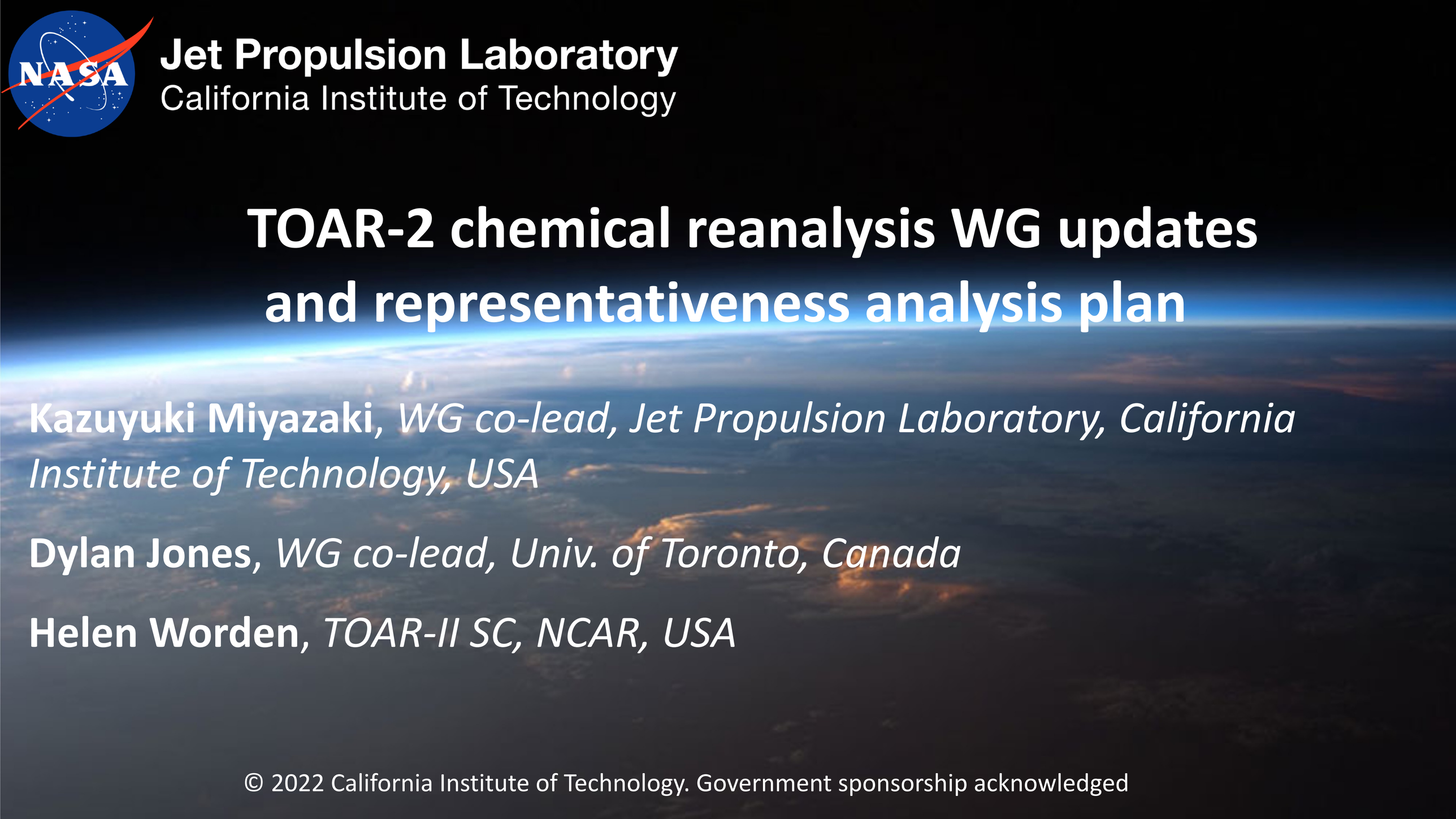


Jet Propulsion Laboratory
California Institute of Technology

TOAR-2 chemical reanalysis WG updates and representativeness analysis plan

Kazuyuki Miyazaki, *WG co-lead, Jet Propulsion Laboratory, California Institute of Technology, USA*

Dylan Jones, *WG co-lead, Univ. of Toronto, Canada*

Helen Worden, *TOAR-II SC, NCAR, USA*

Chemical reanalysis

- A systematic approach to create a long-term data record of atmospheric composition, consistent with model processes and observations, using data assimilation.
- Has the great potential to provide comprehensive information on atmospheric composition variability in order to improve understanding of the processes controlling the atmospheric environment.

Global — **ECMWF CAMS, JPL TCR-2, GEOS-Chem adjoint, RAQMS Aura**

Regional — **Chinese air quality reanalysis (CAQRA), European**

Do they agree/disagree with each other and with new TOAR-II observations?

What is the relative importance of assimilated measurements to improve surface/tropospheric ozone?

TOAR-II chemical reanalysis focus WG

Overview and Goals in support of TOAR-II

- Evaluation of chemical reanalyses with TOAR-II observations and other data (e.g., ozonesonde) will assess the potential of using reanalysis data for studying spatial gradients at regional/global scales and trends in areas with sparse in-situ observations. It will also assist in determining the contribution of precursor emissions/meteorology to observed ozone trends and surface ozone exceedances.
- Sensitivity analyses of the impacts of satellite and in-situ observations of ozone and precursors will assess the relative importance of individual observations to improve surface ozone analyses and help design observing systems that better capture the distribution and regional trends in ozone.
- Inter-comparisons of top-down precursor emissions from reanalyses, and their impacts on surface/tropospheric ozone and subsequent radiative effects, within the reanalysis framework, will facilitate evaluation of emission scenarios and environmental policy in realistic conditions.
- Well-validated chemical reanalysis ozone fields will provide an opportunity to improve the TOAR-II observation quality control processes and representativeness by providing first guess information.

TOAR-II chemical reanalysis focus WG

Synergies with other TOAR-II Focus Working groups and IGAC activities

- facilitate quality control processes (first-guess) and provide representativeness information of various observational measurements for HEGIFTOM Focus Working Group.

- demonstrate the value of individual satellite measurements to study surface/tropospheric ozone, which will be shared with the Satellite Ozone Focus Working Group. Reanalysis products will also be used as transfer functions to inter-compare different satellite products and evaluate representativeness of individual satellite measurements.

- provide observationally-constrained information on the relationship between surface/tropospheric ozone and its precursors while constraining other chemical environments, which will benefit Ozone and Precursors in the Tropics (OPT) Focus Working Group & Tropospheric Ozone "Precursors (TOP) Focus Working Group

- use statistical approach proposed by Statistics Focus Working Group

- IGAC AMIGO, SPARC S-RIP

TOAR-II chemical reanalysis focus WG

Expected Outcomes

- Ability of current reanalysis products to study regional and global ozone trends. We will review and inter-compare global and regional (for many regions) surface/tropospheric ozone from the latest chemical reanalyses validated against TOAR-II observations (***publication 1***).

- What is the effective observing network to study surface/tropospheric ozone variations? We will assess the impact of satellite and in-situ ground-level ozone and precursor measurements on surface/tropospheric ozone analysis using multiple reanalysis systems (***publication 2***)

- Quantitative assessment of the impact of current emission inventories on chemistry/climate model simulations of surface/tropospheric ozone. We will inter-compare top-down and bottom-up precursor emissions inventories and their impacts on surface/tropospheric ozone using multiple reanalysis systems (***publication 3***)

- Provide representativeness information of various in-situ and satellite observational measurements

Publication 1: Overview of the current reanalysis products for studying global and regional variations in ozone

Reanalysis system	Grid	Resolution	Period	Scheme
CAMS (A. Inness)	GLOBAL	T255 (available at 0.75 deg)		4D-Var
GEOS-CHEM (Z. Qu)	GLOBAL	2°x2.5°	2005-2016	4D-Var
TCR2 (K. Miyazaki)	GLOBAL	1.1°x1.1°	2005-2019	EnKF
CAQRA (X. Tang)	CHINA	15 km x 15 km	2013-	EnKF
CMAQ-GSI (R.Kumar)	US, Asia	12 km x 12 km	2005-2018	3D-Var

Outline

1. Introduction
2. Description of reanalysis products
3. Interannual variations
4. Ozone trends
5. Evaluation of ozone precursors
6. Conclusions

Publication 2: Assessing the effective observing network for studying surface and tropospheric variations in ozone

System	Grid	Resolution	Strato/ Column O_3	Tropo O_3	Surface O_3	Precursors	Scheme
MOCAGE (E. Emili)	GLOBAL	2 x 2 deg or 1 x 1 deg	MLS	IASI	TOAR-II		3D-Var
CAMS (A. Inness)	GLOBAL	T255 (at 0.75 deg)	SBUV, OMI, MLS, GOME2, OMPS, SCIAMACHY, MIPAS, TROPOMI			CO, NO2	4D-Var
RAQMS (B. Pierce)	GLOBAL	1x1 degree	OMI, MLS	OMI cloud Cleared		CO, NO2	3D-Var
GEOS-CHEM (Z. Qu)	GLOBAL	2°x2.5°				OMI NO2	4D-Var
TCR2 (K. Miyazaki)	GLOBAL	1.1°x1.1°	MLS	TES, AIRS/ OMI, CrIS		CO, NO2, SO2	EnKF
CAQRA (X. Tang)	China	15 km x 15 km			China	CO, NO2	EnKF
CMAQ-GSI (R.Kumar)	US	12 km x 12 km				CO	3D-Var

Outline

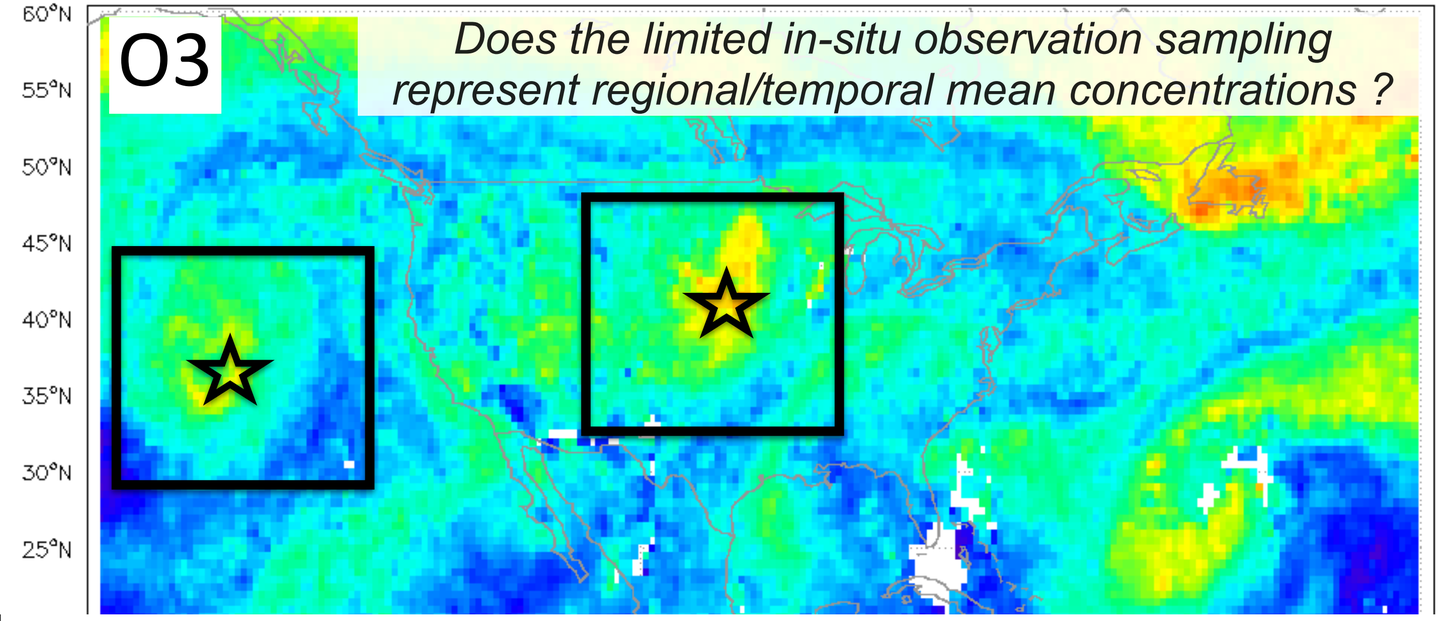
1. Introduction
2. Reanalysis systems
3. Observing System Experiments

- Impact of tropospheric ozone obs
- Impact of ozone precursor obs
- Impact of stratospheric obs

4. Integration of new observations and reanalysis algorithms
5. Discussion (future DA and satellite improvements)
6. Conclusion

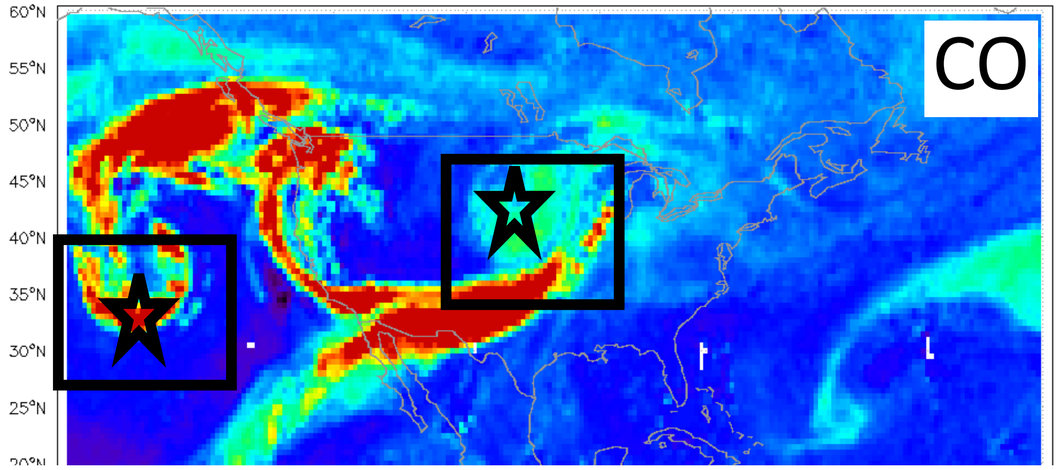
Sampling bias

- Arises due to unrepresentative sampling, which induces spurious features in the average estimates
- In regions where variability is dominated by short-term and/or small-scale variations, limited sampling may lead to a random sampling error.
- The primary technique for sampling bias estimation is to subsample model or reanalysis fields based on the sampling patterns of the measurements and then to quantify differences between the mean fields based on the measurement sampling and those derived from the complete fields.



CrIS at 464 hPa, 2020-09-12

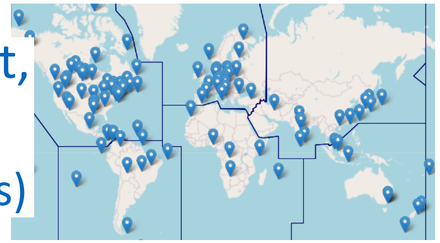
2020 California wildfires

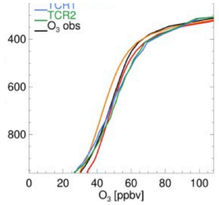


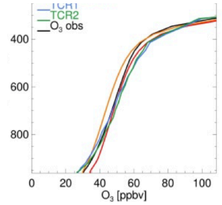
CrIS (JPL TROPESS products) provides detail spatial maps of complicated chemical responses linked to wildfires

Sampling bias

Sonde, aircraft,
Lidar etc
(sparse, profiles)

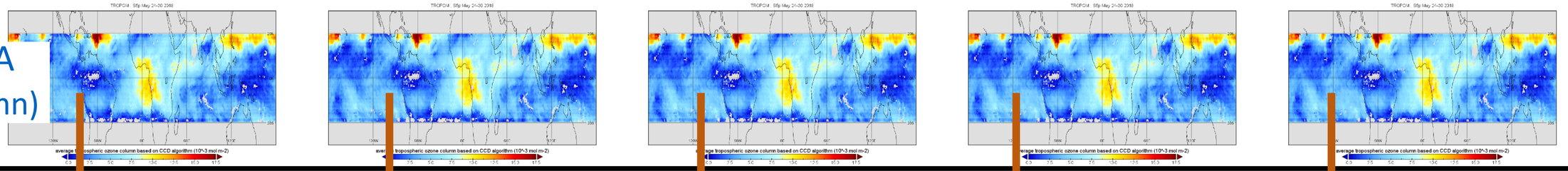




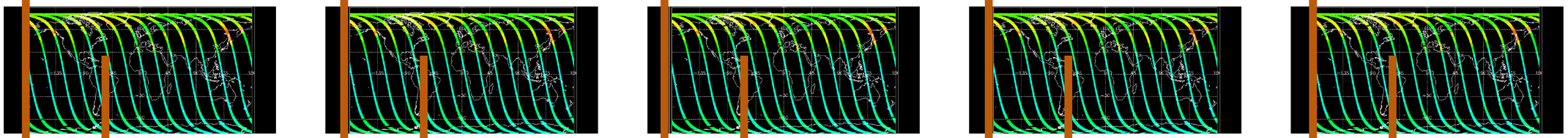


Time

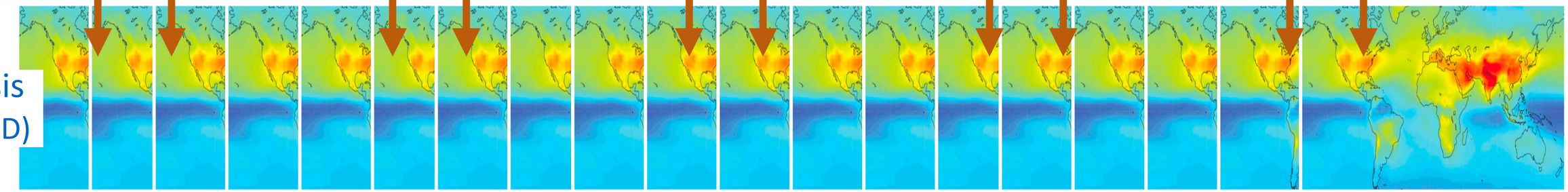
Satellite A
(daily, column)



Satellite B
(daily, column)



Reanalysis
(hourly, 3-D)



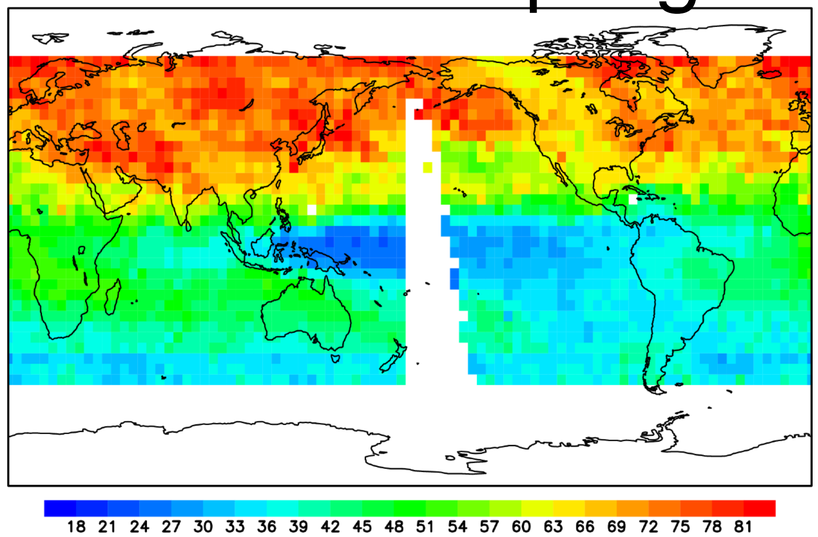
The reanalysis product provides comprehensive and unique information on global ozone distributions for the entire troposphere and on the weakness of the individual measurements and models.

→ limitation of the current ozonesonde network for evaluating temporally-spatially representative ozone fields

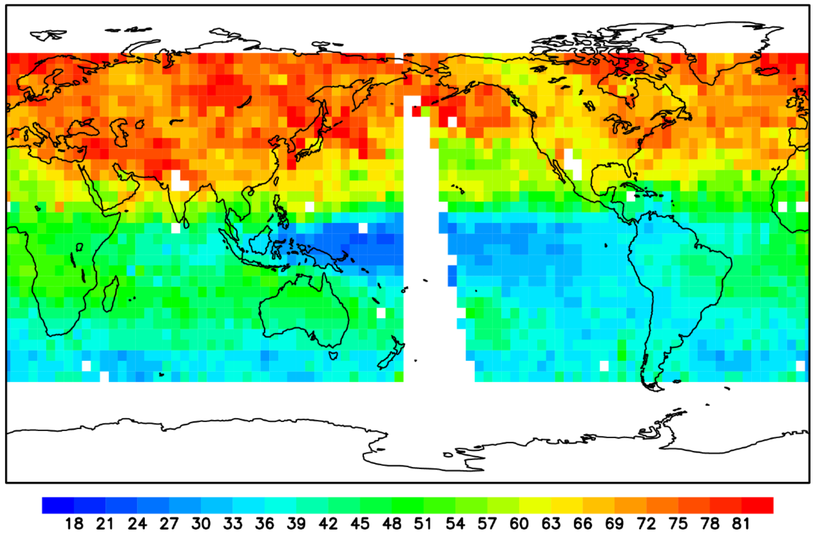
Satellite ozone sampling bias

JPL CrIS L2 data 2018 sampling

Full sampling



50 %



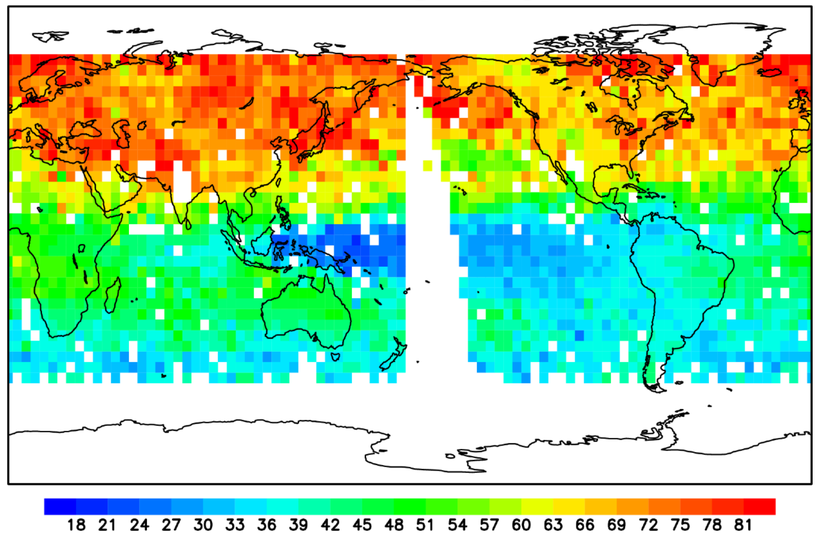
Reanalysis ozone [ppb] with CrIS sampling/AK

2005 annual mean

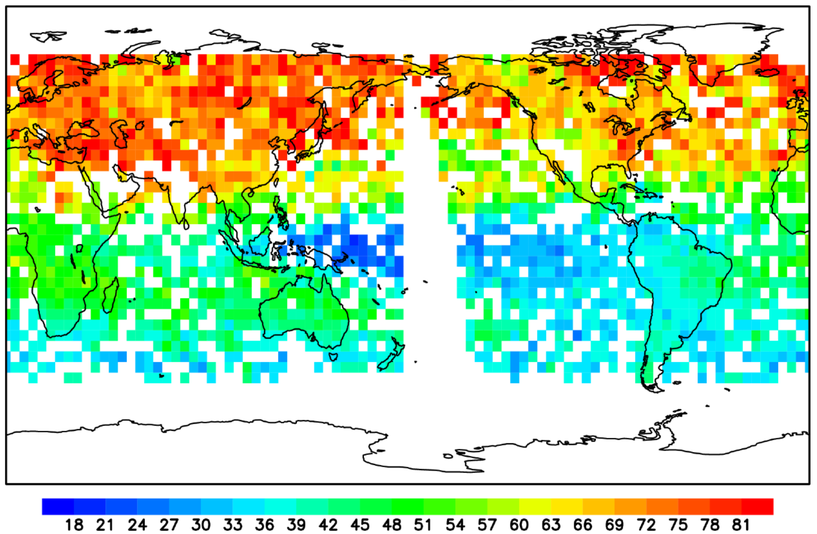
500 hPa

4x4 degree grid

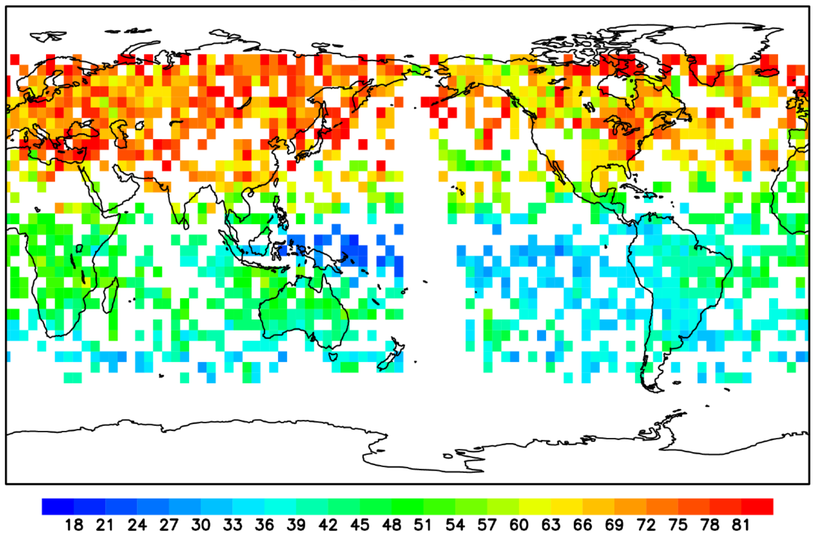
20 %



10 %



5 %

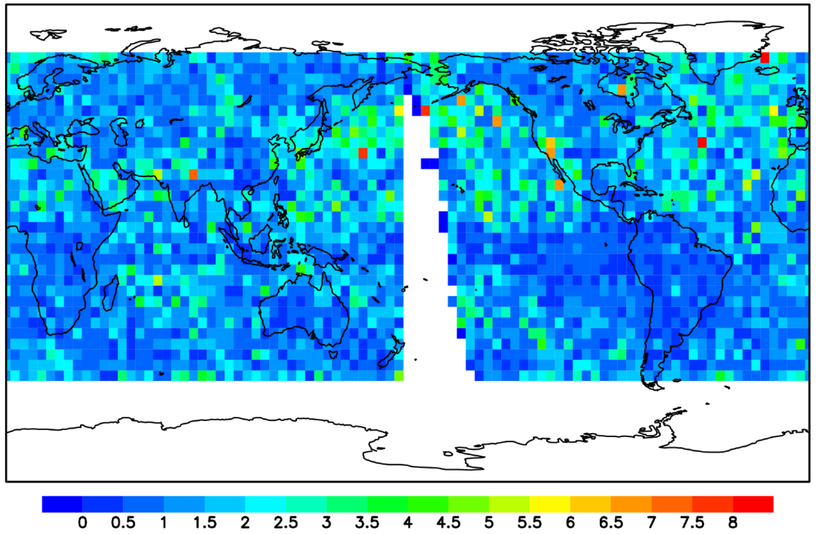


Satellite ozone sampling bias

Sampling	Global mean RMSE [ppb]
5%	4.76
10%	4.12
20%	3.03
50%	1.53

too large to capture spatial patterns?

50 %



RMSE against Full sampling

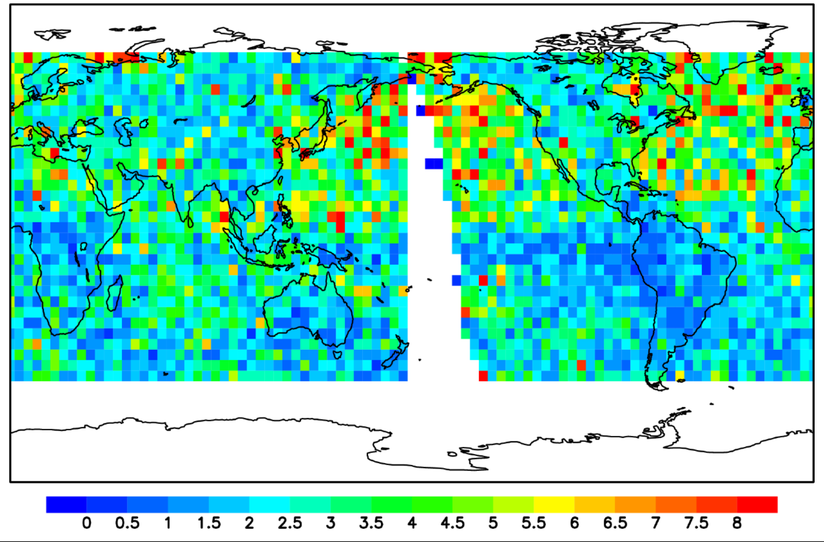
Reanalysis ozone [ppb] with CrIS sampling/AK

2005 annual mean

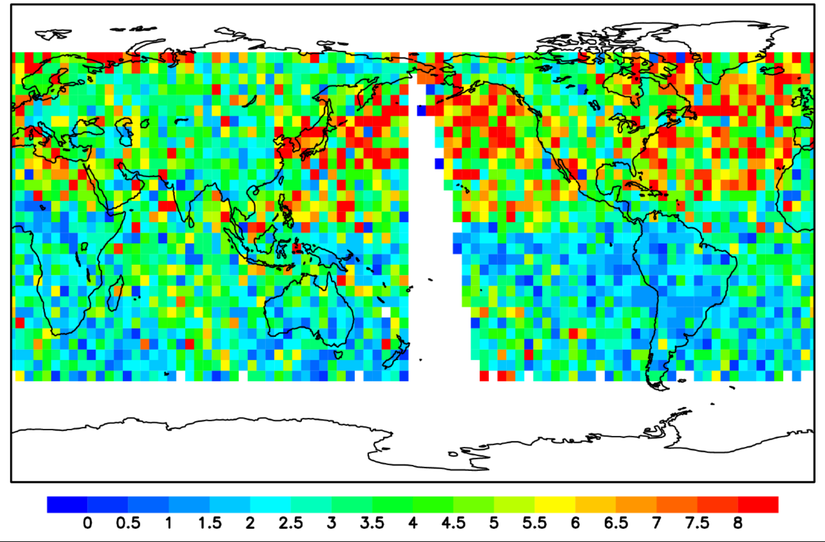
500 hPa

4x4 degree grid

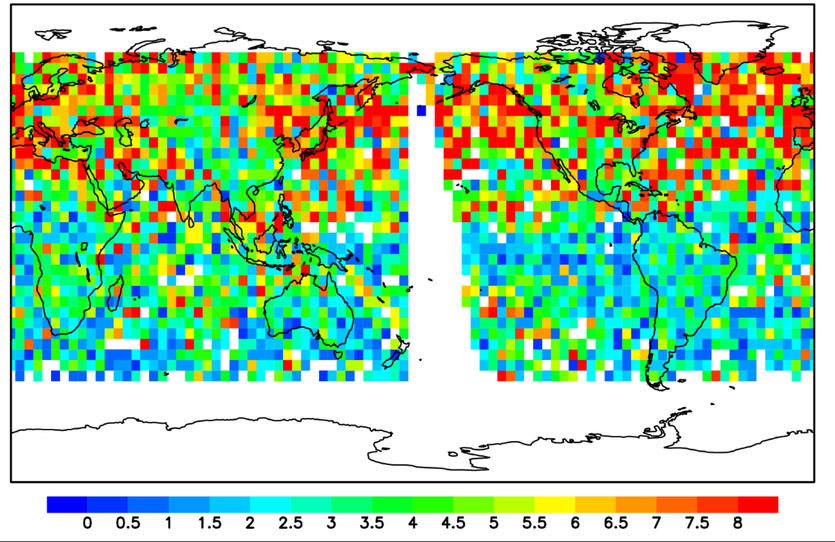
20 %



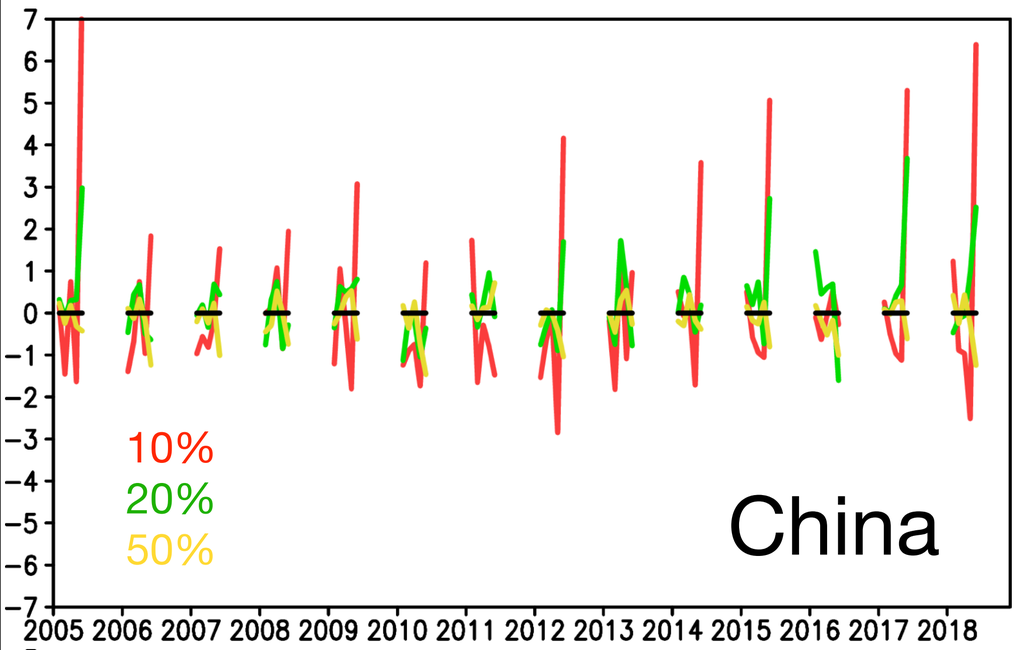
10 %



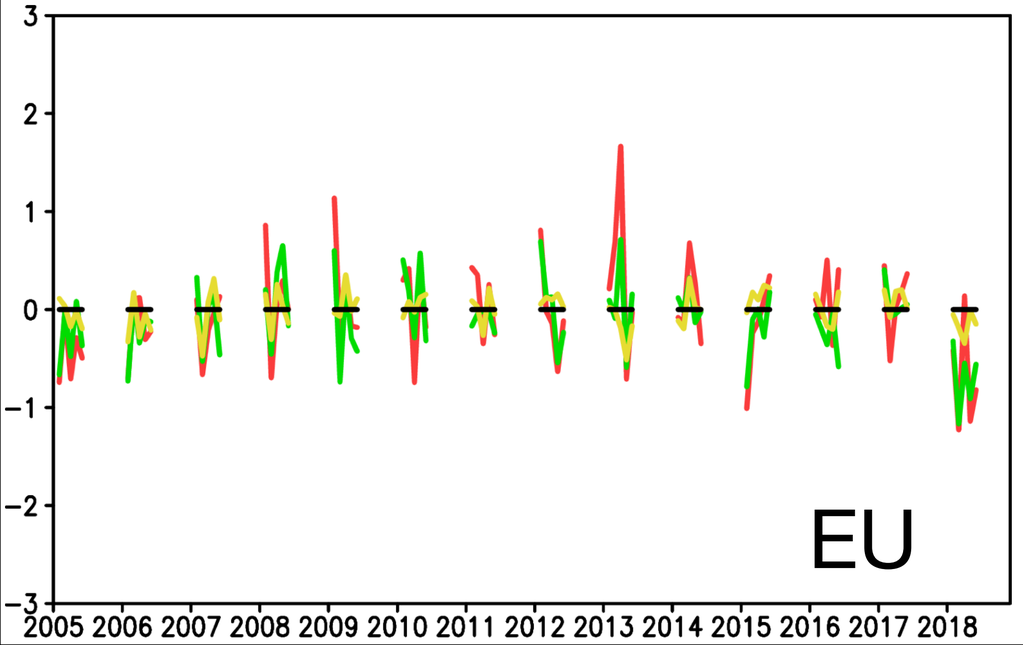
5 %



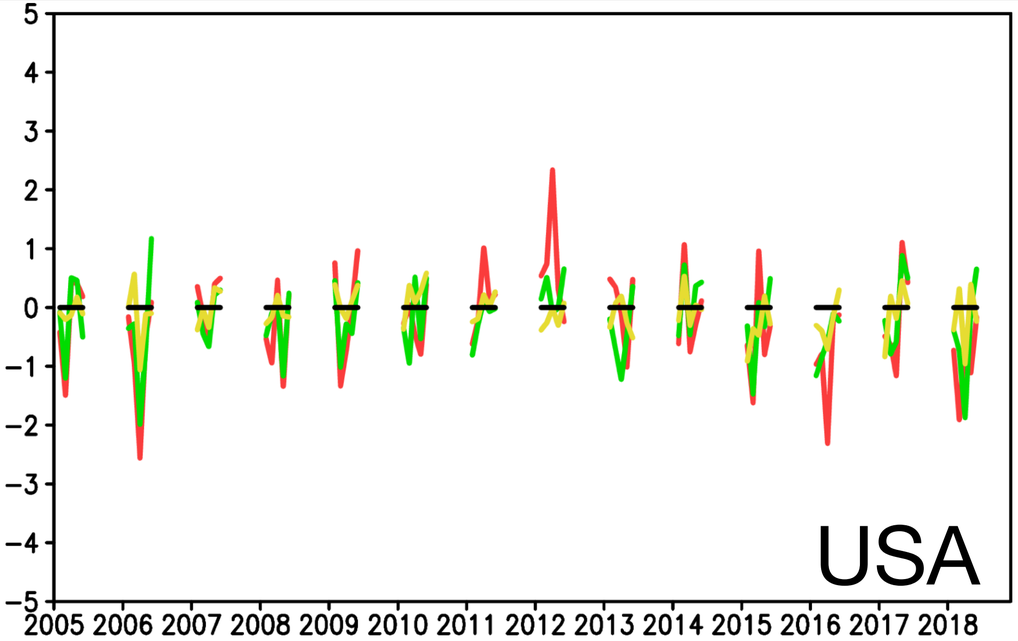
Satellite ozone sampling bias



RMSE [ppb]	
5%	7.06
10%	3.74
20%	1.34
50%	0.29



RMSE [ppb]	
5%	0.78
10%	0.53
20%	0.40
50%	0.13



RMSE [ppb]	
5%	1.11
10%	0.75
20%	0.66
50%	0.15

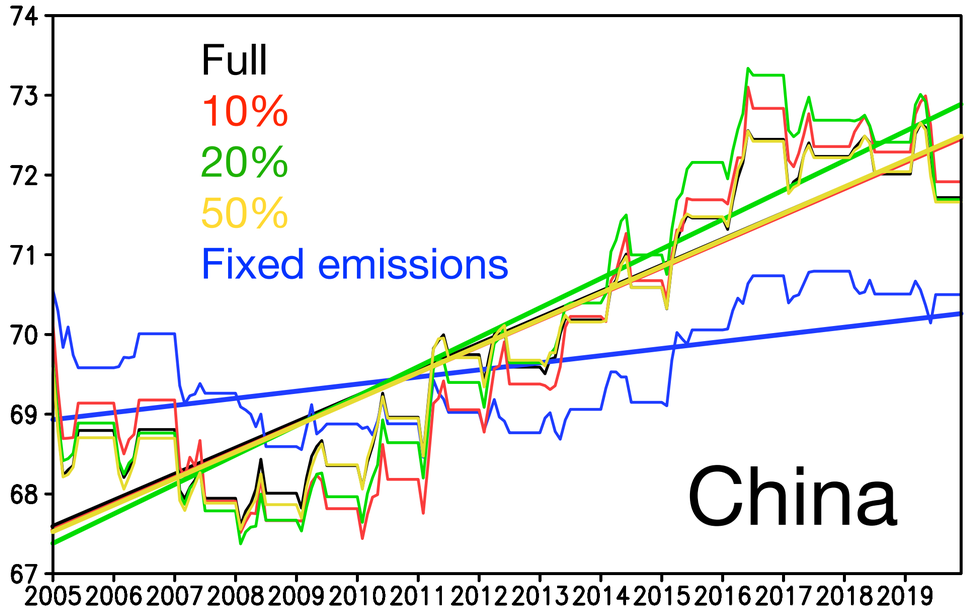
Regional & monthly mean bias against Full sampling

Reanalysis ozone [ppb] with CrIS sampling/AK

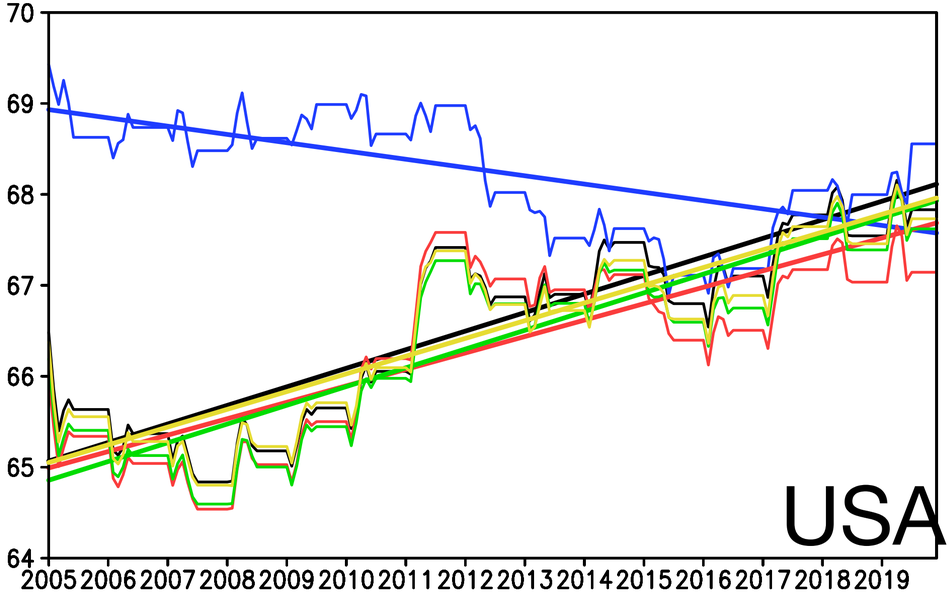
500 hPa

Regional mean

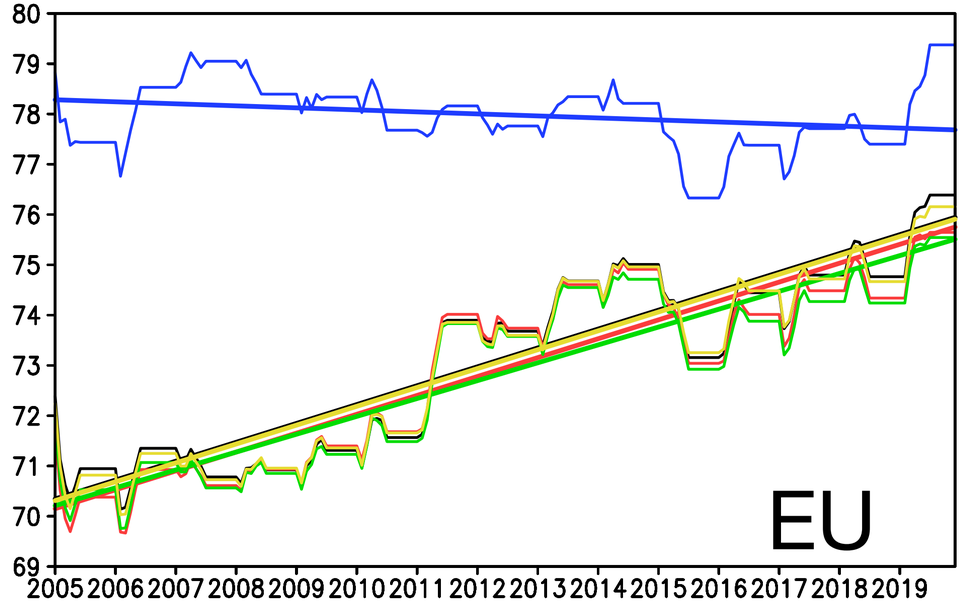
Linear trends and 2-year running means



	Slope	RMSE
Full	0.327	5.29
10%	0.329	6.26
20%	0.36	5.49
50%	0.333	5.29
Fix	0.089	3.49



	Slope	RMSE
Full	0.204	3.68
10%	0.181	3.72
20%	0.206	3.64
50%	0.195	3.73
Fix	-0.102	3.68



	Slope	RMSE
Full	0.375	5.76
10%	0.376	5.68
20%	0.355	5.69
50%	0.375	5.73
Fix	-0.040	4.92

Reanalysis ozone [ppb]
with CrIS sampling/AK

500 hPa

Regional mean

IGAC TOAR-II chemical reanalysis Focus Working Group

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- 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