Multi-constituent chemical data assimilation and AQ-GHG synergies

Kazuyuki Miyazaki (JAMSTEC)

K. W. Bowman, H. Eskes, T. Sekiya, K. Sudo

1. Global EnKF data assimilation systems

- Concentrations + emissions from multi-constituent retrievals
- Tropospheric chemistry reanalysis (2005-2017)
- Multi-model (incl. GEOS-Chem) EnKF inter-comparison

2. AQ-GHG synergies

- through OH coupling (CH_4, O_3)
- joint emission optimization for NOx+CO+CO_2
- transport error diagnostics, combustion process

3. AQ-GHG OSSEs

Tropospheric chemistry reanalyses (TCR)

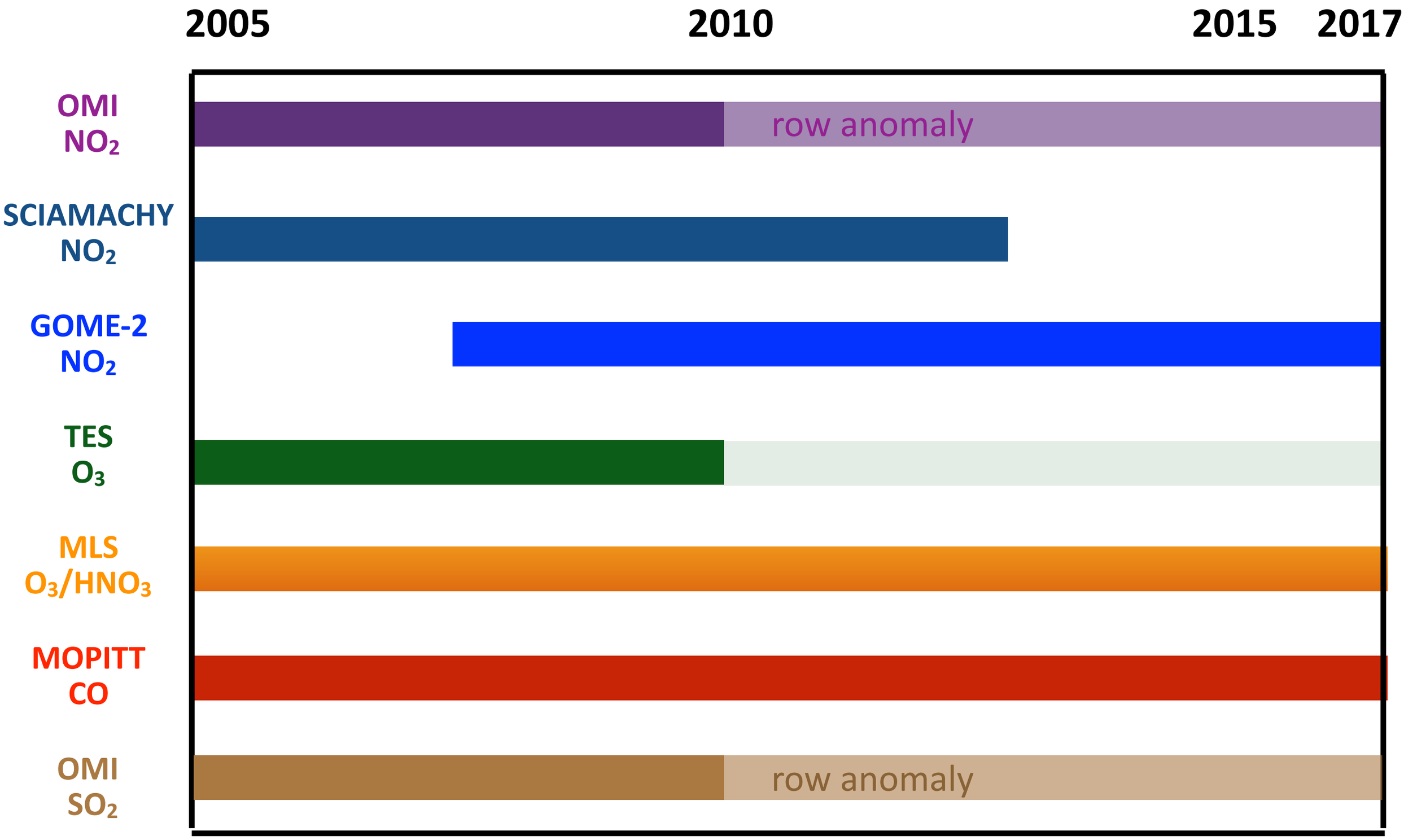
	TCR-1	TCR-2	MACCRA	CAMSiRA
Period	2005-2012	2005-2017	2003-2012	2003-2015
Horizontal resolution	2.8°	1.1°	80 km	110 km
Vertical resolution	32 layers to 4 hPa (sigma)	32 layers to 4 hPa (hybrid)	60 layers to 0.1 hPa	60 layers to 0.1 hPa
Forecast model	CCSR/NIES/FRCGC AGCM-CHASER	MIROC-Chem	C-IFS MOZART-3	C-IFS CB05/ Cariolle ozone
Assimilation scheme	EnKF	EnKF	4D-VAR (w/ bias correction)	4D-VAR (w/ bias correction)
Assimilated measurements	OMI (DOMINO2), TES (v5), MOPITT (v6 NIR), MLS (3.3)	OMI (QA4ECV, PCA), SCIAMACHY, GOME-2 (QA4ECV), TES (v6), MOPITT (v7 TIR/NIR), MLS (v4.2)	GOME, MIPAS, MLS, OMI, SBUV/2, SCIAMACHY, IASI, MOPIITT, MODIS	GOME, MIPAS, MLS, OMI, SBUV/2, SCIAMACHY, IASI, MOPIITT, MODIS
Assimilated species	O3, CO, NO2, HNO3	O3, CO, NO2, SO2, HNO3	O3, CO, AOD	O3, CO, AOD
State vector	Concentrations of 35 species + emissions (NOx, CO, LNOx)	Concentrations of 35 species + emissions (NOx, SO2, diurnal variability, CO, LNOx)	Concentrations	Concentrations
Reference	Miyazaki et al. 2015	Miyazaki et al. in prep	Inness et al., 2013	Flemming et al., 2017

Tropospheric chemistry reanalyses (TCR)

	TCR-1	TCR-2	MACCRA	CAMSiRA
Period	2005-2012	2005-2017	2003-2012	2003-2015
Horizontal resolution	2.8°	1.1°	80 km	110 km
Vertical resolution	32 layers to 4 hPa (sigma)	32 layers to 4 hPa (hybrid)	60 layers to 0.1 hPa	60 layers to 0.1 hPa
Forecast model	CCSR/NIES/FRCGC AGCM-CHASER	MIROC-Chem	C-IFS MOZART-3	C-IFS CB05/ Cariolle ozone
Assimilated species	O3, CO, NO2, HNO3	O3, CO, NO2, SO2, HNO3	O3, CO, AOD	O3, CO, AOD
State vector	Concentrations of 35 species + emissions (NOx, CO, LNOx)	Concentrations of 35 species + emissions (NOx, SO2, diurnal variability, CO, LNOx)	Concentrations	Concentrations
Reference	Miyazaki et al. 2015	Miyazaki et al. in prep	Inness et al., 2013	Flemming et al., 2017

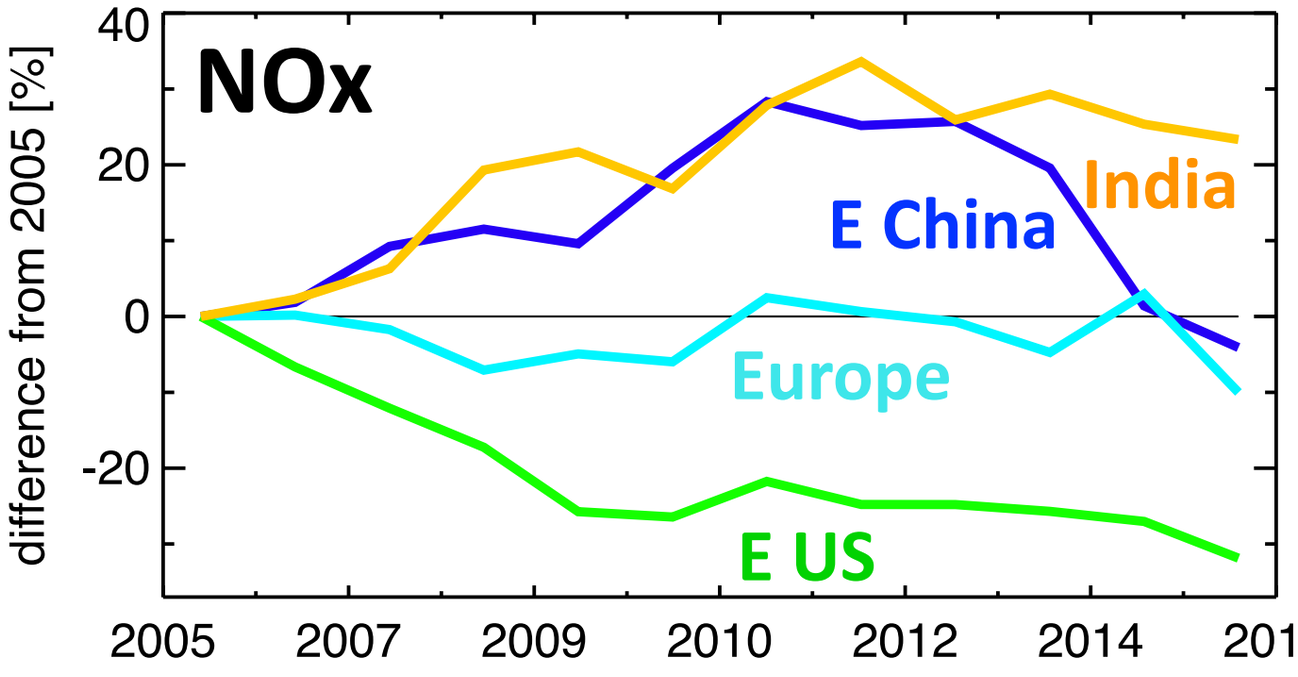
- Multiple-species assimilation provides comprehensive constraints on emissions while improving chemical lifetimes (OH) and reducing model errors
- The improved representations of the emission variability benefit the atmospheric concentration analysis through a reduction in model forecast error.

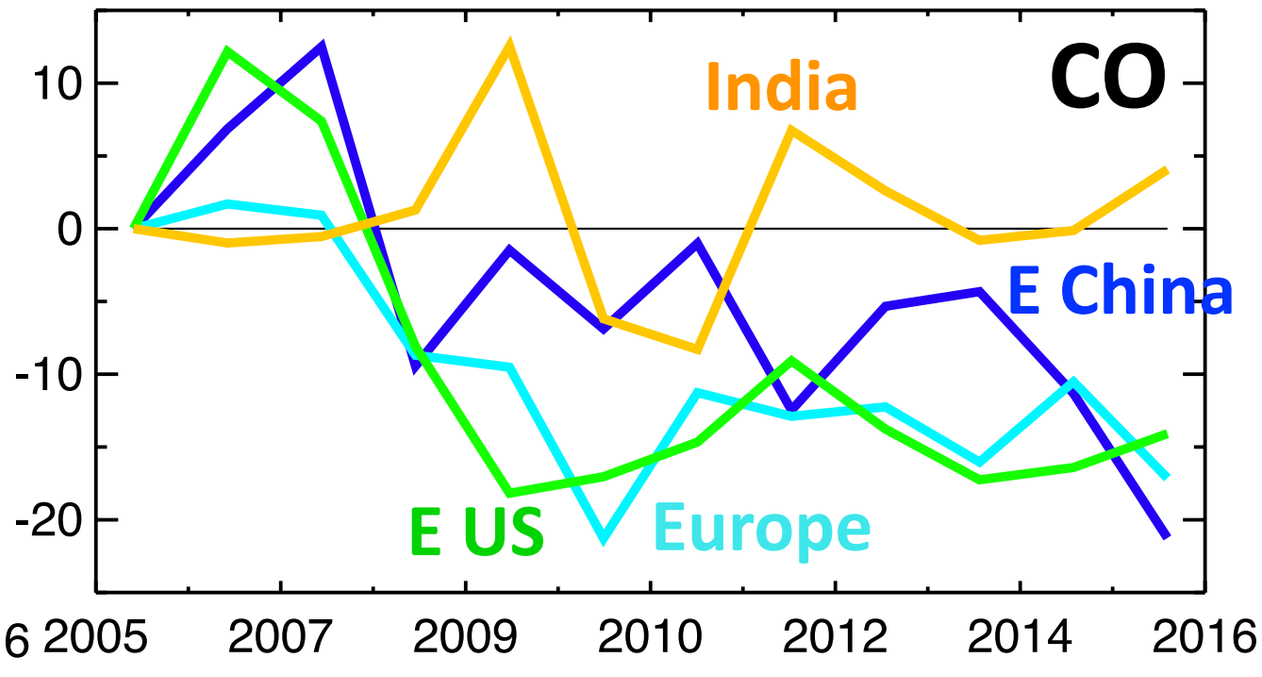
Tropospheric Chemistry Reanalysis (TCR-2)



Global NOx and CO trends from TCR

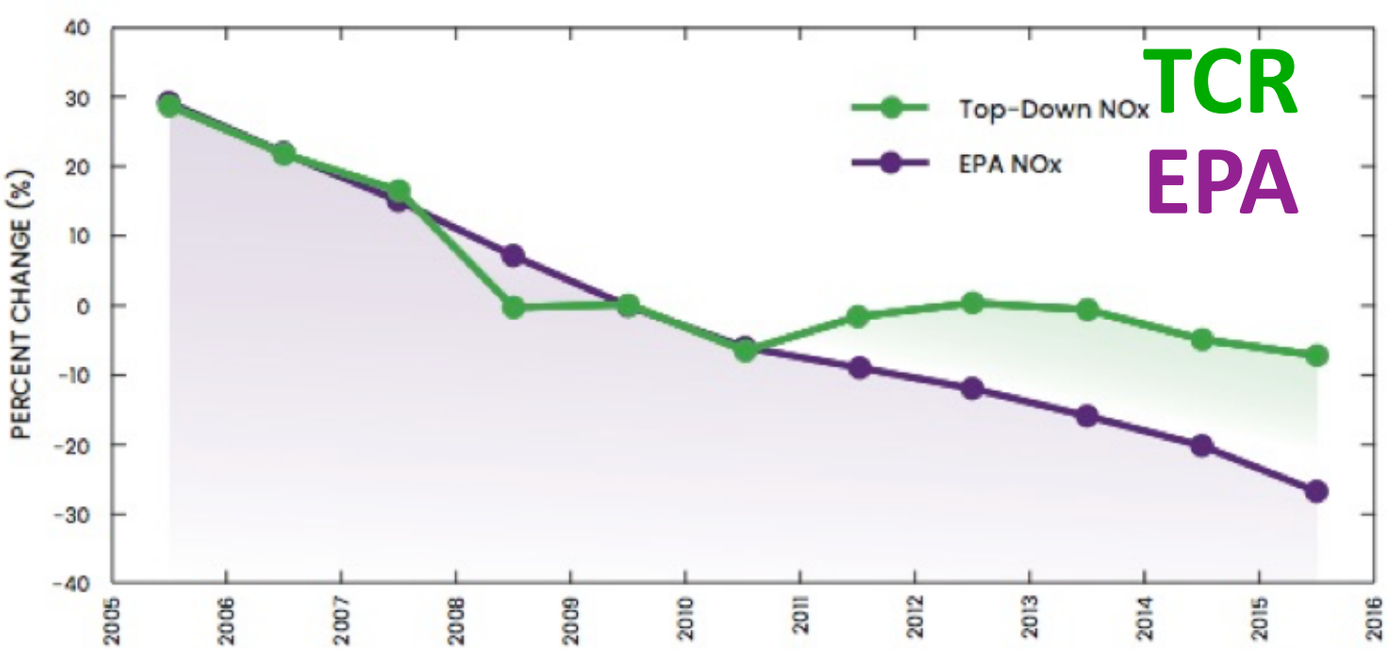
Miyazaki et al., ACP, 2017

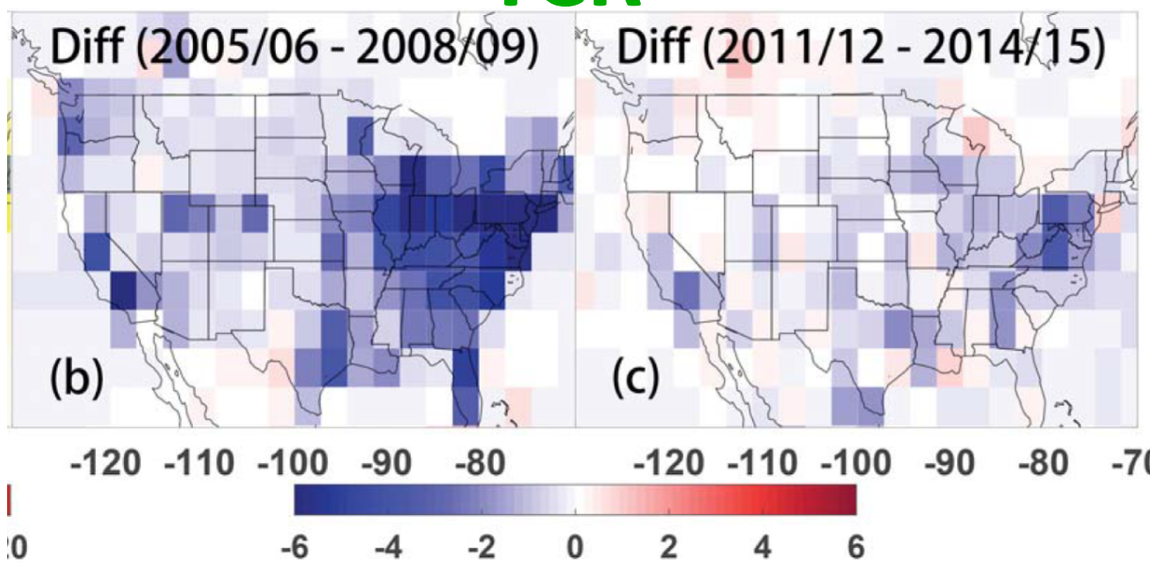




Unexpected slowdown of US pollutant emission reduction

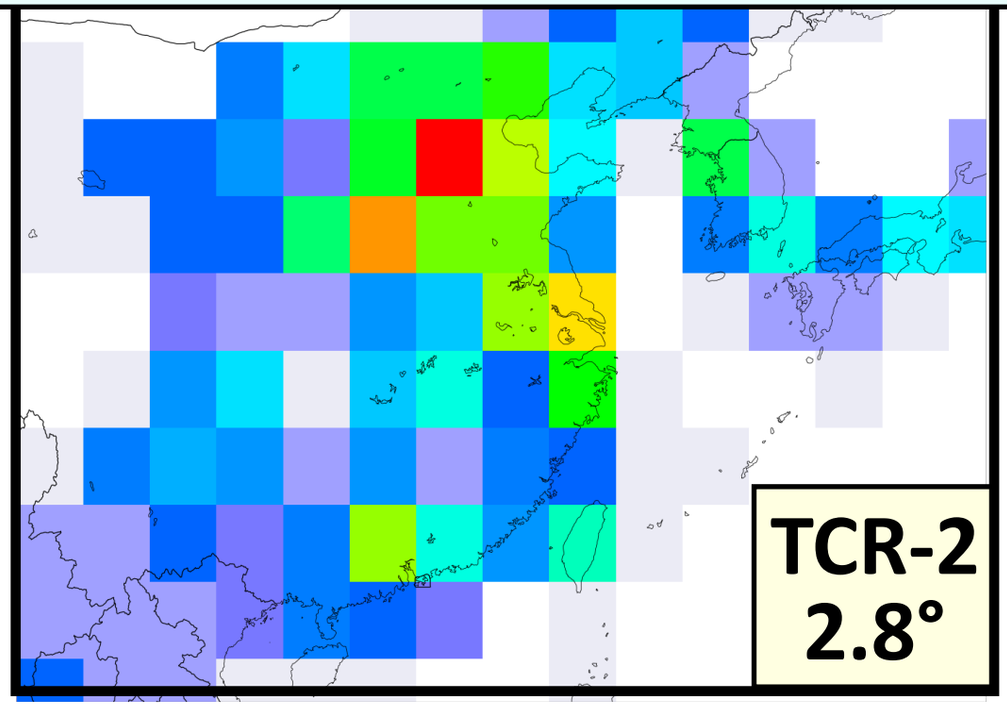
Jiang et al., PNAS, 2018

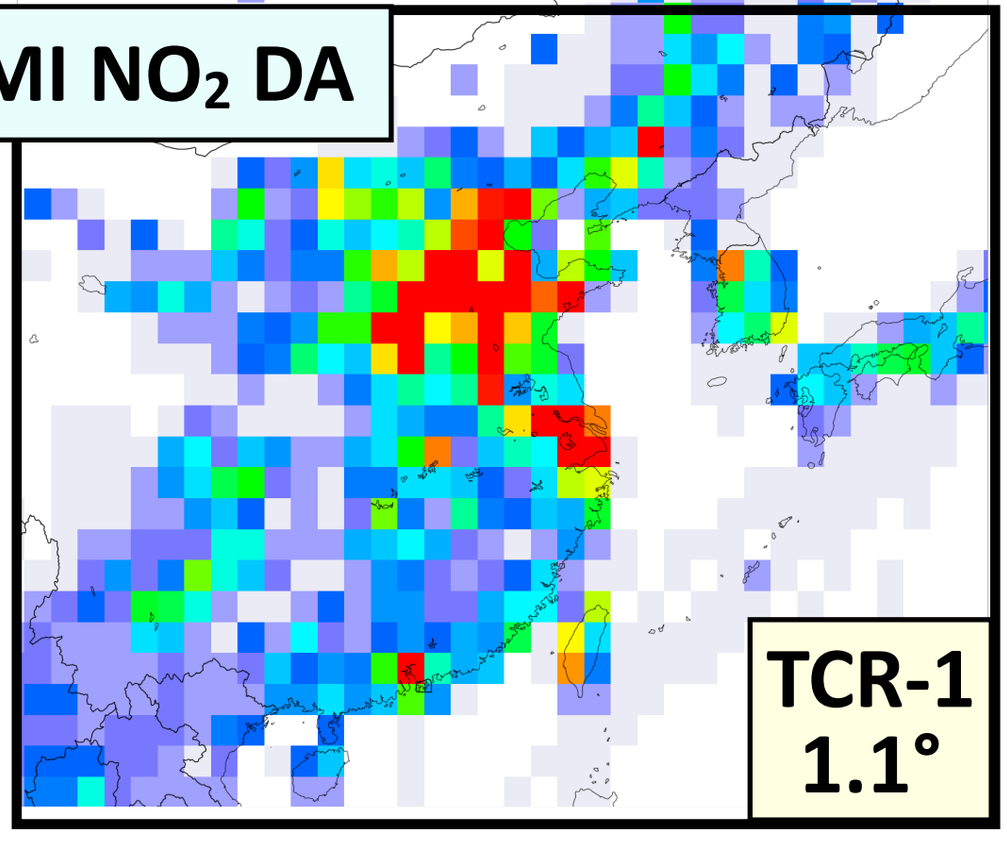




Top-down emission (TCR) estimates show that the decline has slowed dramatically in recent years.

Estimated NOx emissions from QA4ECV OMI NO_2 DA





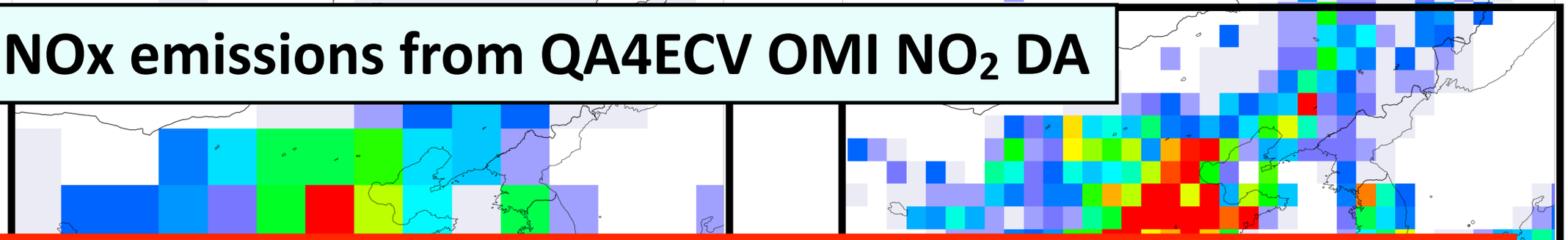
Estimated NOx emissions from QA4ECV OMI NO_2 DA

TCR-2
2.8°

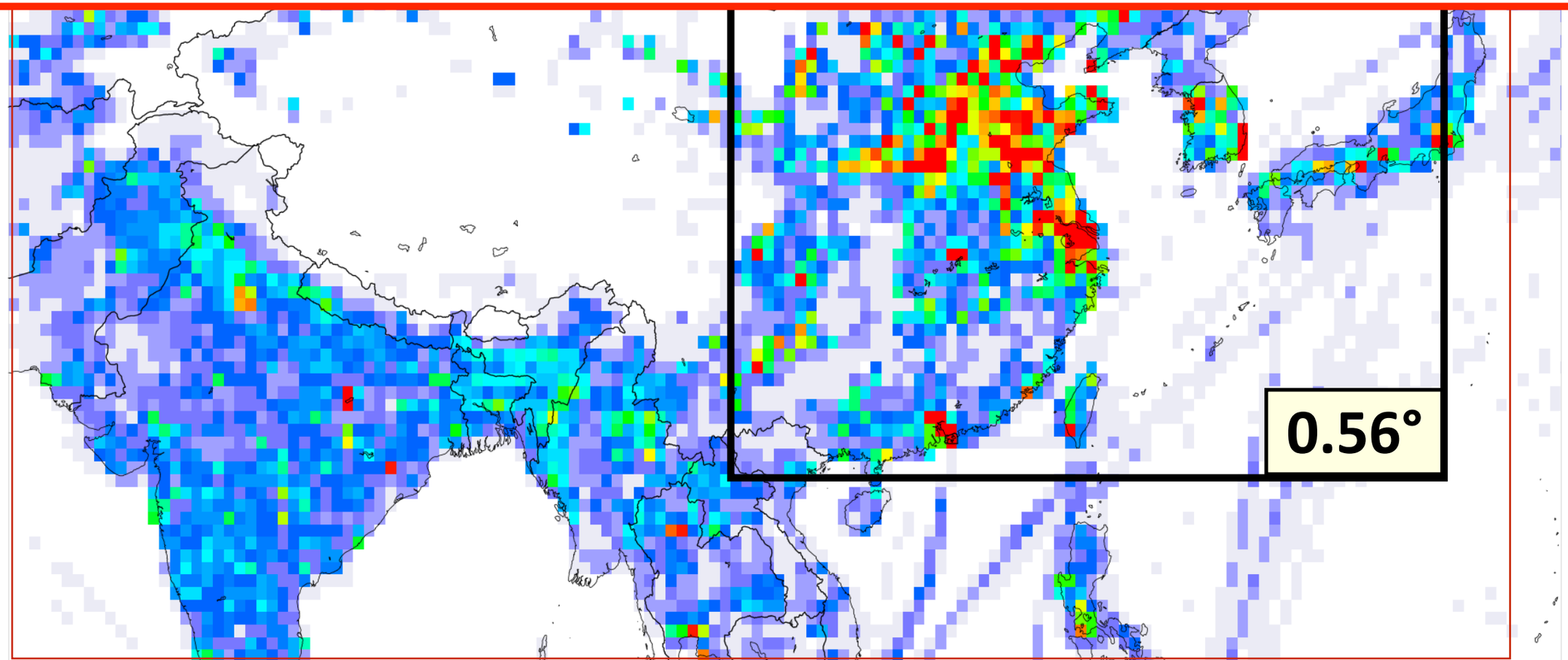
TCR-1
1.1°

0.56°

Estimated NOx emissions from QA4ECV OMI NO_2 DA

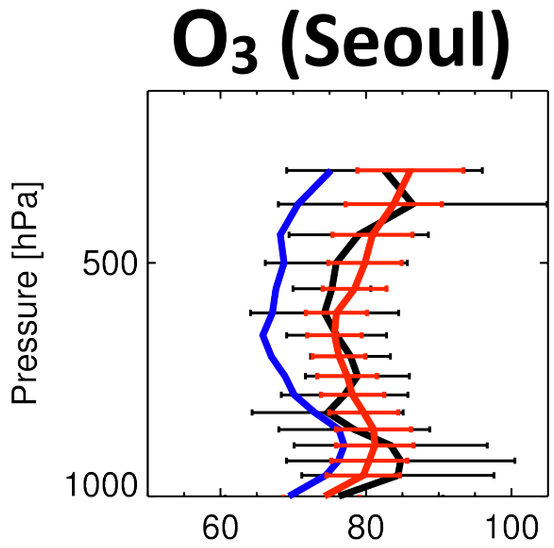


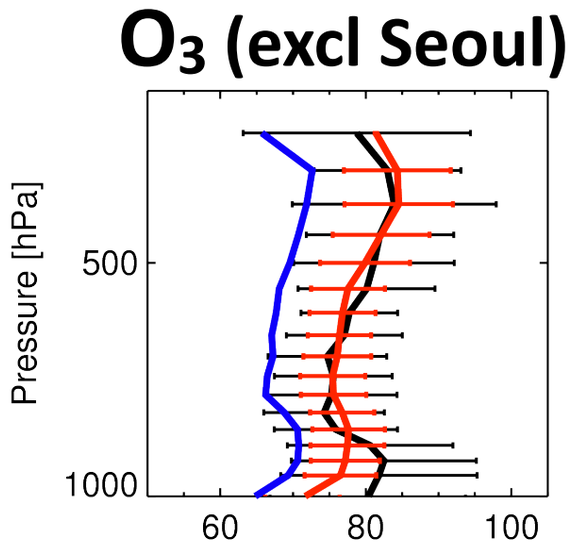
- **1.1° TCR-2 for 2005-2017:** will be released soon. For decadal atmospheric composition variability at megacity-scale
- **0.56° DA**: multi-constituent (NOx, CO, SO_2, O_3, HCHO) data from TROPOMI and 3-GEOs
- Aerosol and GHG DA may be included in the future

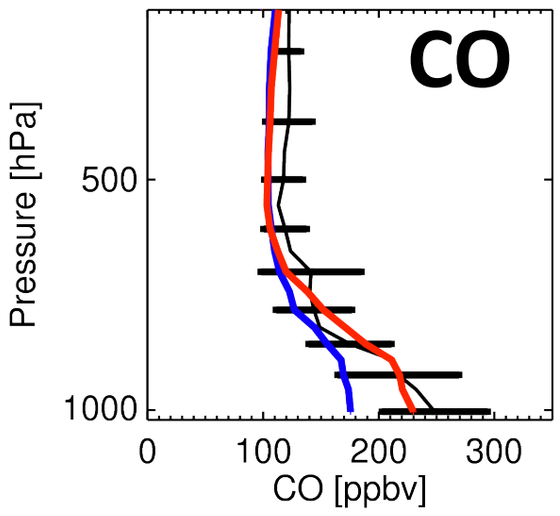


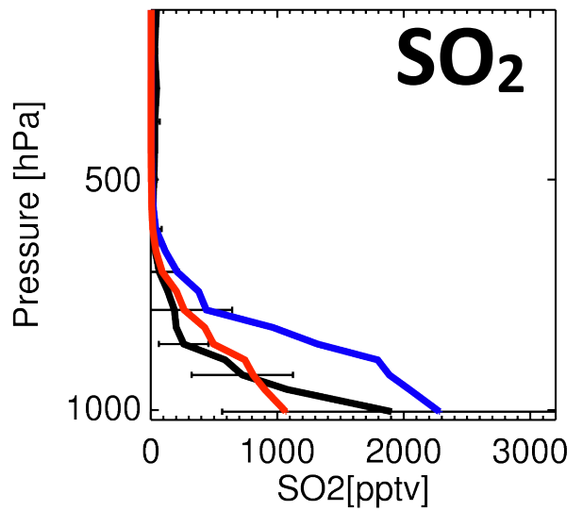
TCR-2 validation: Mean DC-8 profiles

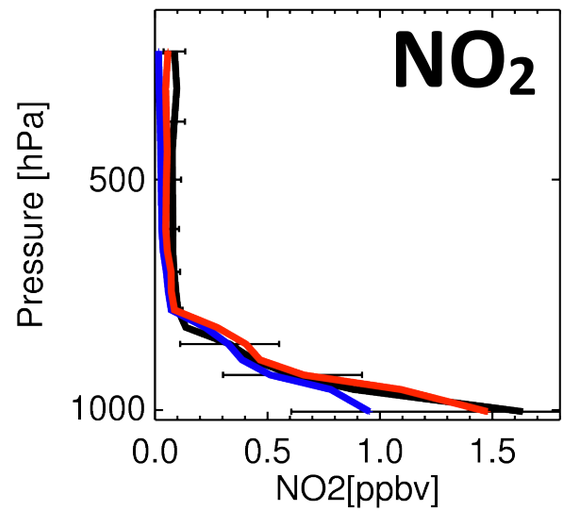
KORUS-AQ

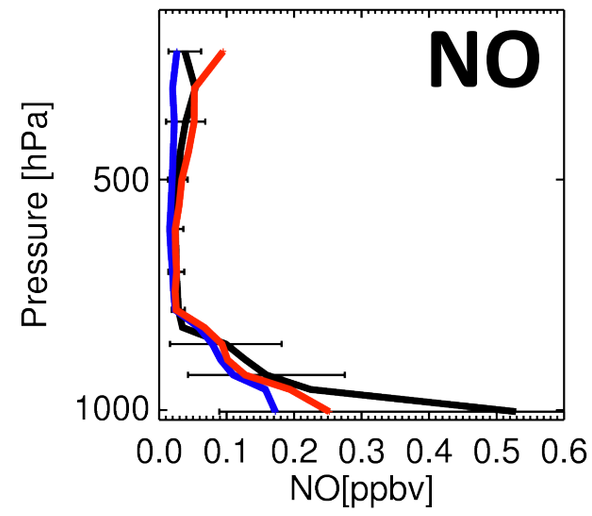


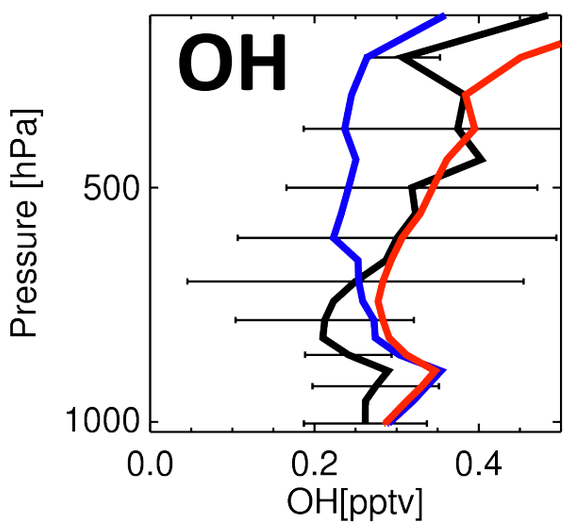


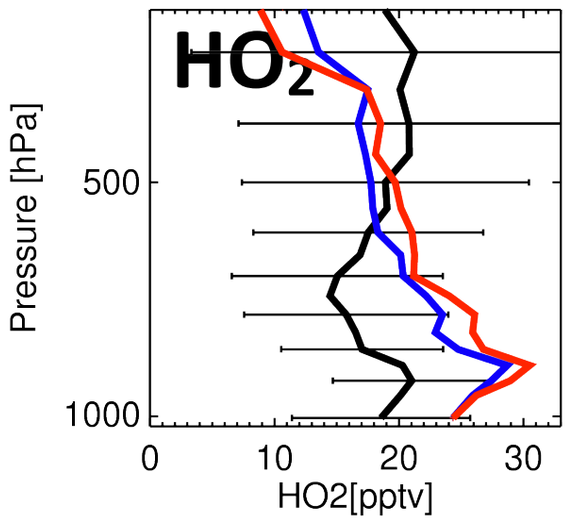


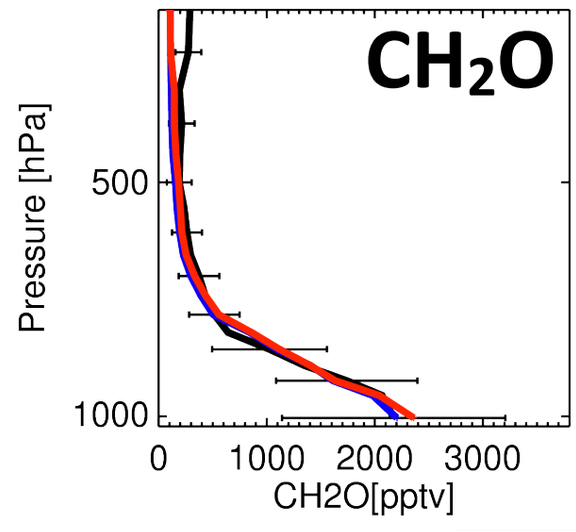


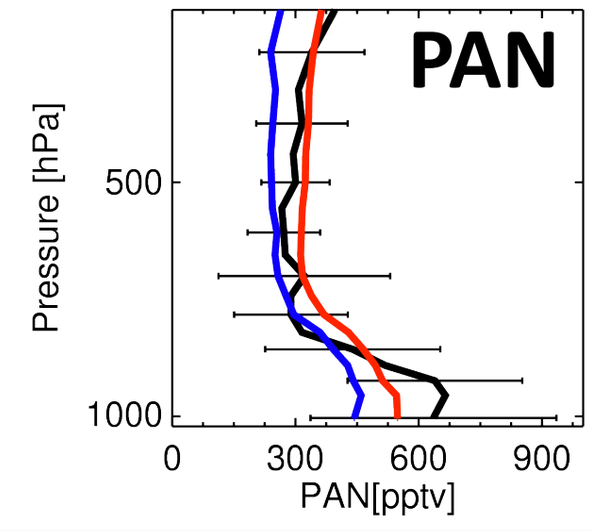












Observation **Model** **TCR-2**

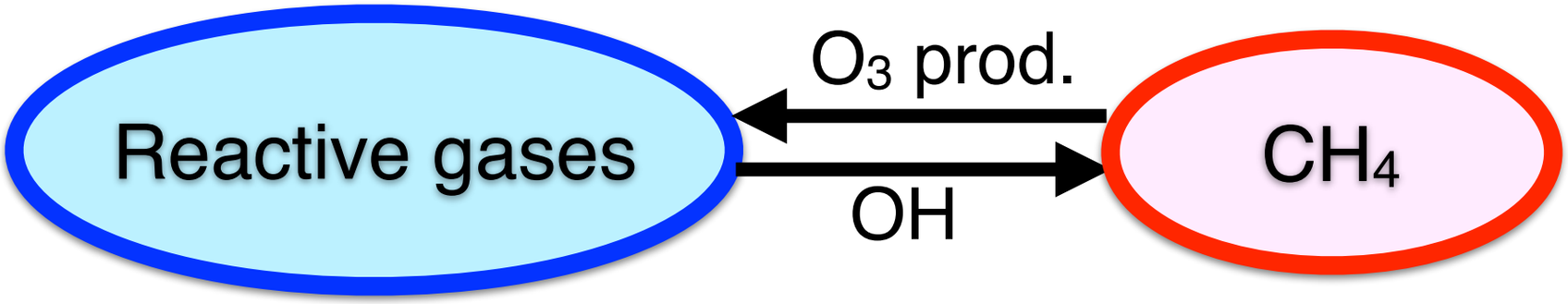
Miyazaki et al., submitted

AQ-GHG synergies

NOx-CO-O_3 +α → OH → CH_4

(from monthly to decadal scales)

TCR + any CTMs (CH4 inversion)



OMI, TES, MLS
SCIAMACHY,
GOME-2, MOPITT,
TROPOMI
(NOx, CO, SO2, O3, HCHO)

GOSAT
TROPOMI

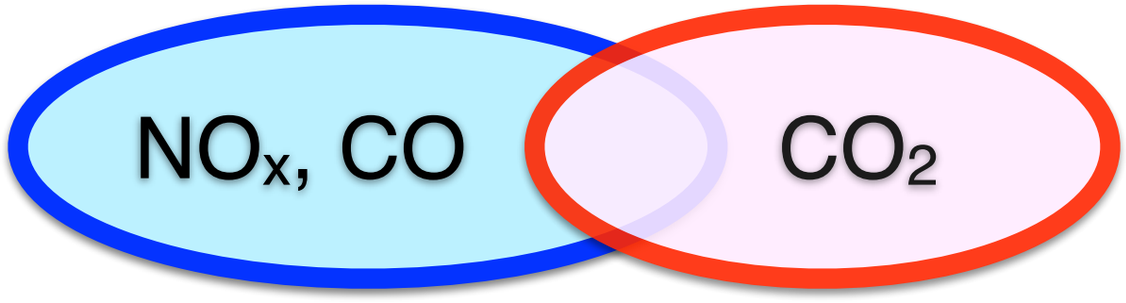
AQ-GHG synergies

NOx-CO-CO_2 joint emission inversion

Transport error diagnostics

Changes in composition due to anthropogenic combustion

TCR + CO_2 inversions (JAMSTEC and others)



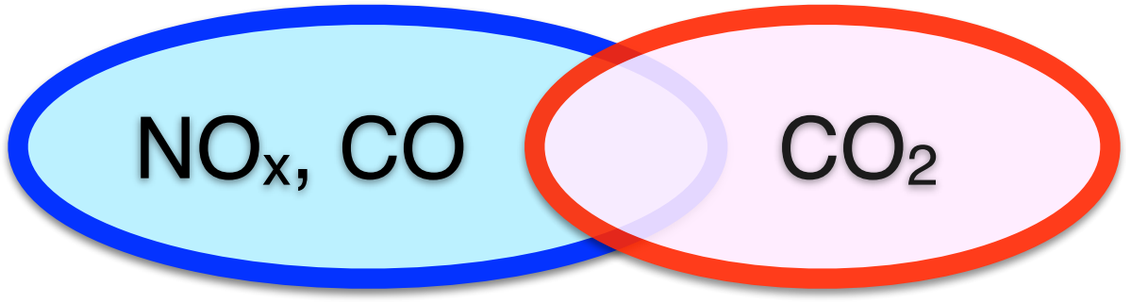
AQ-GHG synergies

NOx-CO-CO_2 joint emission inversion

Transport error diagnostics

Changes in composition due to anthropogenic combustion

TCR + CO_2 inversions (JAMSTEC and others)



	GOSAT	GOSAT-2	GOSAT-3
Species	CO_2, CH_4	CO_2, CH_4, CO	????
OSSE	No	No	Yes?

	1. GEOS-Chem	2. CHASER (TCR-1)	3. MIROC	4. MIROC-H (TCR-2)
Horizontal resolution	2°x2.5°	2.8°x2.8°	2.8°x2.8°	1.1°x1.1°
Vertical resolution	47 layers to 0.1 hPa (hybrid)	32 layers to 4 hPa (sigma)	32 layers to 4 hPa (hybrid)	32 layers to 4 hPa (hybrid)
Forecast model	GEOS-Chem v9 (adjoint v35)	CCSR/NIES/FRCGC AGCM-CHASER	MIROC-Chem	MIROC-Chem
Chemistry	43 species, 318 reactions	47 species, 88 reactions	92 species, 262 reactions	92 species, 262 reactions
Met data	GEOS-5	Nudged to NCEP-DOE/ AMIP-2	Nudged to ERA-Interim	Nudged to ERA-Interim
A priori emissions	EDGAR, NEI2008, RETRO, GFED2,	EDGAR 4.2, GFED 3.1, GEIA	EDGAR 4.2, GFED 3.1, GEIA	HTAP2, GFED4, GEIA
Assimilated measurements	OMI (DOMINO2), TES (v5), MOPITT (v6 NIR), MLS (3.3)	OMI (DOMINO2), TES (v5), MOPITT (v6 NIR), MLS (3.3)	OMI (DOMINO2), TES (v5), MOPITT (v6 NIR), MLS (3.3)	OMI (QA4ECV, PCA), SCIAMACHY, GOME-2 (QA4ECV), TES (v6), MOPITT (v7J), MLS (v4.2)
Assimilated species	O3, CO, NO2, HNO3	O3, CO, NO2, HNO3	O3, CO, NO2, HNO3	O3, CO, NO2, SO2, HNO3
State vector	Concentrations of 43 species + emissions (NOx, CO, LNOx)	Concentrations of 35 species + emissions (NOx, diurnal variability, CO, LNOx)	Concentrations of 35 species + emissions (NOx, diurnal variability, CO, LNOx)	Concentrations of 35 species + emissions (NOx ,diurnal variability, CO, SO2, LNOx)
Reference	Miyazaki et al. 2018b (in prep.)	Miyazaki et al. 2012a,b 2013, 2014, 2015	Miyazaki et al. 2017	Miyazaki et al. 2018a (in prep.)

	1. GEOS-Chem	2. CHASER (TCR-1)	3. MIROC	4. MIROC-H (TCR-2)
Horizontal resolution	2°x2.5°	2.8°x2.8°	2.8°x2.8°	1.1°x1.1°
Vertical resolution	47 layers to 0.1 hPa (hybrid)	32 layers to 4 hPa (sigma)	32 layers to 4 hPa (hybrid)	32 layers to 4 hPa (hybrid)
Forecast model	GEOS-Chem v9 (adjoint v35)	CCSR/NIES/FRCGC AGCM-CHASER	MIROC-Chem	MIROC-Chem
Chemistry	43 species, 318 reactions	47 species, 88 reactions	92 species, 262 reactions	92 species, 262 reactions
Met data	GEOS-5	Nudged to NCEP-DOE/ AMIP-2	Nudged to ERA-Interim	Nudged to ERA-Interim
A priori emissions	EDGAR, NEI2008, RETRO, GFED2,	EDGAR 4.2, GFED 3.1, GEIA	EDGAR 4.2, GFED 3.1, GEIA	HTAP2, GFED4, GEIA
Assimilated measurements	OMI (DOMINO2), TES (v5), MOPITT (v6 NIR), MLS (3.3)	OMI (DOMINO2), TES (v5), MOPITT (v6 NIR), MLS (3.3)	OMI (DOMINO2), TES (v5), MOPITT (v6 NIR), MLS (3.3)	OMI (QA4ECV, PCA), SCIAMACHY, GOME-2 (QA4ECV), TES (v6), MOPITT (v7J), MLS (v4.2)
Assimilated species	O3, CO, NO2, HNO3	O3, CO, NO2, HNO3	O3, CO, NO2, HNO3	O3, CO, NO2, SO2, HNO3
				Concentrations of 25
Reference	Miyazaki et al. 2018b (in prep.)	Miyazaki et al. 2012a,b 2013, 2014, 2015	Miyazaki et al. 2017	Miyazaki et al. 2018a (in prep.)

Observation sensitivity assessment based on multi-model DA systems would help to evaluate the value of observing systems

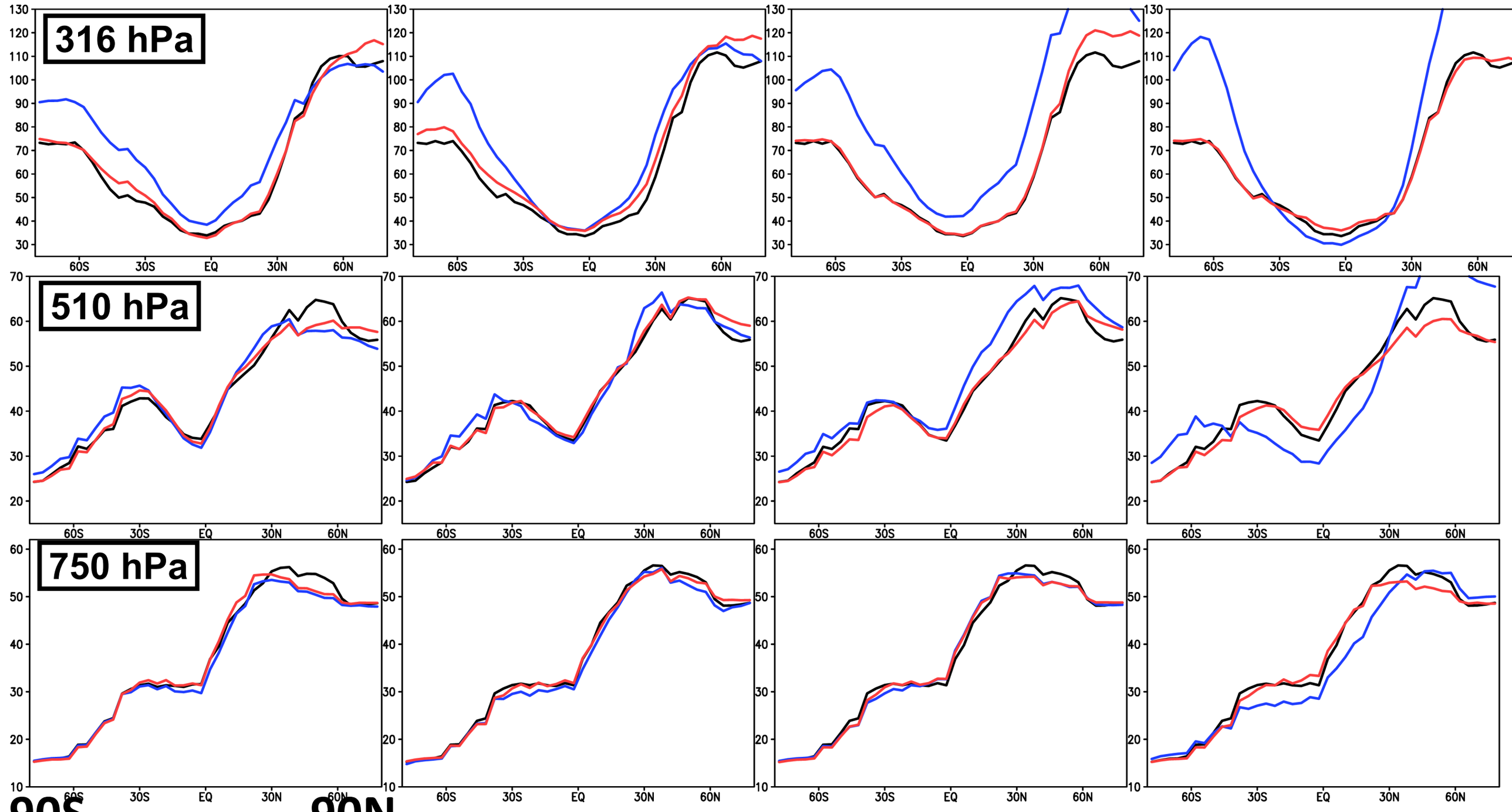
TES ozone (ppbv): zonal mean

GC | CHASER (TCR-1) | MIROC | MIROC-H (TCR-2)

316 hPa

510 hPa

750 hPa

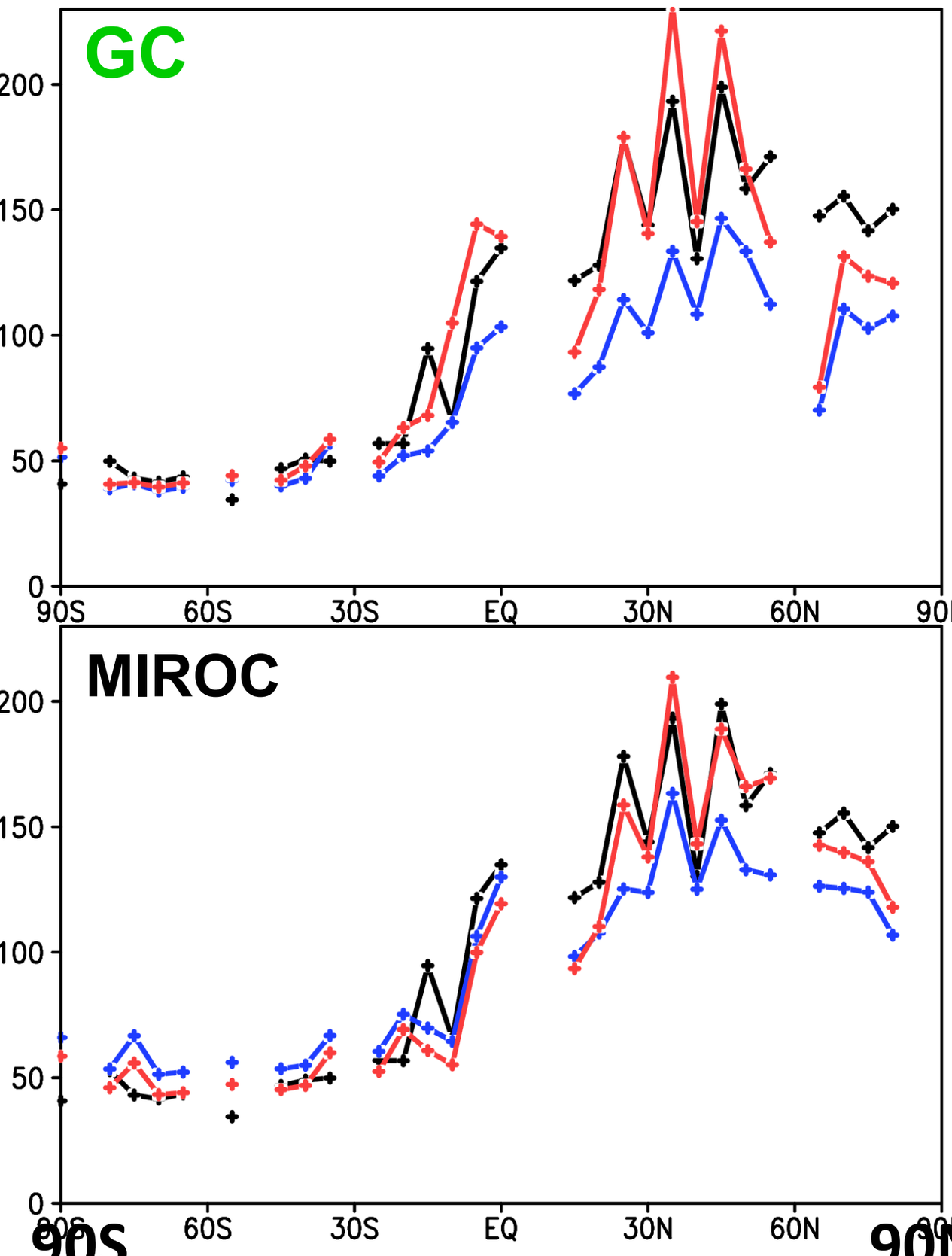


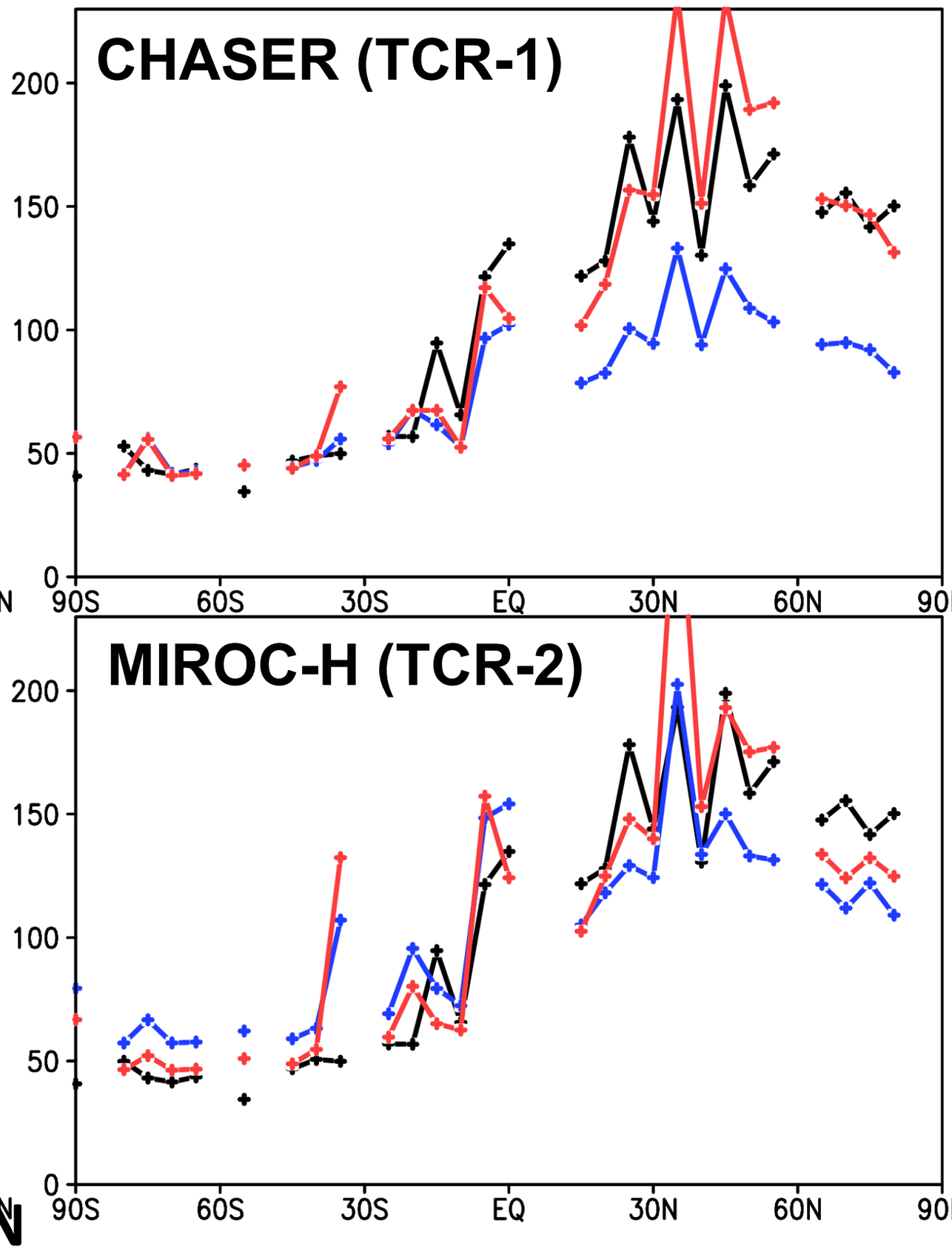
90S 90N

Obs Model DA

March 2007

WDCGG surface CO (ppbv): zonal mean





90S **90N**

Obs **Model** **DA**

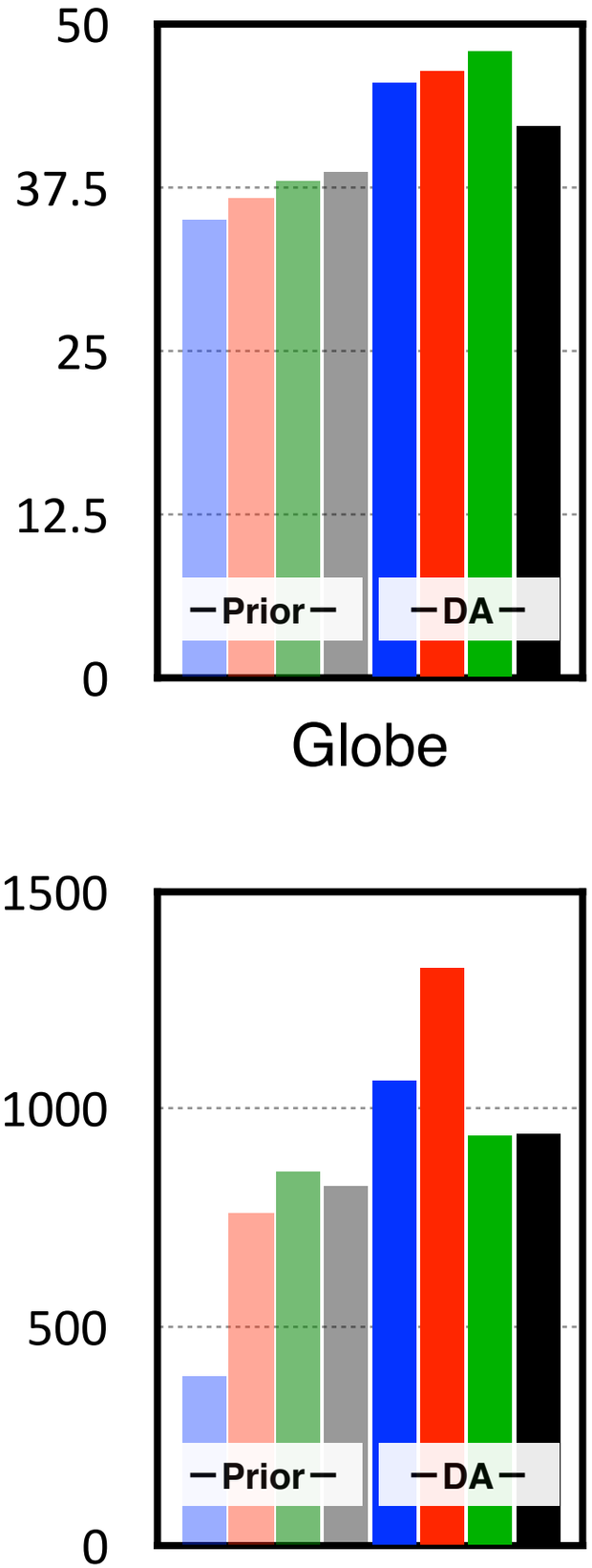
March 2007

Emissions

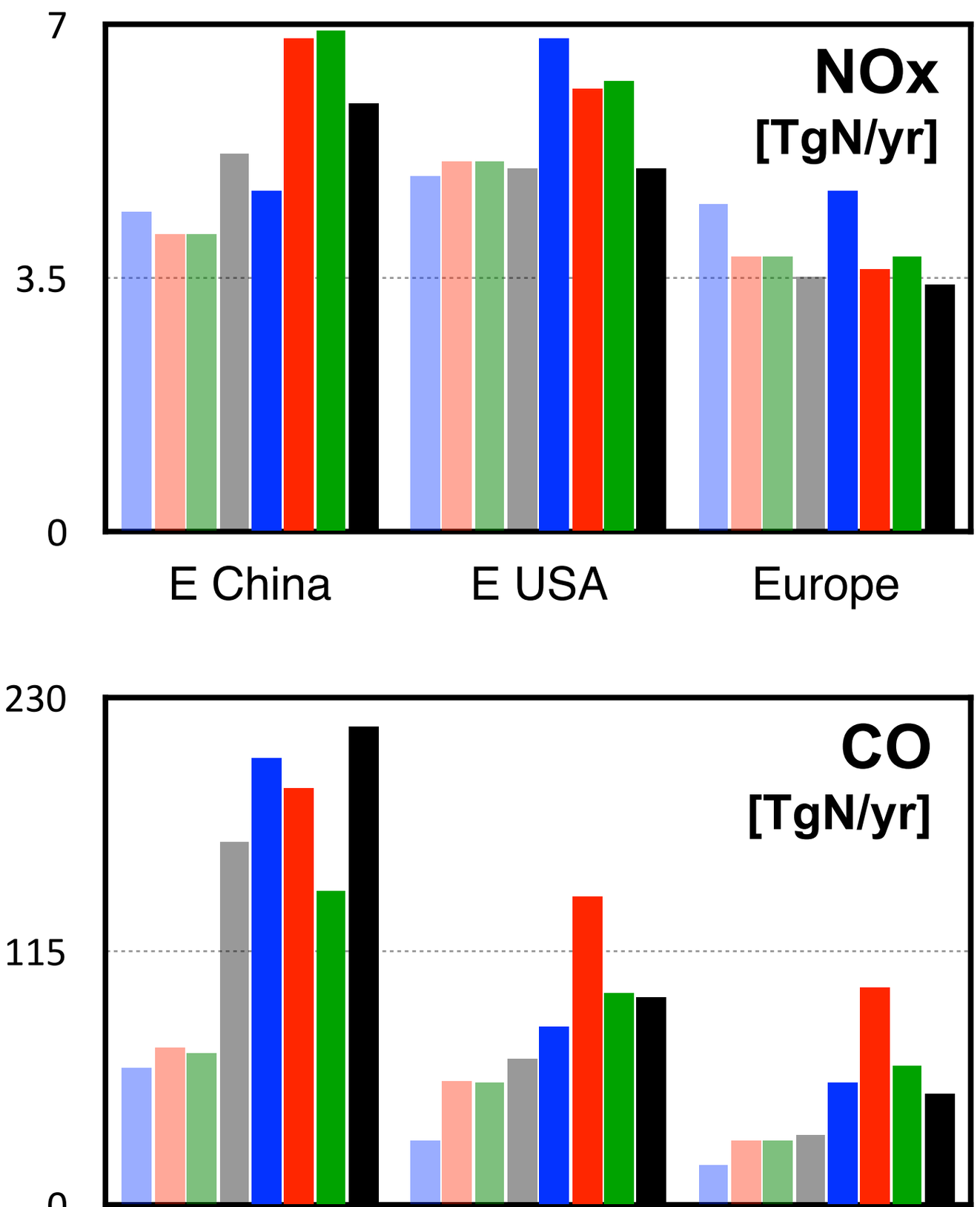
A priori: GC, CHASER, MIROC, MIROC-H
A posteriori: GC DA, CHASER DA, MIROC DA, MIROC-H DA

NOx [TgN/yr]

Globe



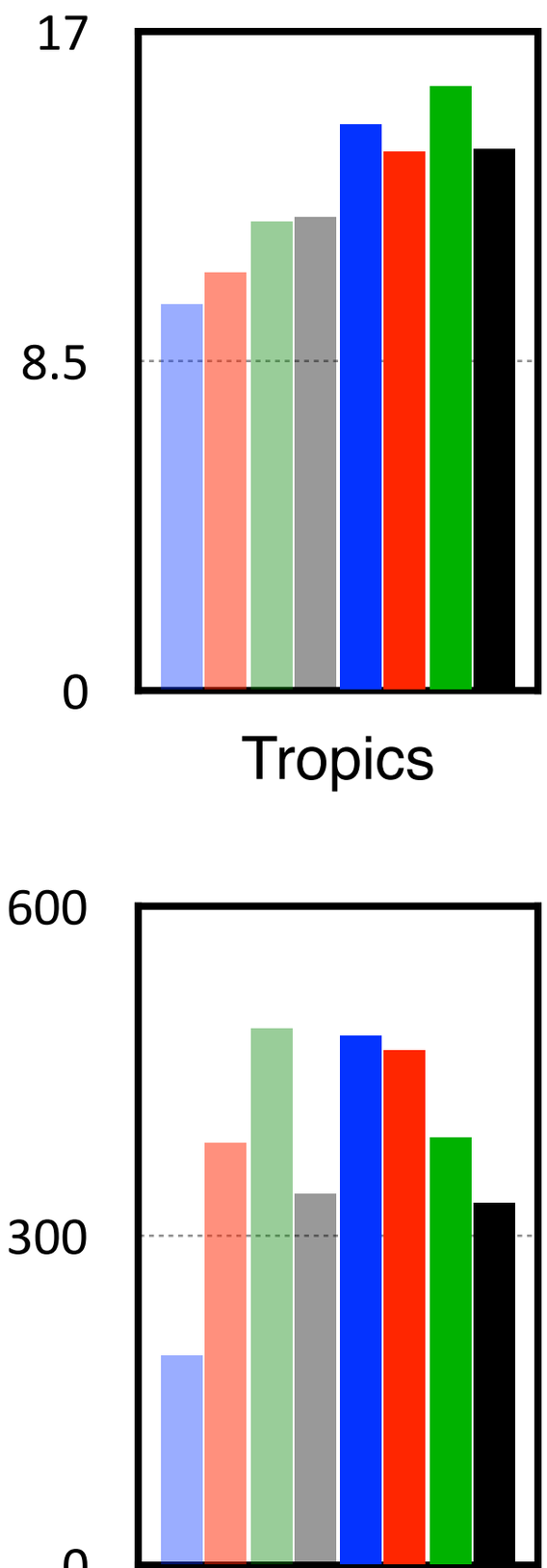
E China



E USA

Europe

Tropics



CO [TgN/yr]

Globe

E China

E USA

Europe

Tropics

OH at 700 hPa

March 2007

GC

CHASER (TCR-1)

MIROC

MIROC-H (TCR-2)

Model

DA

DA-Model (%)

-40%

-40%

+30%

+60%

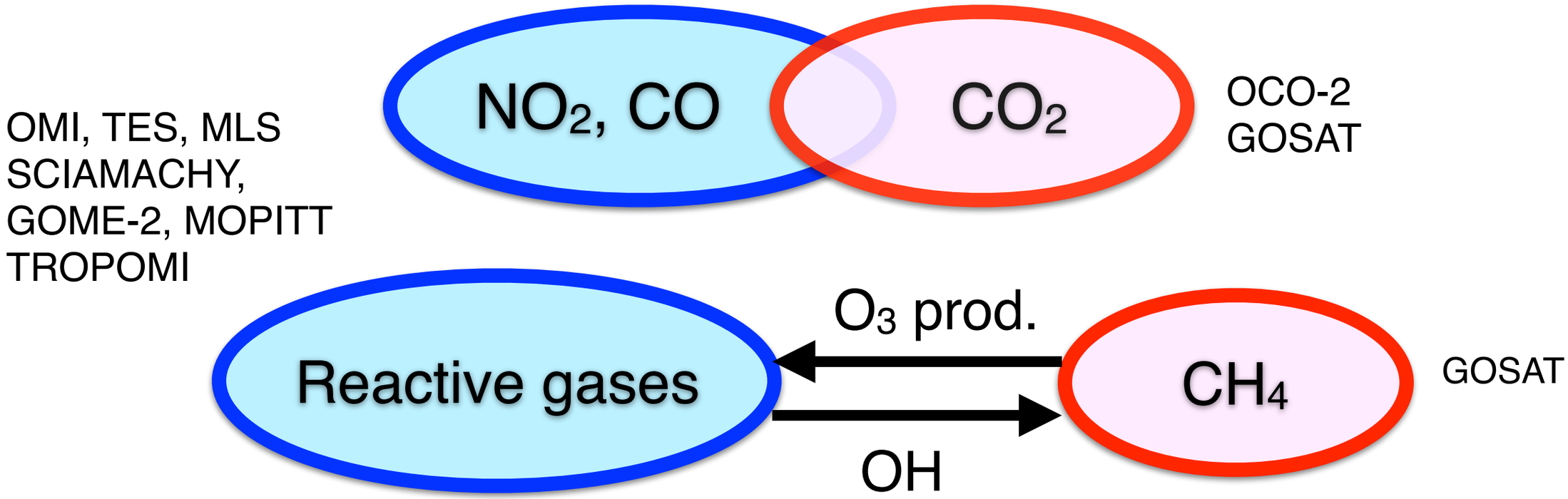
- Multi-constituent DA decreased NH/SH OH ratio (by 4-12%) in all systems
- Better agreements among the models after DA

AQ-GHG synergies

GEOS-Chem-EnKF + *CMS flux*

NOx-CO-CO_2 joint emission inversion

Changes in composition due to anthropogenic combustion

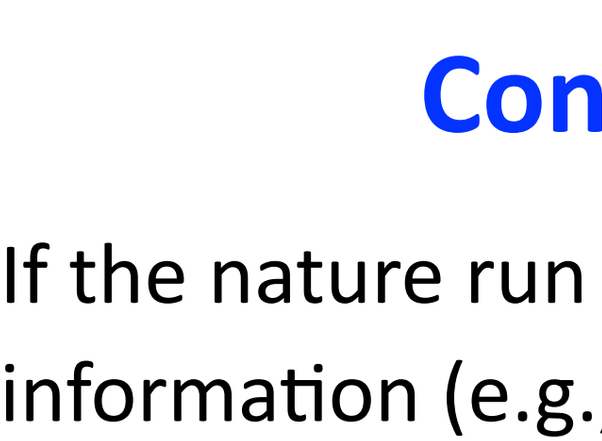


High computer efficiency of GEOS-Chem-EnKF → High resolution GCHP

Contributions to AQ-GHG OSSEs

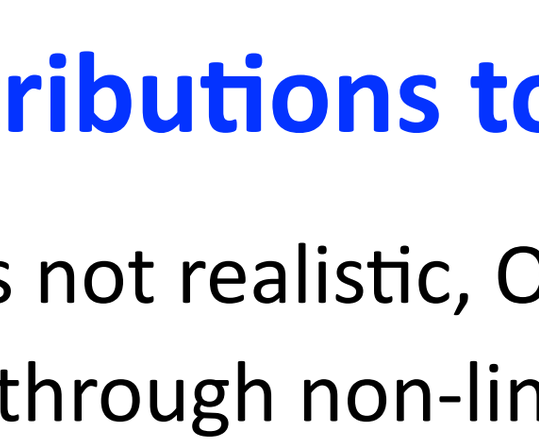
- If the nature run is not realistic, OSSEs could produce biased information (e.g., through non-linear chemistry).
- Chemical reanalysis fields could be used as a nature run, and to evaluate the observation impacts under realistic conditions.

Truth= Chemical reanalysis



Global CTM "CHASER"

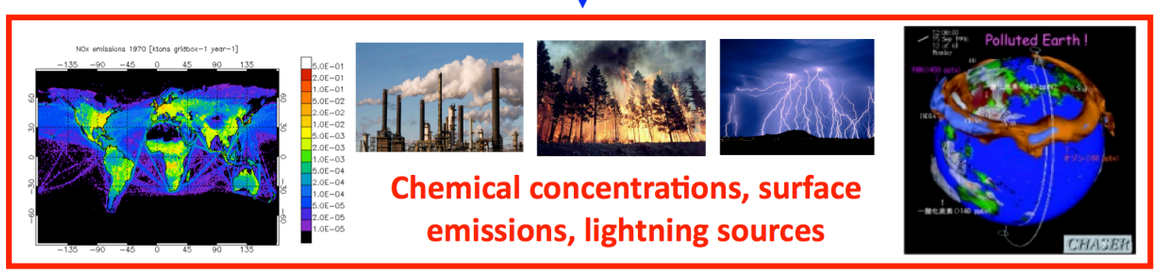
+



OMI
TES
MLS
MOPITT

Observations

Ensemble Kalman Filter
Data Assimilation



Chemical concentrations, surface emissions, lightning sources

Future sensors or idealized cases

Synthetic obs

Chemical DA

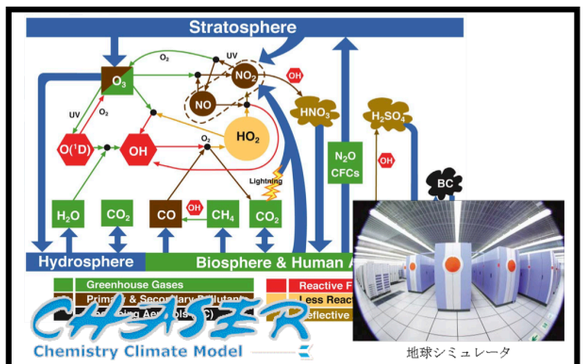
Validation

- with different emissions
- Cross-OSSE avoid over-optimistic results

Contributions to AQ-GHG OSSEs

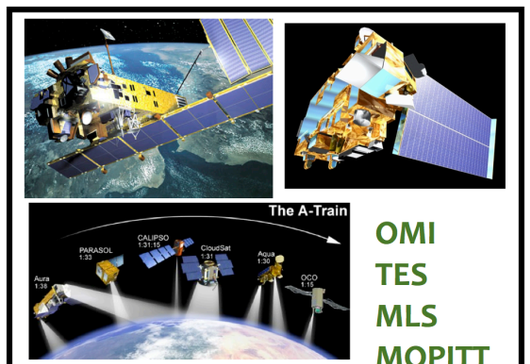
- The multi-constituent DA framework can be used to produce synthetic observations for current observing systems and to explore the ideal potential of current observing systems

Truth= Chemical reanalysis



Global CTM "CHASER"

+



OMI
TES
MLS
MOPITT

Observations

Ensemble Kalman Filter
Data Assimilation

Chemical concentrations, surface emissions, lightning sources

Existing real obs (x,y,t,AK,R, a priori)

Synthetic obs

CHASER-based DA

Validation

Validation

Sonde etc

Compare

- DA/OSSE calibration
- Retrieval/DA problems

Summary

- An updated chemistry reanalysis, TCR-2, will be released soon.
- A global 0.56° resolution DA system will be used to assimilate multi-constituent retrievals from TROPOMI and 3-GEOs.
- Multi-constituent DA sytems will be extended to AQ-GHG synergies.

AQ system	TCR	TCR	GEOS-Chem-EnKF
GHG system	**CO_2 inversion**	**any CTM (CH_4)**	**CMS-flux**
OH coupling	×	○	×
Joint emission opt	○	×	△
Combustion process	○	△	○
Satellite	○	○ (TROPOMI)	○ (OCO-2)
High resolution	△ (○AQ)	△ (○AQ)	△ (GCHP)

- Multi-model based EnKF DA systems and chemical reanalysis would help to (better) evaluate the observation impacts.