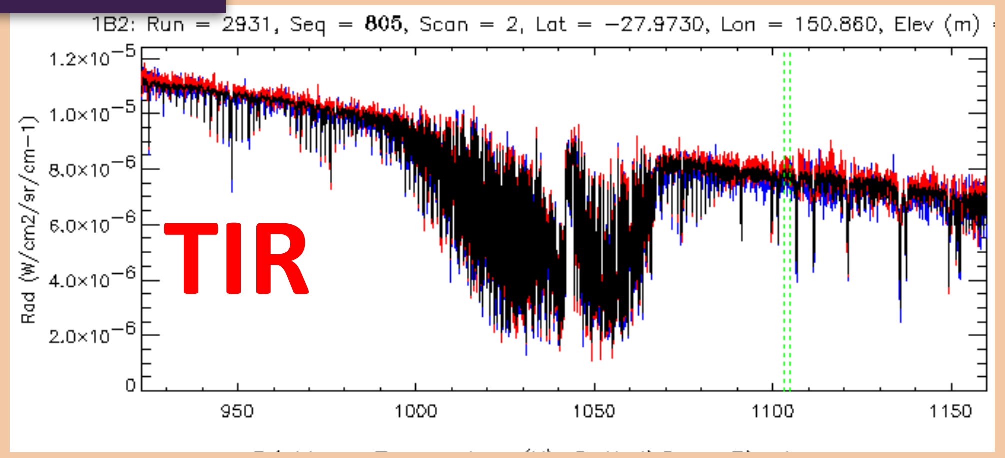
AIRS/OMI ozone monitoring and assimilation

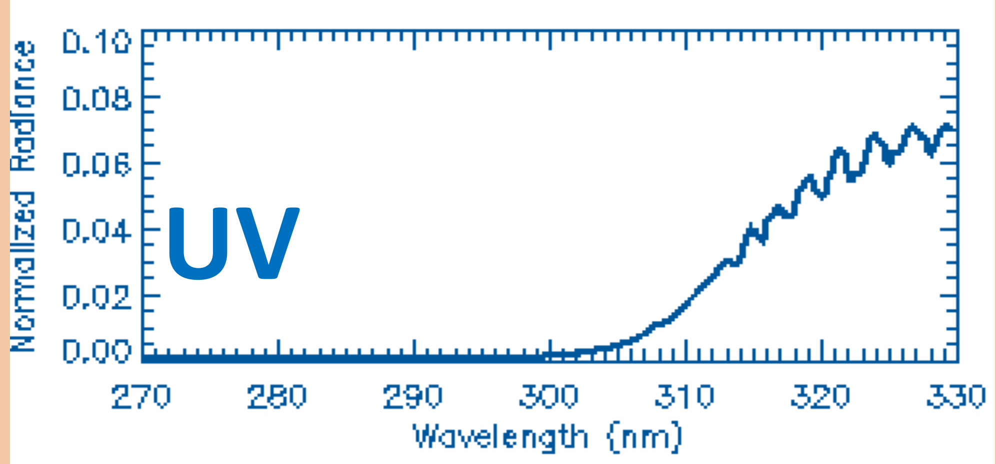
Joint LW/SW or ultra-high spectral resolution measurements distinguish upper/lower troposphere.

- TIR observations are sensitive to the free-tropospheric trace gases.
- UV-Vis-NIR observations are sensitive to the column abundances of trace gases.

How are retrievals used?

MUlti-SpEctra, MUlti-SpEcies, MUlti-SEnsors (MUSES) Retrieval Algorithm

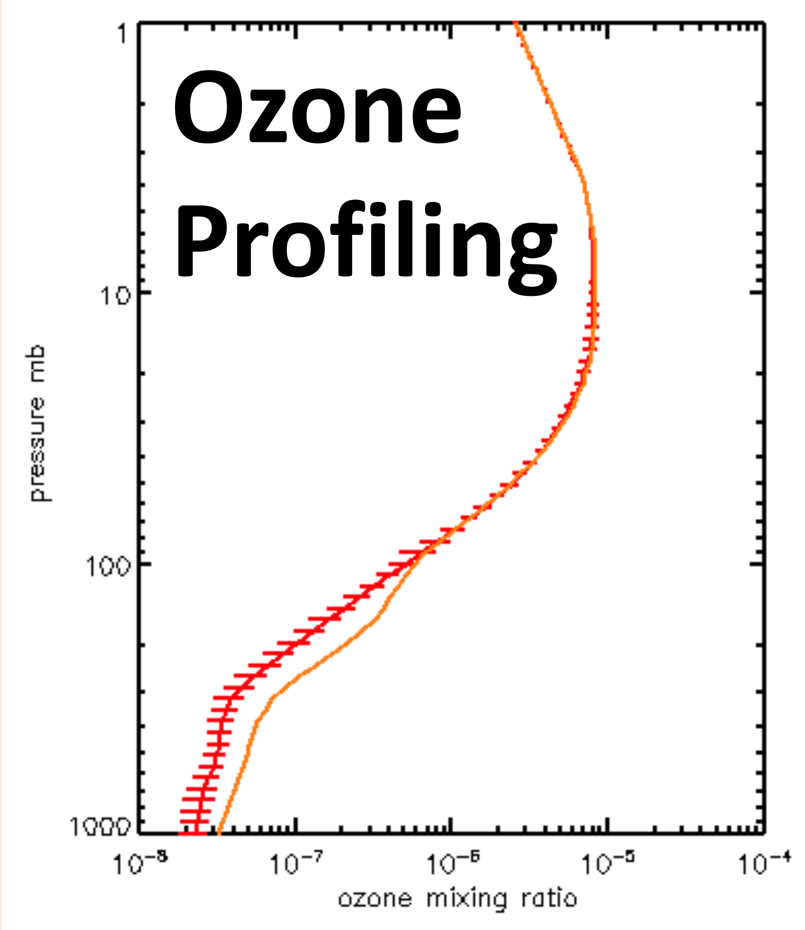




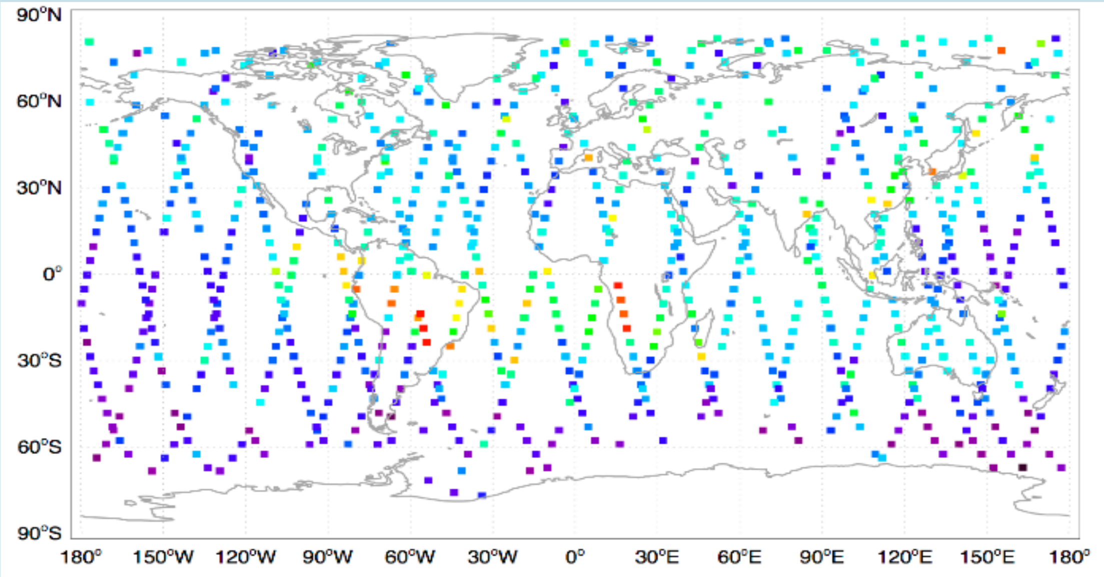
$$\|\mathbf{y}-\mathbf{F}(\mathbf{x}_a)\|^2_{\mathbf{S}_n^{-1}} + \|\mathbf{x}-\mathbf{x}_a\|^2_{\mathbf{S}_a^{-1}}$$

NASA Retrieval Algorithm

$$\hat{\mathbf{x}} = \mathbf{x}_a + \mathbf{A}(\mathbf{x}-\mathbf{x}_a) + \mathbf{G}\mathbf{n}$$

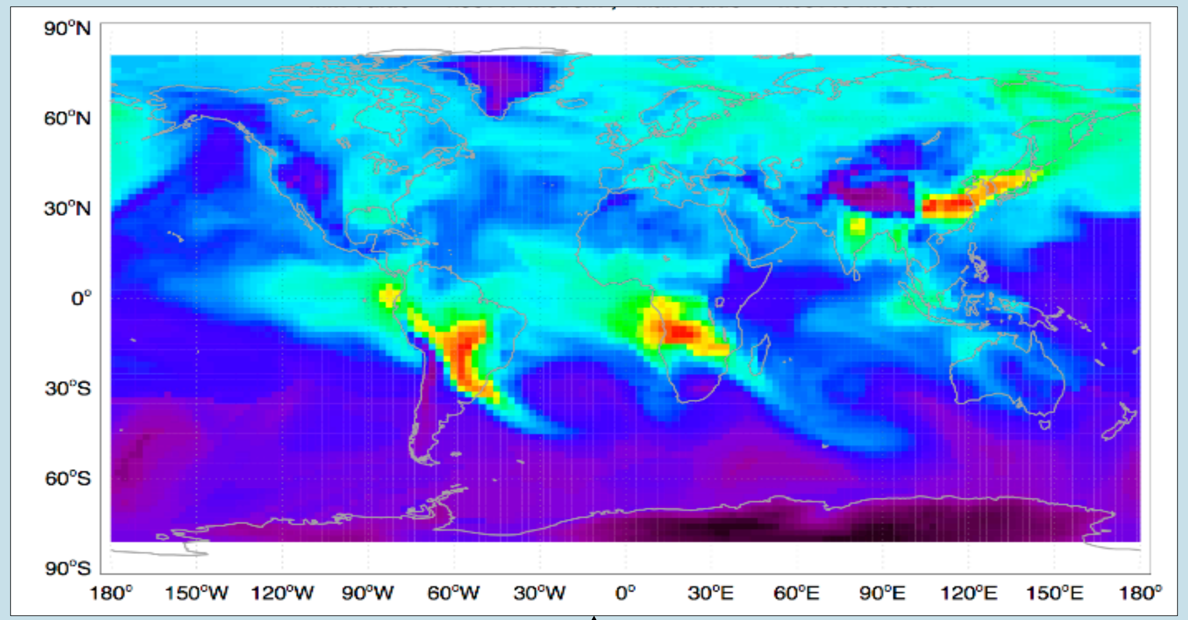


Operational Data Processing



Data Assimilation

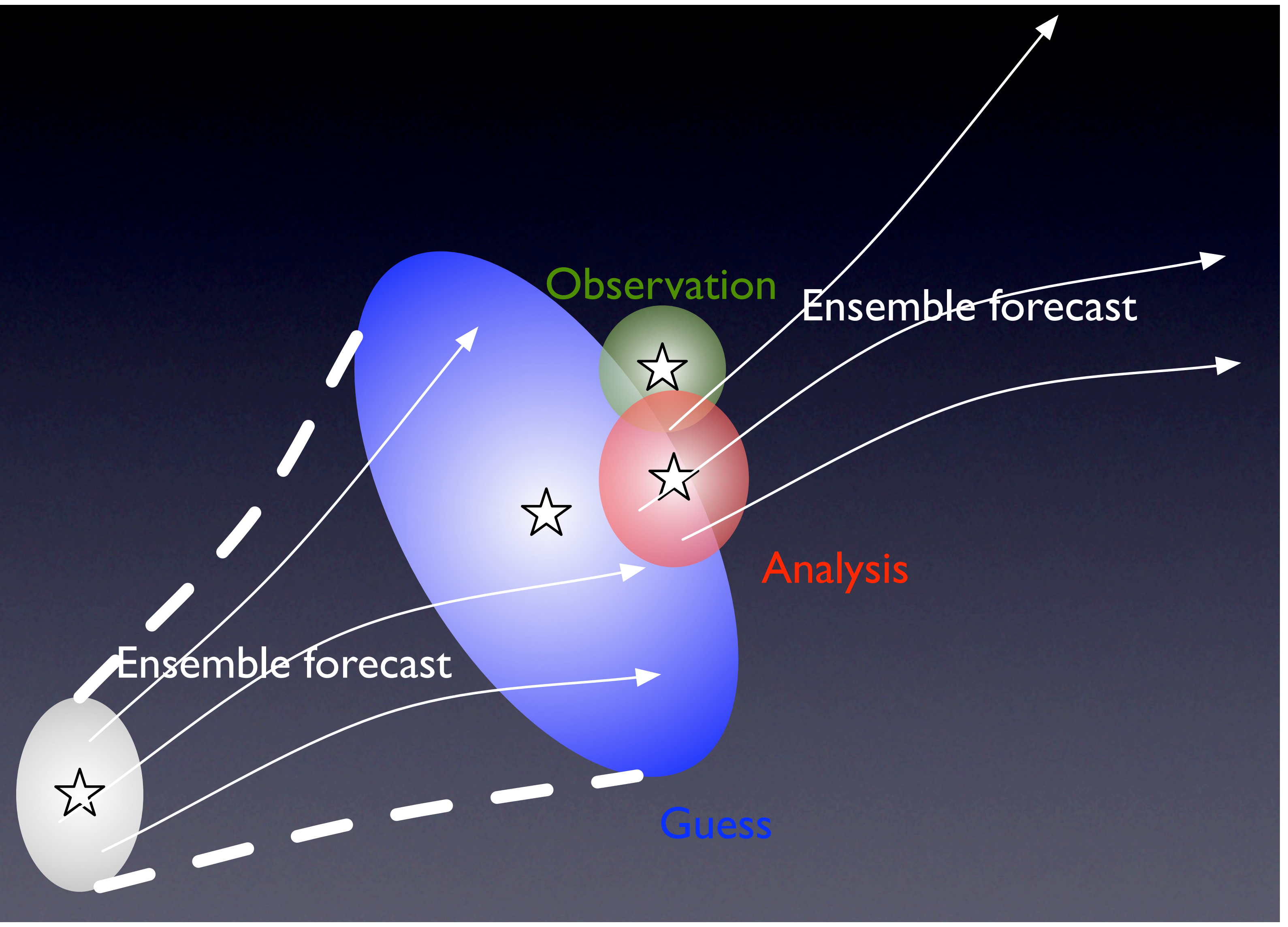
$$\mathbf{H}_i(\bullet) = \mathbf{x}_a + \mathbf{A}_i(\bullet - \mathbf{x}_a)$$



$$\sum_i \|\hat{\mathbf{x}}_i - \mathbf{H}_i(\mathbf{x})\|^2_{(\mathbf{G}_i\mathbf{S}_n^i\mathbf{G}_i^T)^{-1}} + \|\mathbf{x}_0 - \mathbf{x}_B\|^2_{\mathbf{B}^{-1}}$$

Fu et al., 2019

EnKF: The forecast error covariance is advanced by the model itself (flow-dependent forecast error covariance), which allow us to fully take advantage of the CTM.



Background error covariance

(assuming that background ensemble perturbations sample the forecast errors)

$$\mathbf{P}^b = \mathbf{X}^b(\mathbf{X}^b)^T. \qquad \overline{\mathbf{x}^b} = \frac{1}{k}\sum_{i=1}^{k}\mathbf{x}_i^b \;;\;\; \mathbf{X}_i^b = \mathbf{x}_i^b - \overline{\mathbf{x}^b}.$$

Analysis ensemble mean and its perturbation

$$\overline{\mathbf{x}^a} = \overline{\mathbf{x}^b} + \mathbf{X}^b\tilde{\mathbf{P}}^a(\mathbf{Y}^b)^T\mathbf{R}^{-1}(\mathbf{y}^o - \overline{\mathbf{y}^b}),$$

How are retrievals used?

- **The observation operator (H)** converts the model profiles (x) to the profile that would be retrieved from satellite measurements (y^b).

$$y^b = H(x) = x_a + \mathbf{A}(S(x) - x_a).$$

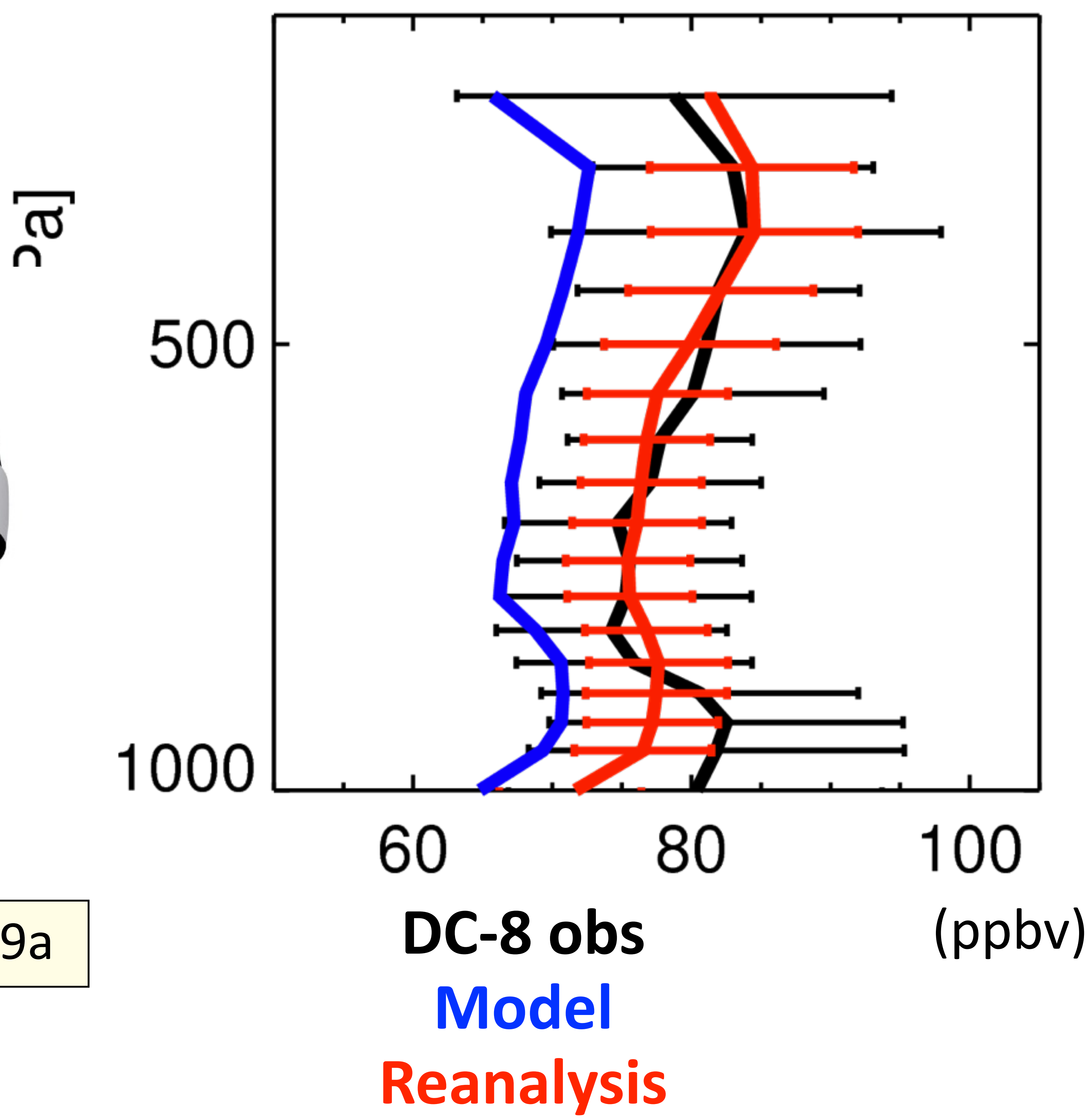
- The model-satellite difference is not biased by the retrieval a priori profile.

$$y^o - y^b = \mathbf{A}(x_{true} - S(x)) + \epsilon,$$

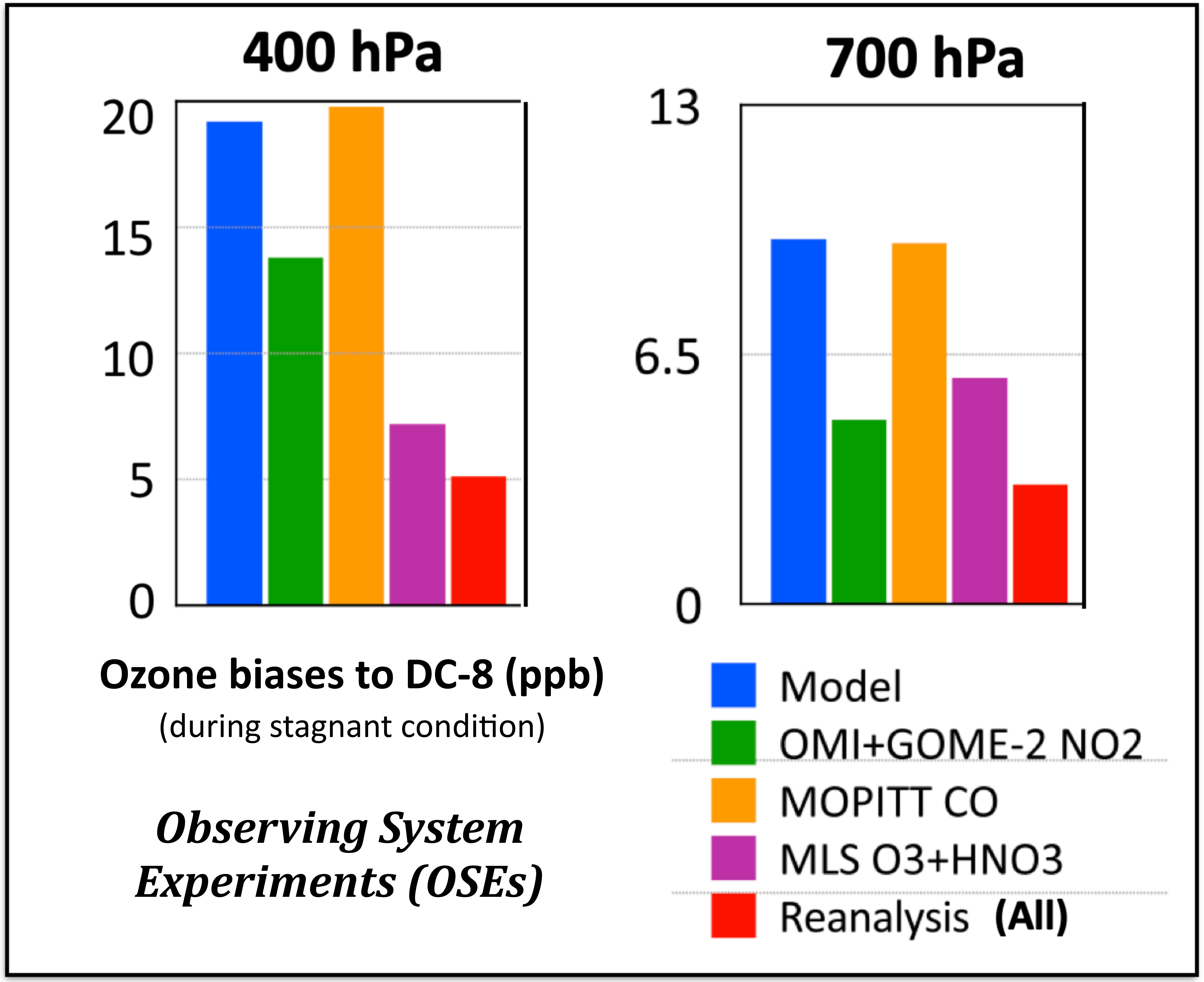
(Rodgers, 2000; Eskes and Boersma, 2003)

What is the impact of IR soundings in regional and global models?

Mean ozone profile



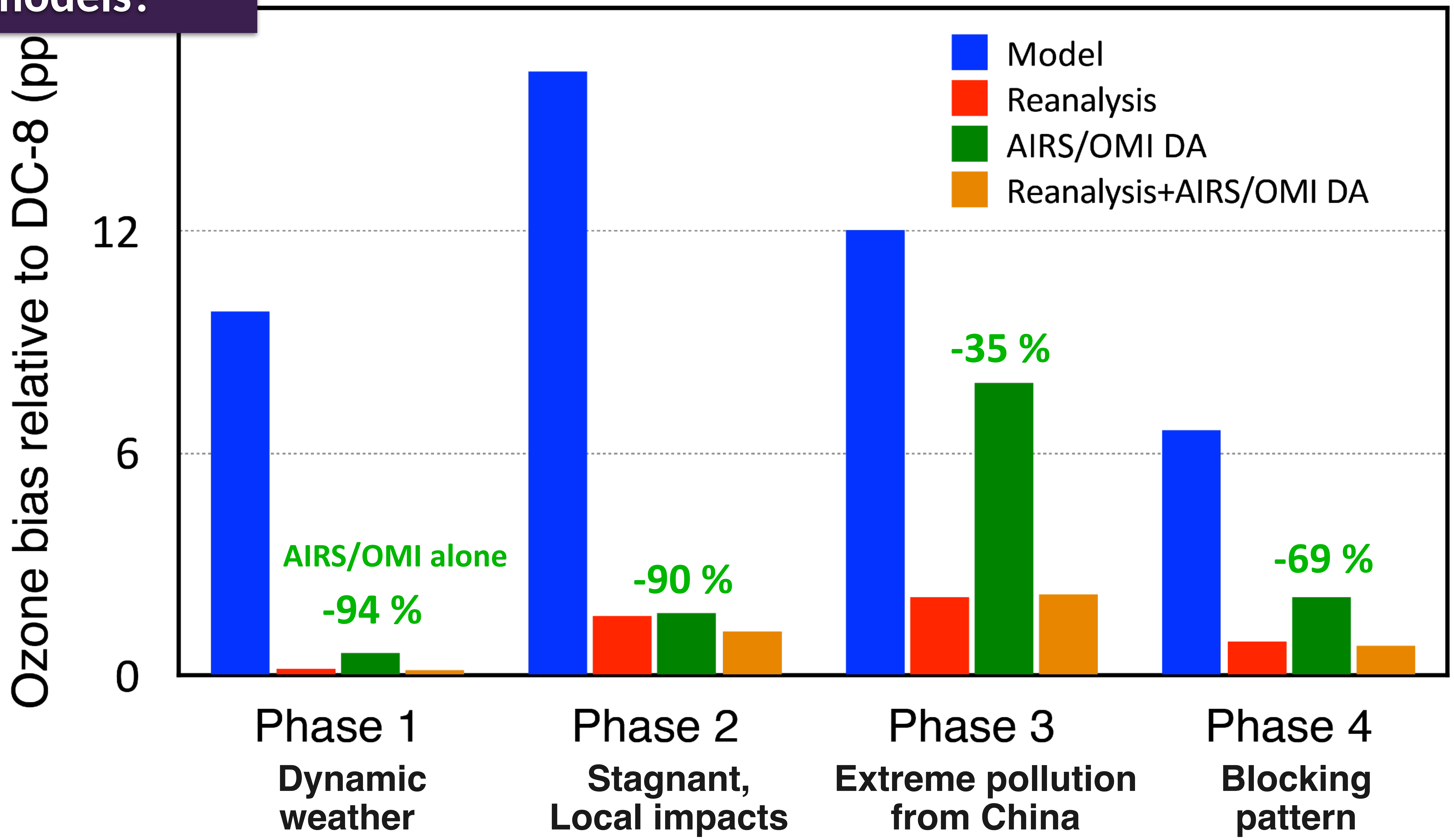
Miyazaki et al., 2019a



- **OMI + GOME-2 NO_2** → Improved the lower tropospheric ozone
- **MLS O_3/HNO_3** → Additional important corrections throughout the troposphere.
- **Multi-constituent (Reanalysis)** → correct the entire tropospheric ozone profile

What is the impact of IR soundings in regional and global models?

…nparisons against KORUS-AQ DC8 ozone at 650 hPa



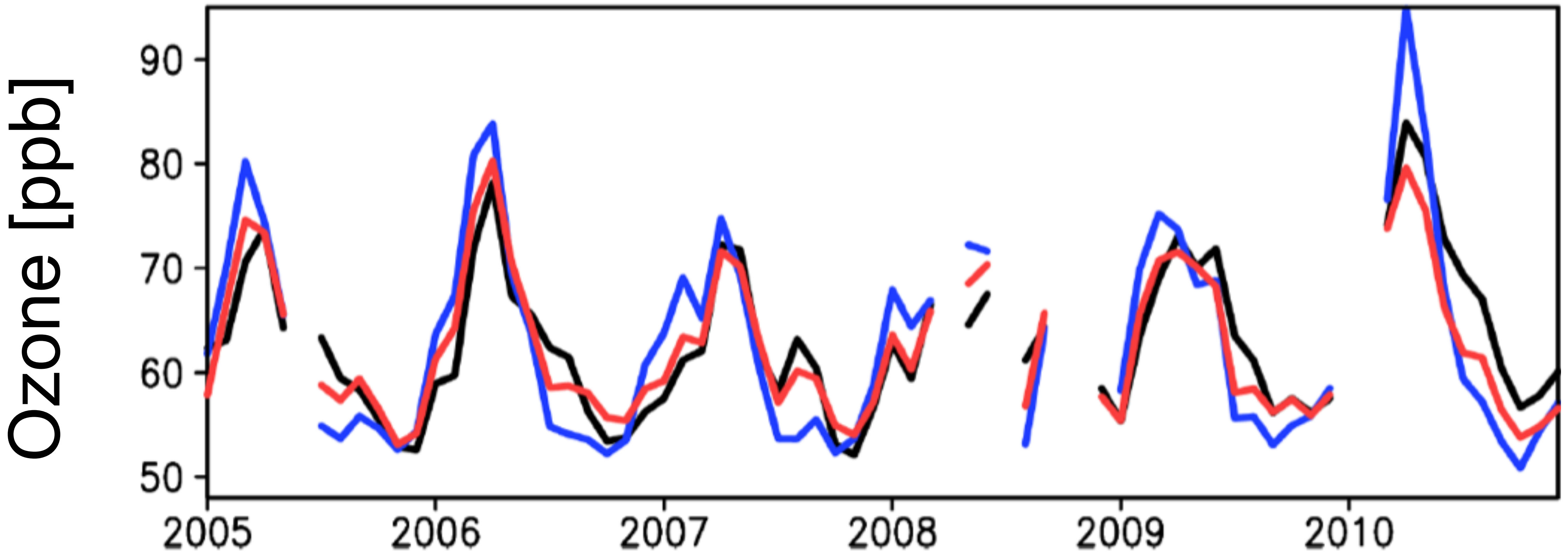
Miyazaki et al., 2019a

- **AIRS/OMI ozone retrievals** provided the largest corrections for dynamic weather conditions (P1), whereas the improvement was limited just after stagnant conditions (P3).
- **Combining precursors' emission optimization and direct ozone assimilation** is an effective method to obtain sufficient corrections on ozone for any meteorological condition.

Free tropospheric and surface ozone validation

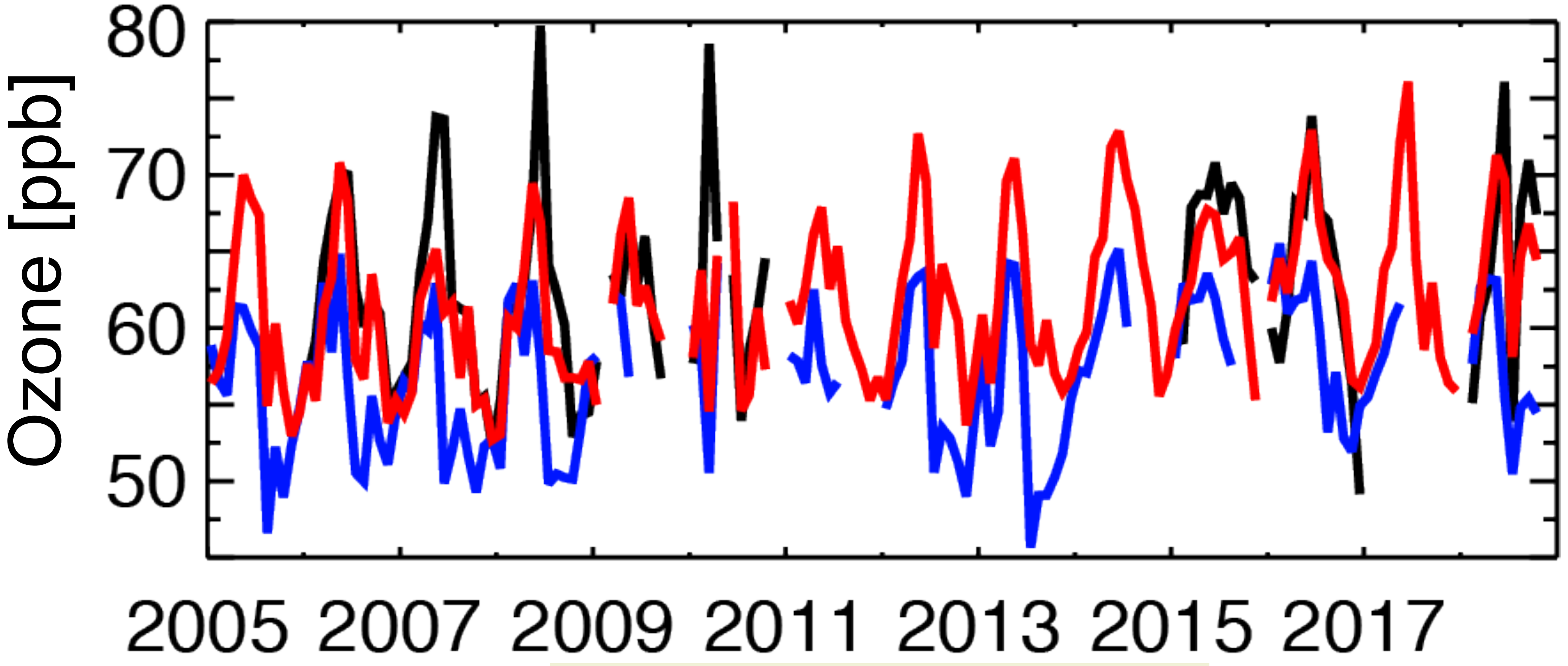
700-300 hPa: against TES (China)

AIRS/OMI
Model
Reanalysis
(w/o TES)



700-500 hPa: against AIRS/OMI (China)

AIRS/OMI
Model
Reanalysis

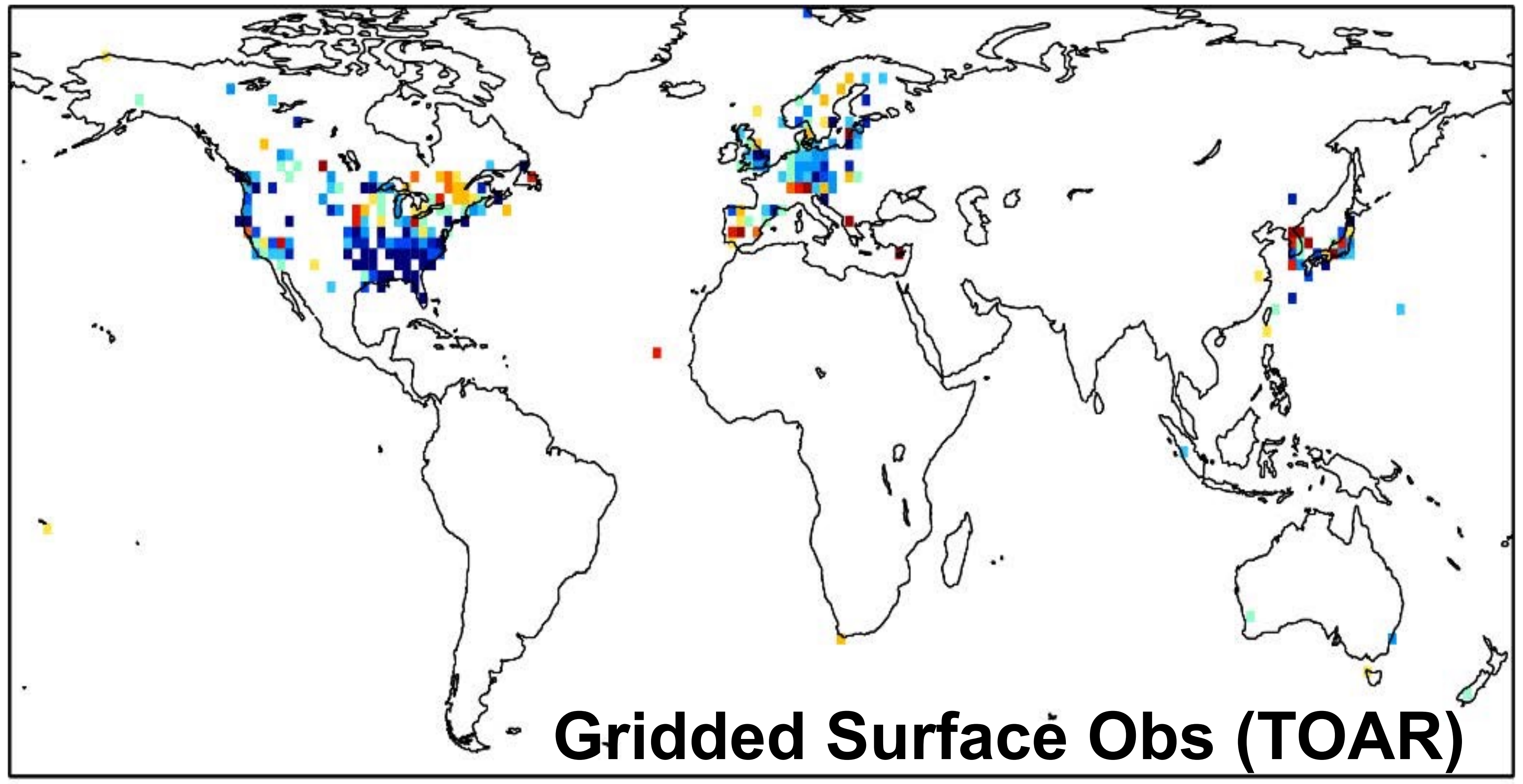


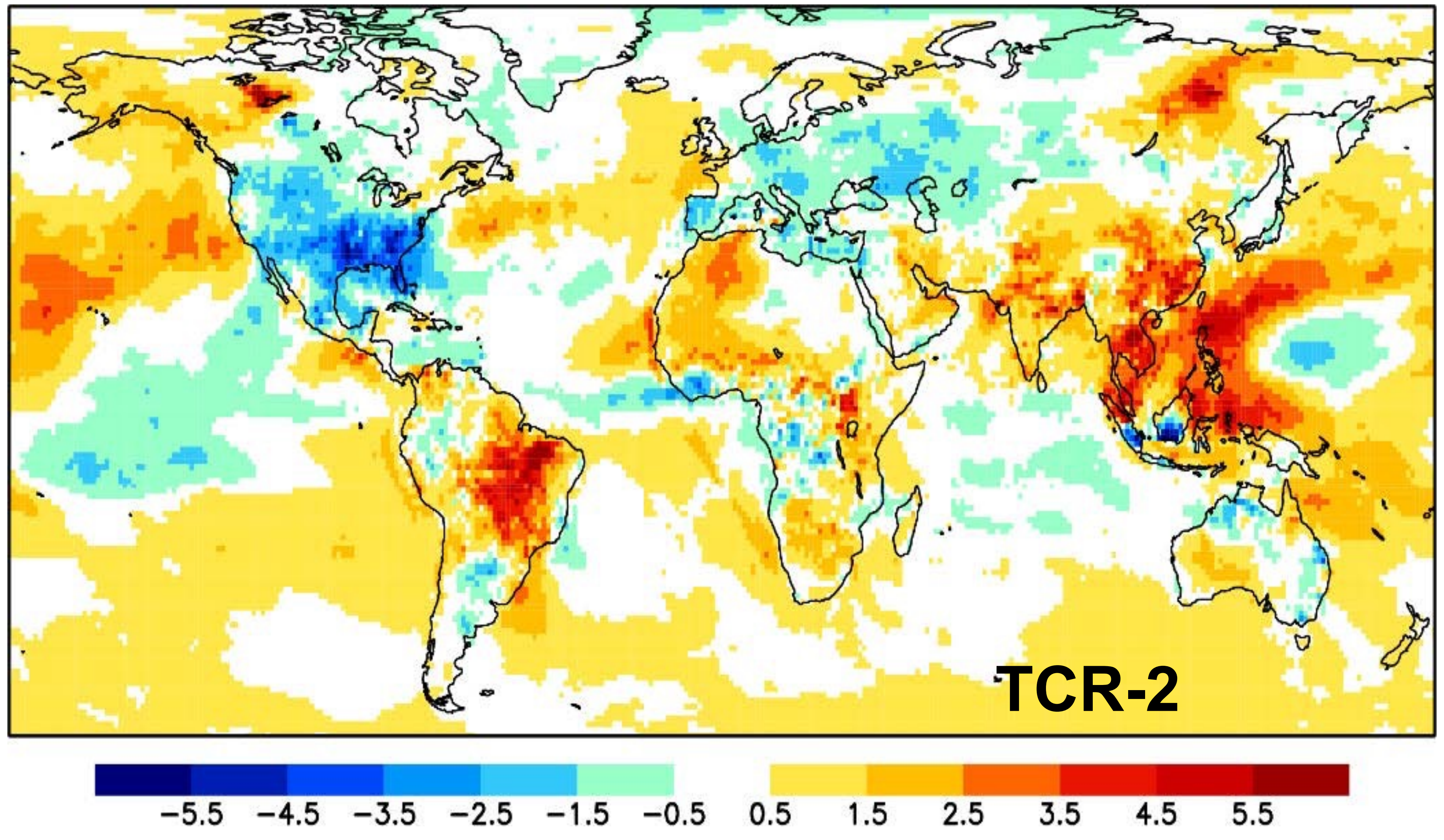
Monitoring → DA

Miyazaki et al., 2020b

TES/OMI multispectral ozone products have also been used to infer surface ozone (Colombi et al., 2021)

Surface ozone changes: 2005-2014

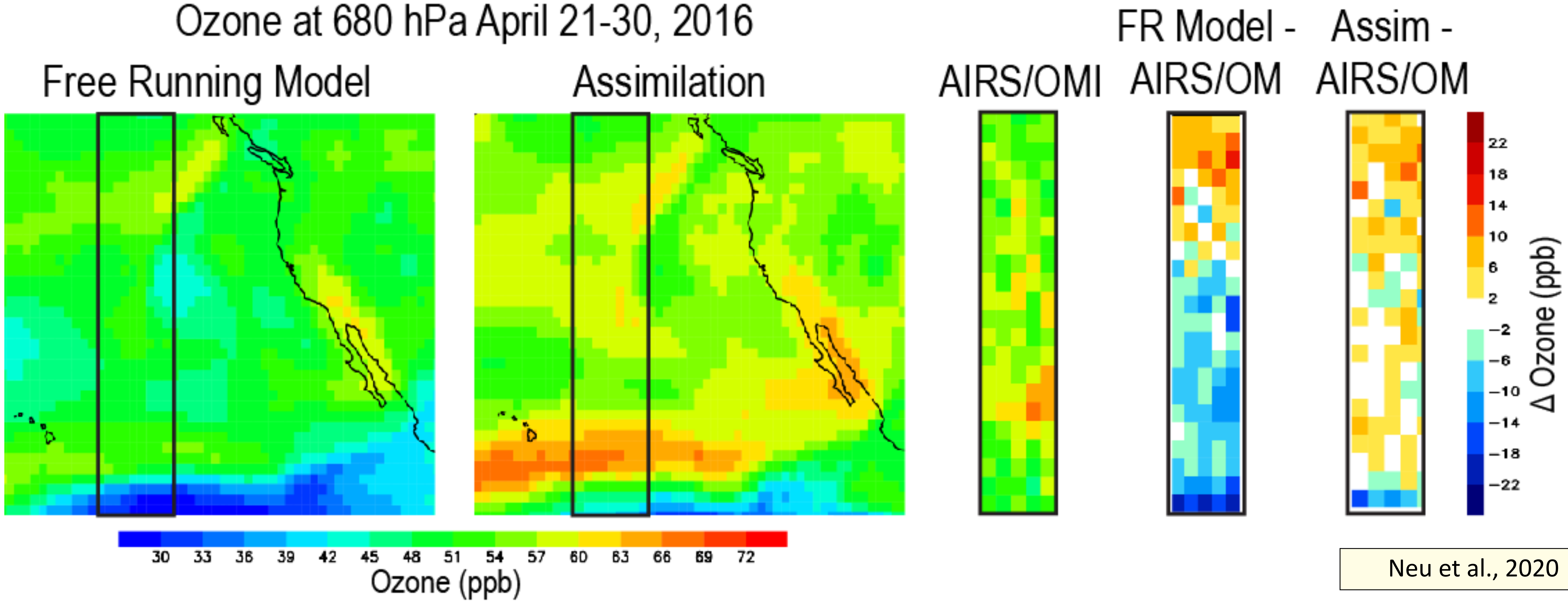




Regional model boundary conditions: Evaluation using AIRS/OMI

What is the impact of IR soundings in regional and global models?

NASA HAQAST



Neu et al., 2020

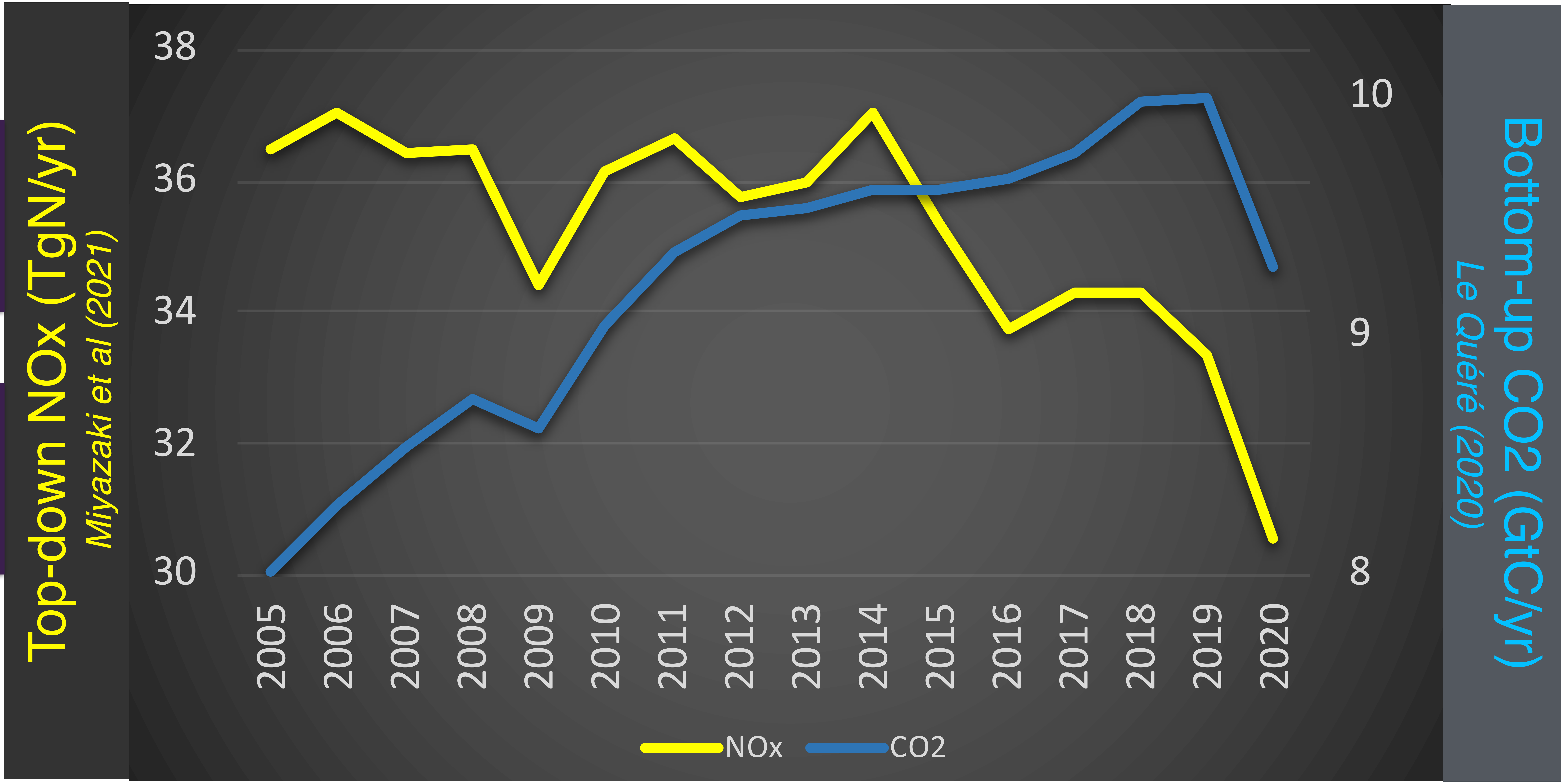
- The assimilation improves the representation of plume transport across the Pacific relative to AIRS/OMI
- Further improvements may be seen with assimilation of AIRS/OMI O_3.


Human activity
COVID-19
natural experiment
Environmental policy to
reduce human health risk
from air pollution
Human activity and technology
Air pollutant emissions (NOx etc)
Complex chemical mechanisms
Air pollution level (Ozone, PM2.5)
Human health
& Climate
??
Answer!!
(observables)
Can be inferred
Implications for
effective policy making
Sinuses
Windpipe
(trachea)
Lungs
Miyazaki et al.,
Science Adv. 2021
Laughner et al.,
PNAS 2021

Global anthropogenic emission reductions in 2020: 7% (CO_2) 8% (NOx)

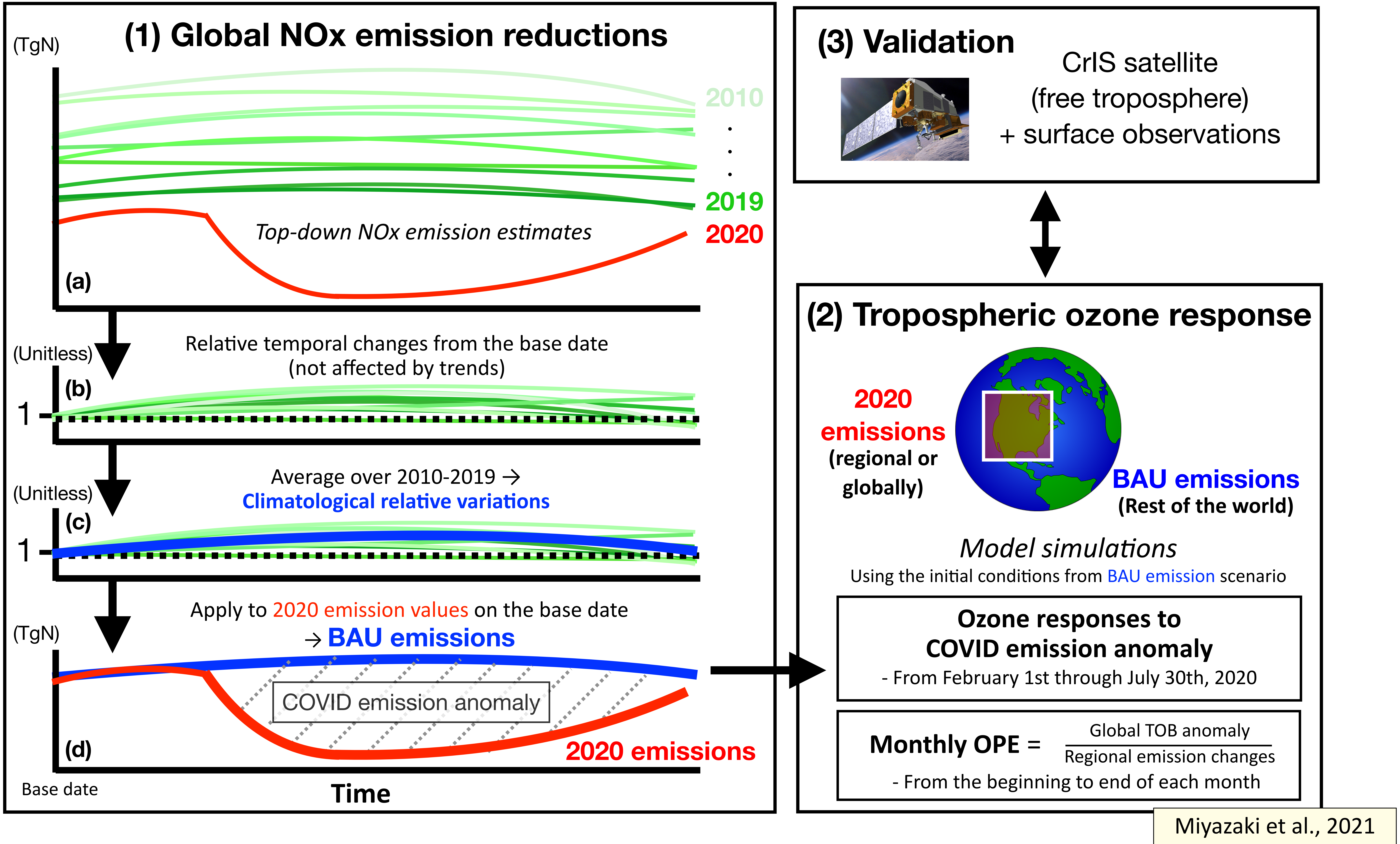
What is the optimum latency for regional and global models?

Impact of IR sounders on reanalysis for climate studies

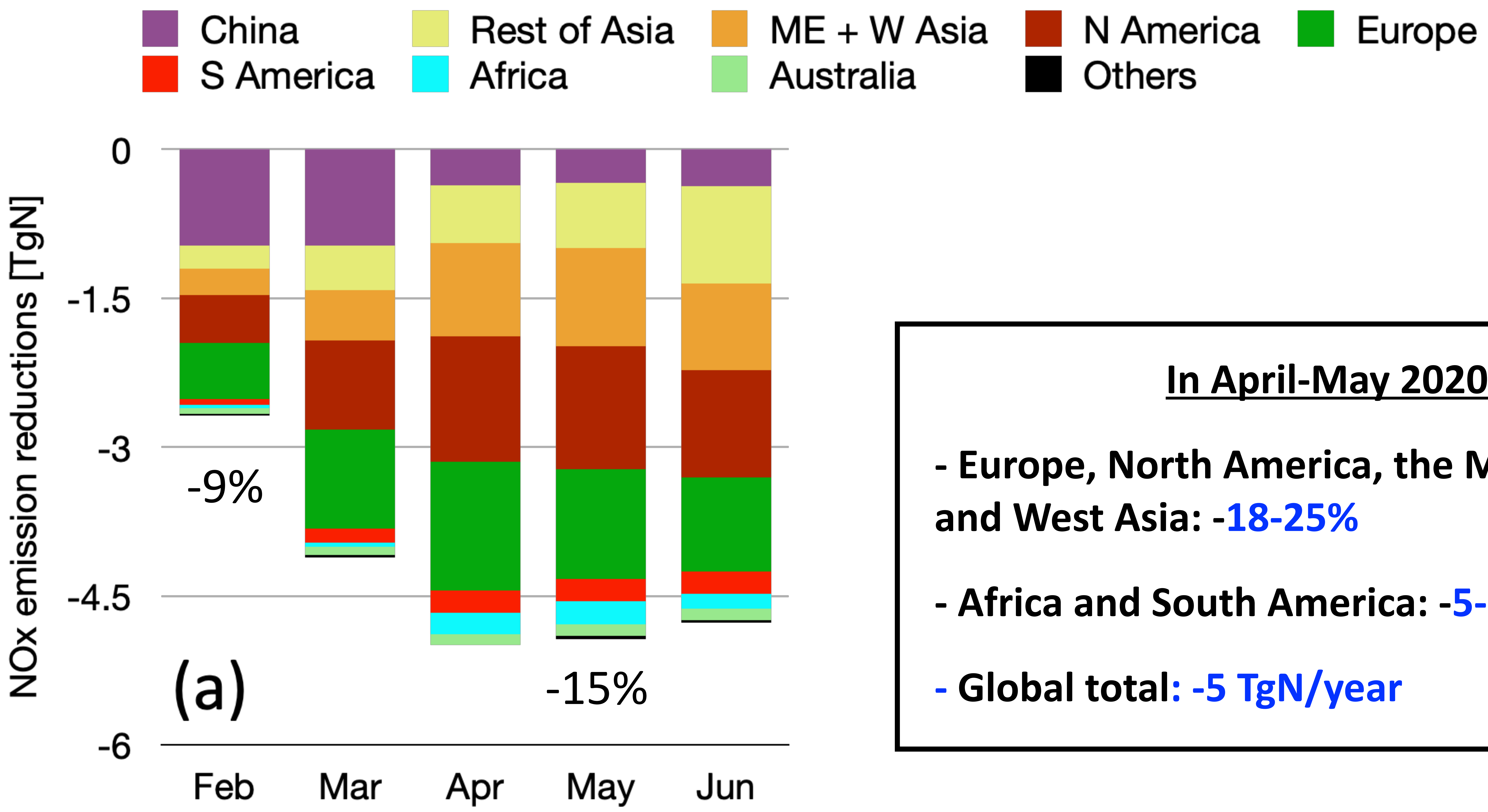


Laughner et al., PNAS 2021

1. Emissions (NOx, SO2, CO) → **2. Concentrations** → **3. Health and climate Impacts**


(1) Global NOx emission reductions
(TgN)
2010
2019
2020
Top-down NOx emission estimates
(a)
Relative temporal changes from the base date
(not affected by trends)
(Unitless)
(b)
1
Average over 2010-2019 →
Climatological relative variations
(Unitless)
(c)
1
Apply to 2020 emission values on the base date
→ BAU emissions
(TgN)
COVID emission anomaly
(d)
2020 emissions
Base date
Time
(3) Validation
CrIS satellite
(free troposphere)
+ surface observations
(2) Tropospheric ozone response
2020
emissions
(regional or
globally)
BAU emissions
(Rest of the world)
Model simulations
Using the initial conditions from BAU emission scenario
Ozone responses to
COVID emission anomaly
- From February 1st through July 30th, 2020
Monthly OPE = Global TOB anomaly / Regional emission changes
- From the beginning to end of each month
Miyazaki et al., 2021

Estimated NOx emissions



1. Emissions (NOx)

<u>In April-May 2020</u>

- **Europe, North America, the Middle East and West Asia: -18-25%**
- **Africa and South America: -5-10%**
- **Global total: -5 TgN/year**


Feb 01 2020
Ozone Anomaly
-6
-3
0
3
6
parts per billion
Values between -1.0 and 1.0 ppb culled for clarity
200 mb
400 mb
600 mb
800 mb
1000 mb

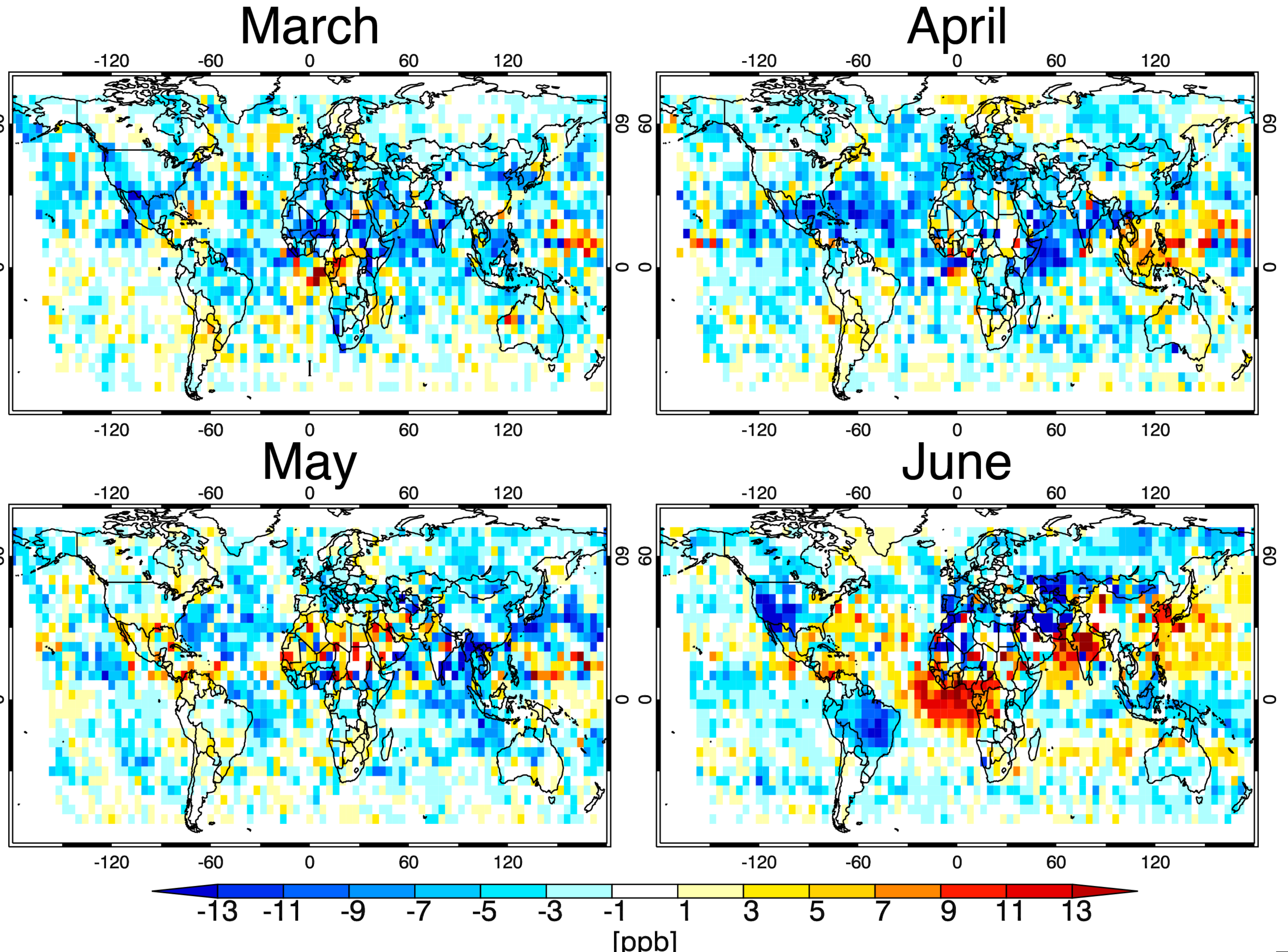

Feb 17 2020
Ozone Anomaly, United States
-6 -5 -4 -3 -2 -1 0
parts per billion
Ozone Anomaly, Non-China Asia
-6 -5 -4 -3 -2 -1 0
parts per billion
200 mb
400 mb
600 mb
800 mb
1000 mb

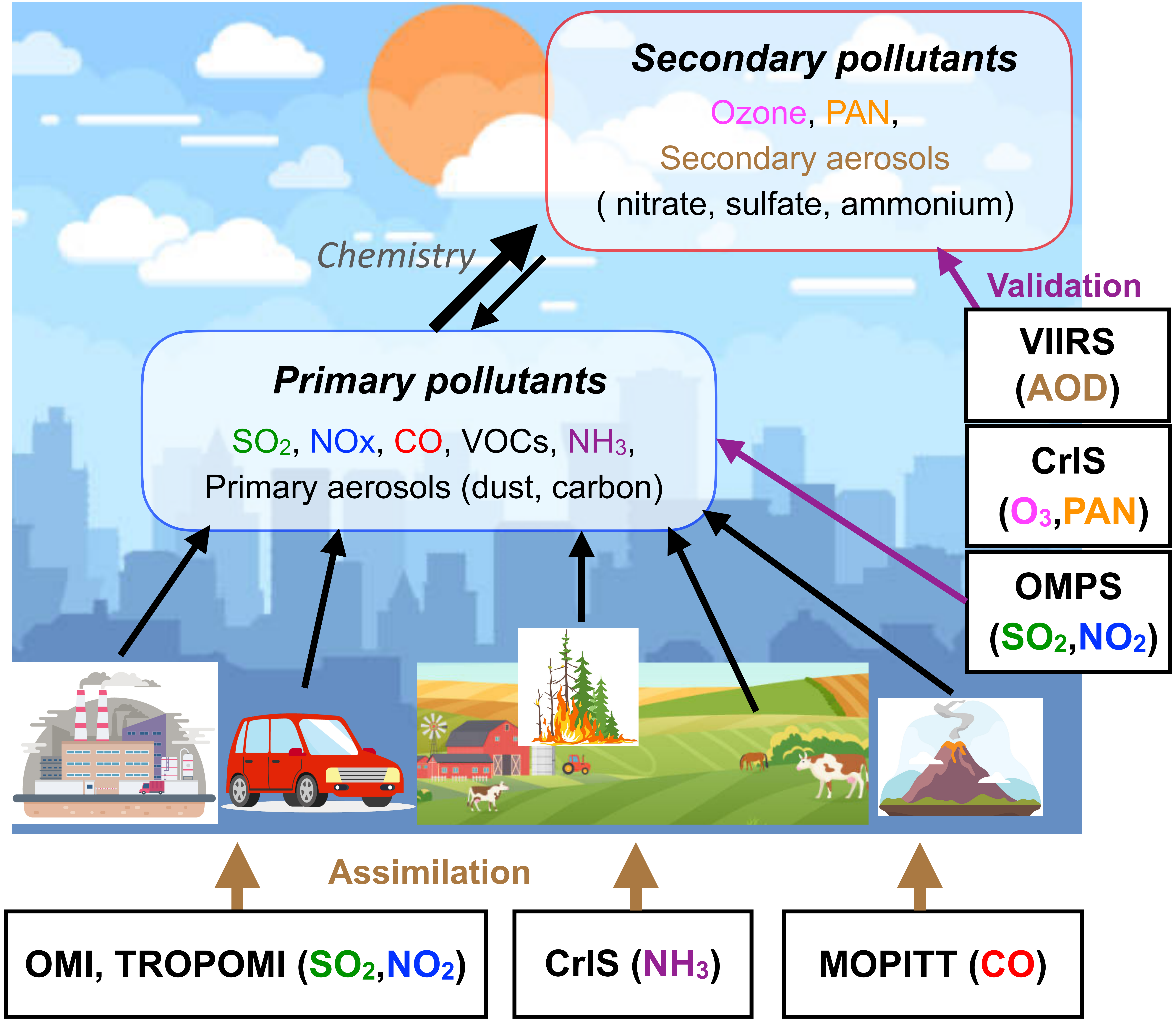
Global ozone response: Comparisons against CrIS satellite

CrIS (JPL TROPESS) ozone 700 hPa: 2020 minus 2019

2. Concentrations

tropess




Secondary pollutants
Ozone, PAN,
Secondary aerosols
(nitrate, sulfate, ammonium)
Chemistry
Validation
VIIRS
(AOD)
CrIS
(O3,PAN)
OMPS
(SO2,NO2)
Primary pollutants
SO2, NOx, CO, VOCs, NH3,
Primary aerosols (dust, carbon)
Assimilation
OMI, TROPOMI (SO2,NO2)
CrIS (NH3)
MOPITT (CO)

Summary

- The chemical reanalysis data, combined with suborbital and ground-based measurements, has been used to improve our understanding of atmospheric composition and to evaluate new satellite data products including AIRS/OMI and CrIS.

- *Answers to the meeting questions*: (1) IR soundings have a big impact on global and regional studies as well as climate. (2) Low data latency would be important for predictions (e.g., wildfire impacts) while attribution analysis w/o low data latency is also important. (3) Assimilation of retrievals are efficient and sufficient for science applications.

- New LEO and GEO measurements and multi-spectral retrievals of composition provide much-improved spatial and temporal resolution and coverage in conjunction with the chemical reanalysis. They should lead to greater usefulness of satellite measurements for climate and air quality applications. E.g., GEMS NO_2 with CrIS/TROPOMI O_3 would better isolate sources and attribute sectors and their influences on ozone at daily scales.