

# Recent developments in chemical data assimilation for atmospheric gases and aerosols in Japan

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# Motivations/Purposes

- **We have developed chemical data assimilation systems for monitoring atmospheric environment in East Asia since 2009. - CO<sub>2</sub>, aerosols, and ozone.**
- **The data assimilation systems developed by four Japanese research institutes employ a same data assimilation scheme, a localized EnKF (LETKF).**
- **The data assimilation approach allows to simultaneously optimize forecast variables (i.e., concentrations) and parameters (i.e., emissions).**
- **This presentation: introduction of our recent activities on chemical data assimilation for atmospheric gases and aerosols.**

# Ensemble Kalman Filter

	<b>4D-Var</b>	<b>4D-EnKF</b>
Background error statistics	Flow-dependent	Flow-dependent
Program code	Complicated	<b>Simple</b>
Adjoint matrix	Necessary	<b>Unnecessary</b>
Observation operator	Requires tangent linear & adjoint operators	<b>Requires only a forward transform operator</b>
Asynchronous observations	Handles at each observational time	Handles at each observational time
Analysis error covariance	Not provided	Explicitly provided

**1. Stratospheric ozone**  
**(MLS, OMI)**

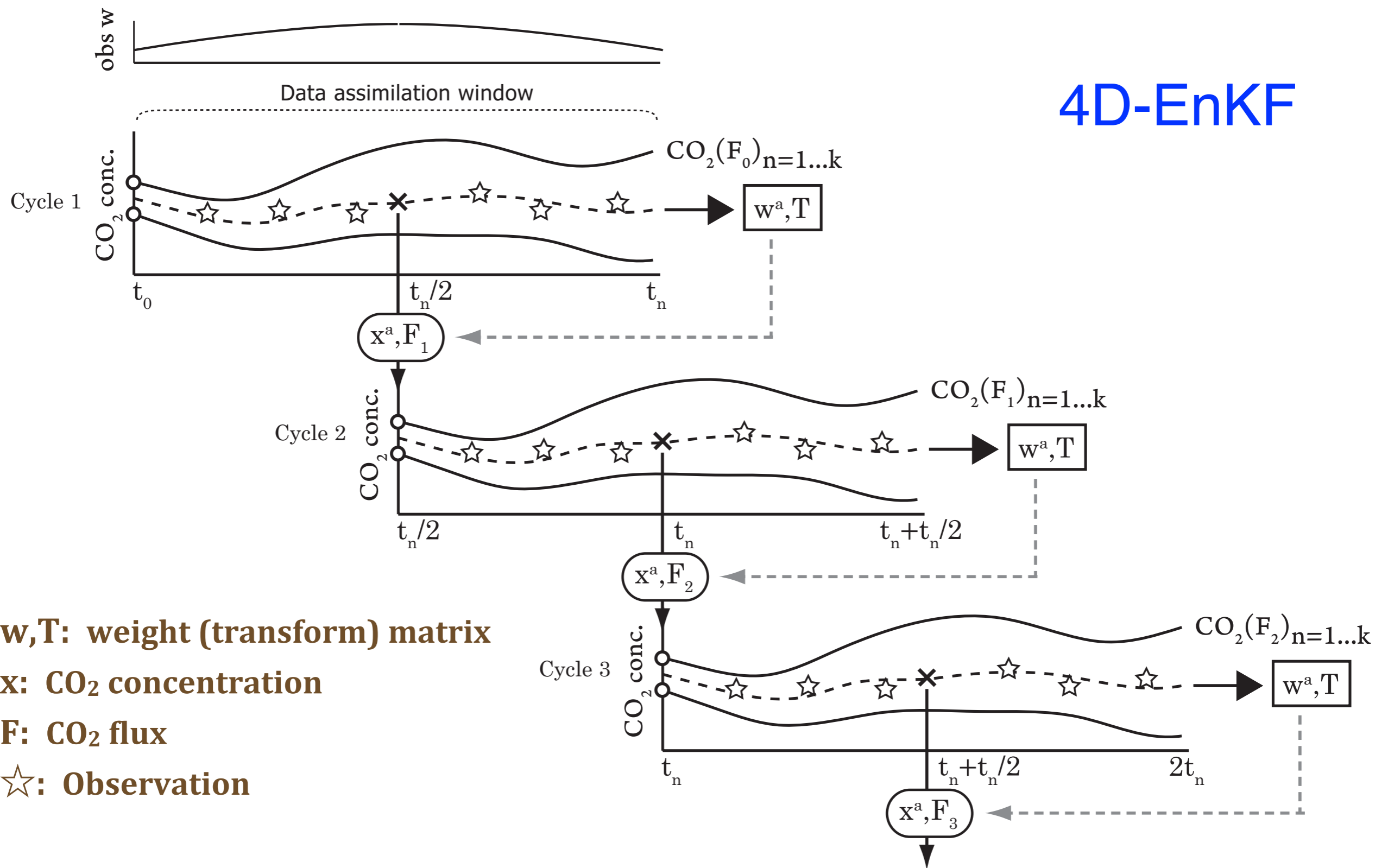
**2. Aerosols**  
**(CALIPSO, ground-based  
lidar)**

**Japanese  
CTMs/CCMs  
& 3D/4D-LETKF**

**3. Surface CO<sub>2</sub> flux**  
**(GOSAT, CONTRAIL)**

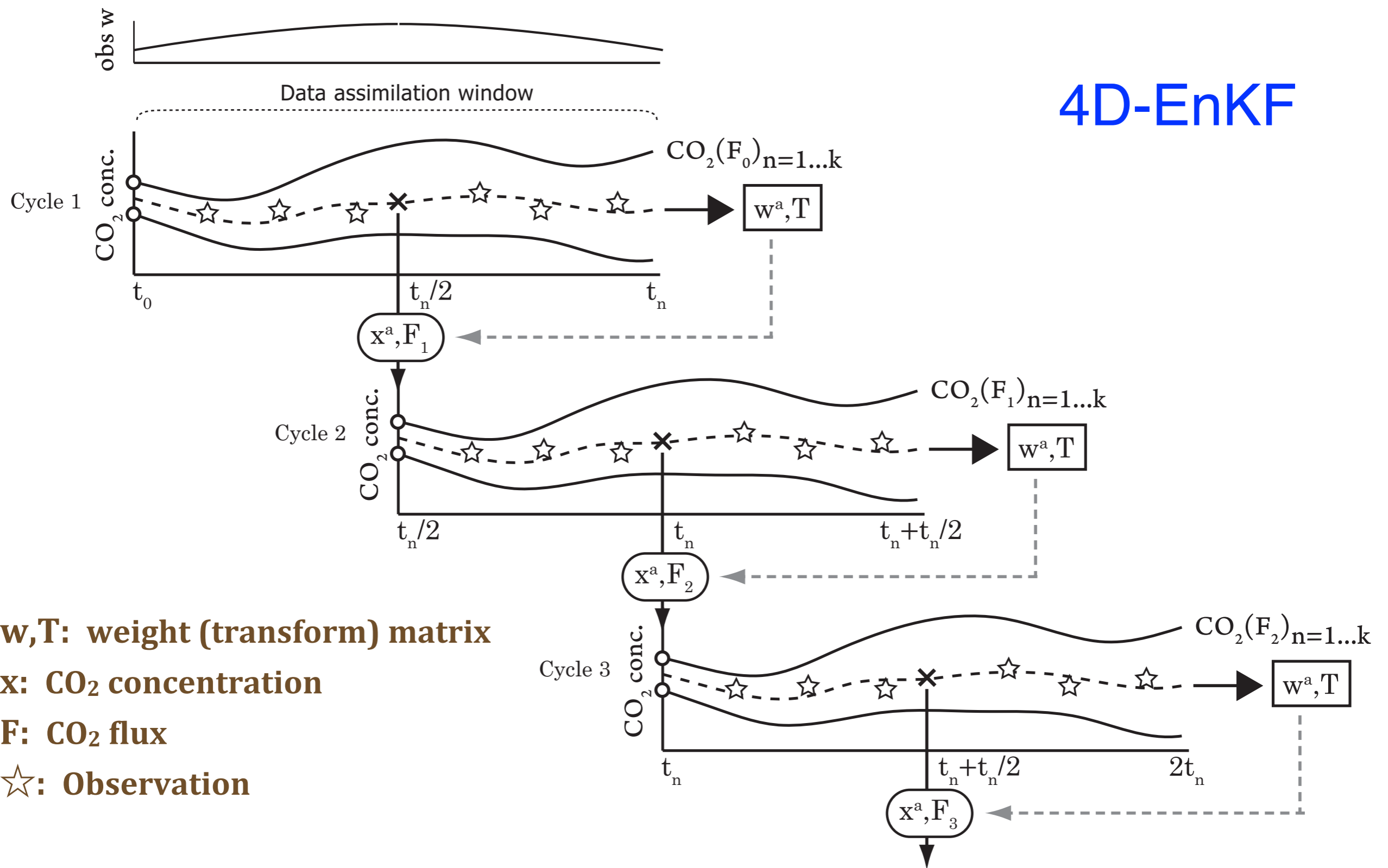
**4. Air quality**  
**(OMI, SCIAMACHY...)**

# 4D-EnKF



**In a 4D EnKF, the observations in a data assimilation window are simultaneously assimilated, and the assimilation window includes analysis time.**

# 4D-EnKF



**w, T: weight (transform) matrix**

**x: CO<sub>2</sub> concentration**

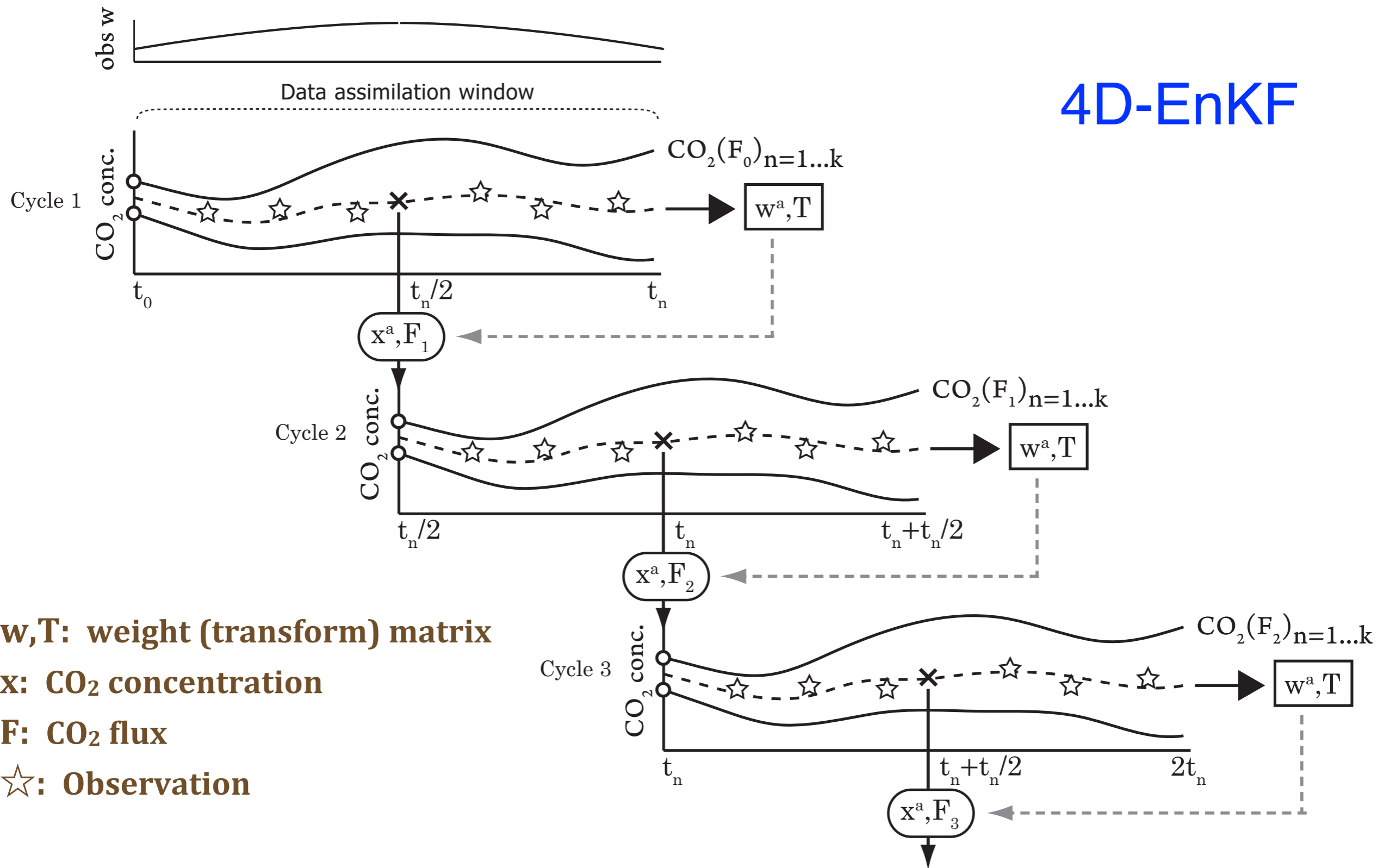
**F: CO<sub>2</sub> flux**

**☆: Observation**

**A weight matrix (w, T) used to obtain the local analysis increment is estimated at the end of the window using all observations and the corresponding background perturbations within the window.**



# 4D-EnKF



**w, T: weight (transform) matrix**

**x: CO<sub>2</sub> concentration**

**F: CO<sub>2</sub> flux**

**☆: Observation**

**The weight (w) is valid at any time in the assimilation window.**

# Comparison with the fixed lag Kalman Smoother

- Fixed lag Kalman smoother (e.g., Peters et al., 2005) uses the expanded state vector and the multiple time analysis.
- has major advantages in analyzing long term variations of global surface fluxes at a large scale.
- since the approach allows the use of large constraints obtained from a long data assimilation window (possibly) w/o serious model error growth with time and sampling errors.
- It might be difficult to obtain meaningful constrains from remote data on surface flux variations especially at a fine scale.



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- since the approach allows the use of large constraints obtained from a long data assimilation window (possibly) w/o serious model error growth with time and sampling errors.
- It might be difficult to obtain meaningful constrains from remote data on surface flux variations especially at a fine scale.
- Our method, with localized analyses, has advantages in analyzing fine scale structures in surface fluxes, if provided sufficient observational information is available in a localized space. However, when the analysis increment is too localized, some areas are possibly under-constrained.

# 1. Stratospheric ozone

## Forecast models:

(1) **CCSR/NIES CCM** (Akiyoshi et al., 2009)

T42L34 p-top=0.01 hPa

(2) **MRI CCM2** (Shibata and Deushi, 2008, Deushi and Shibata 2011)

T42L68 p-top=0.01 hPa

(3) **CHASER** (Sudo et al., 2002) *not shown here*

T42L32 p-top=3 hPa

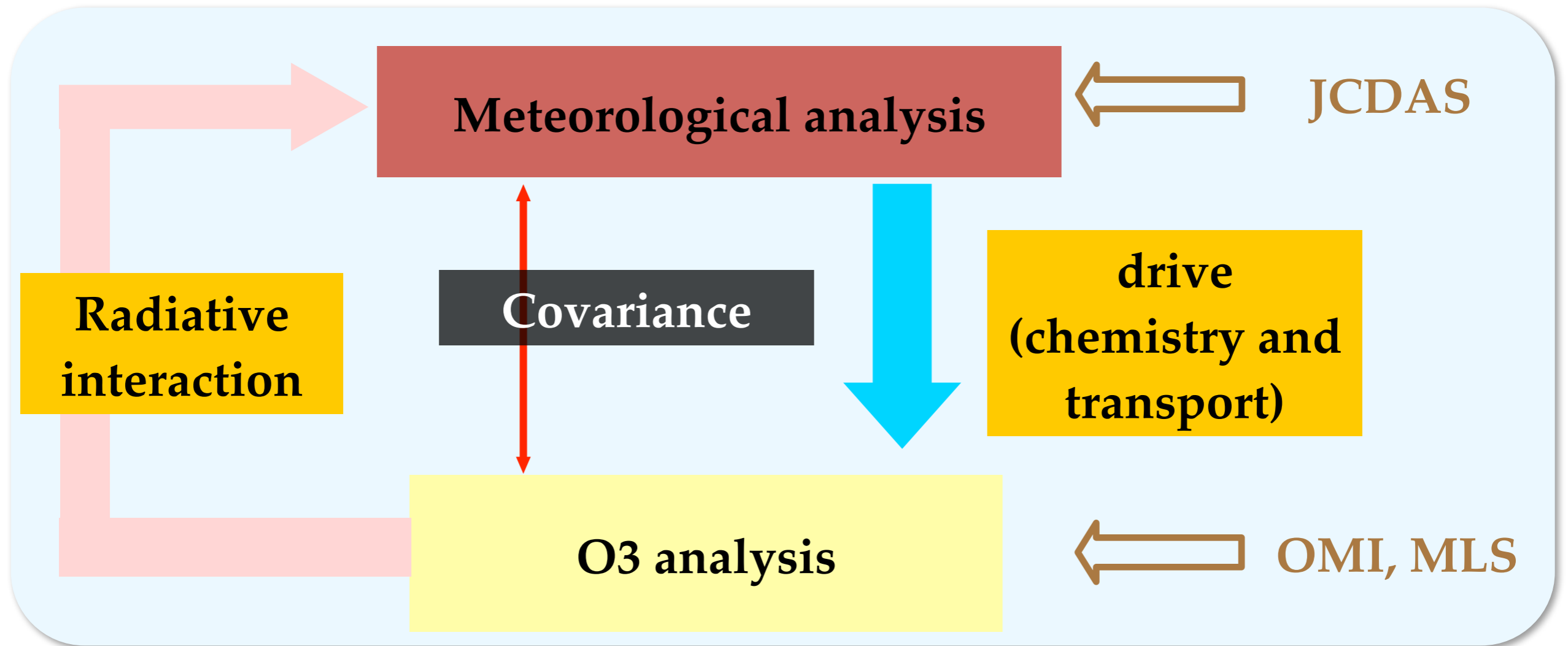
**A multi-model comparison provides an opportunity to examine the effects of the model bias on the assimilation performance.**

**Assimilated data:** MLS O3 profile, OMI O3 column, JCDAS (regarded as met. data, simplifying the system)

**Control variables:** O3, U, V, T

**Assimilation setting:** 3D analysis with 6-hourly cycle

# Meteorology-chemistry coupling data assimilation



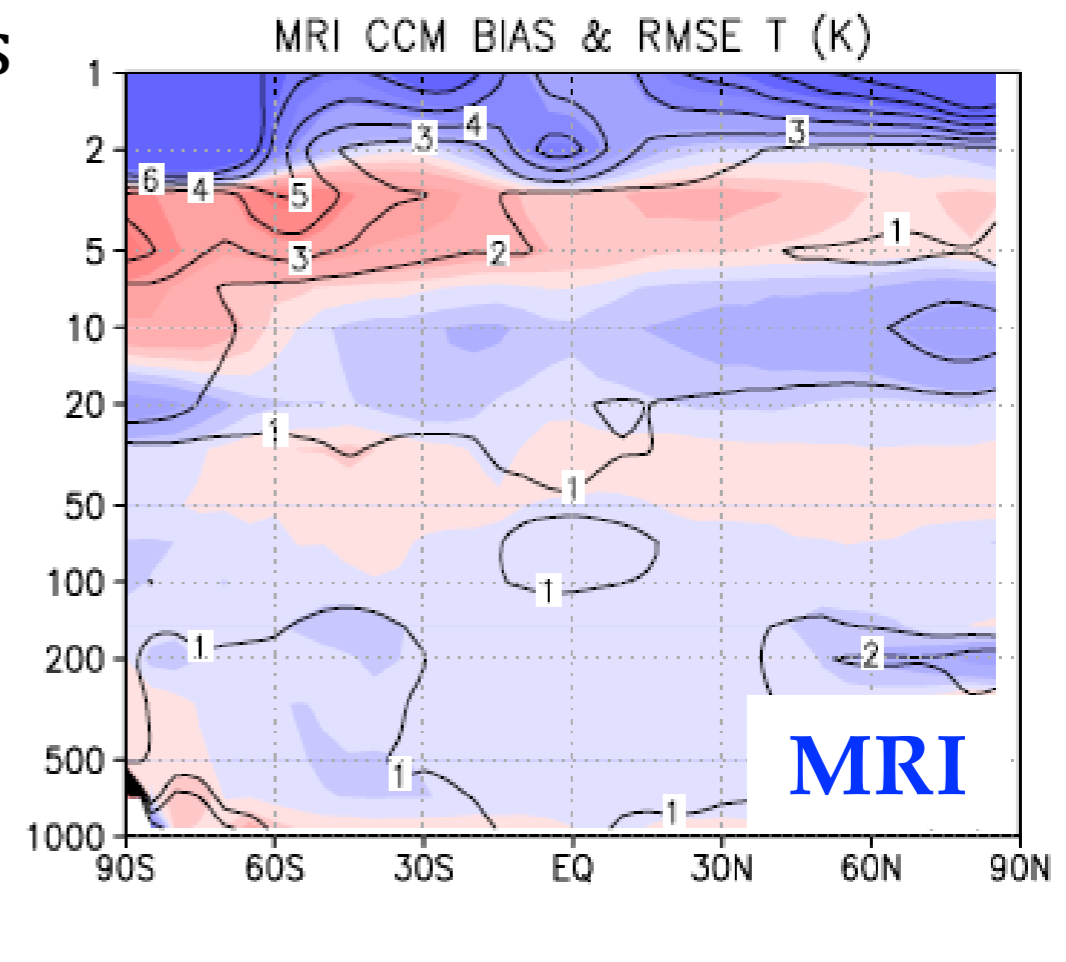
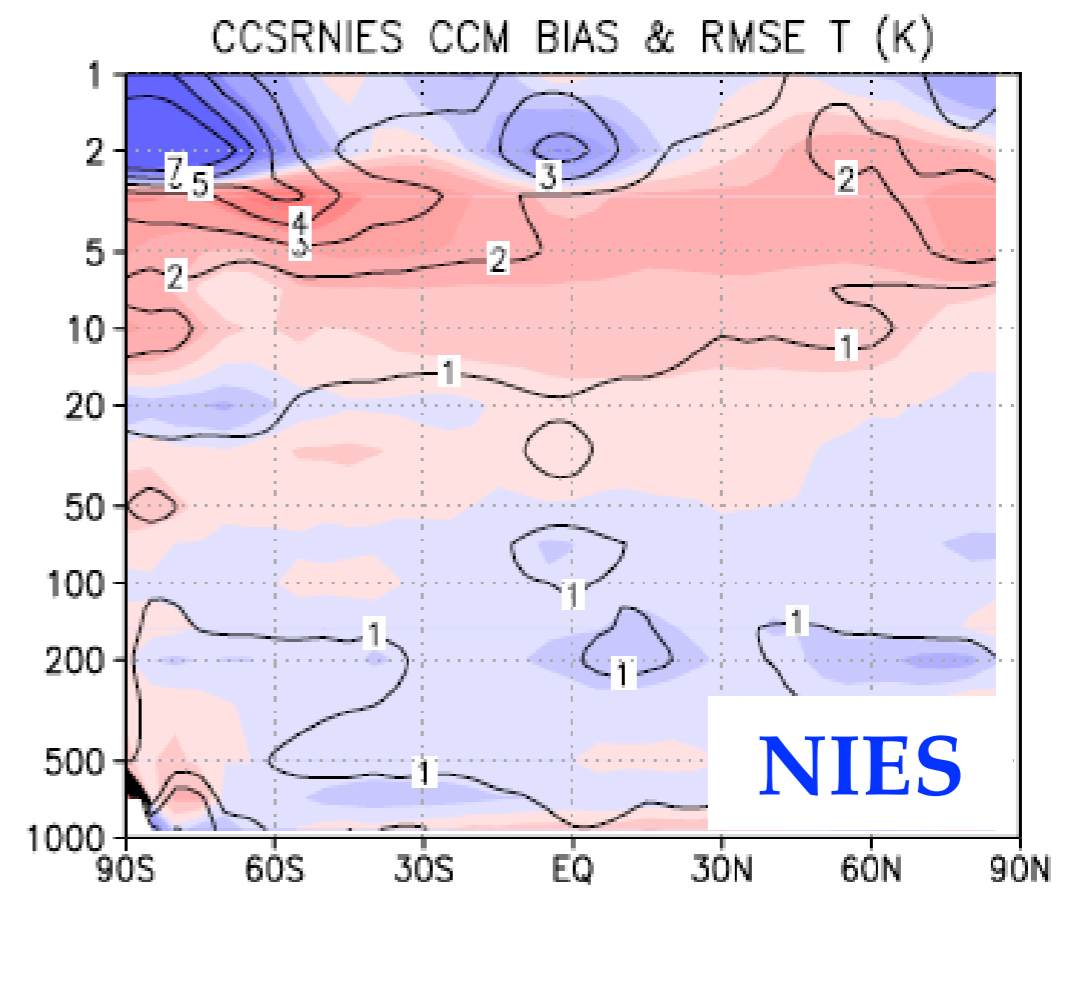
**How does the ozone data assimilation improve the meteorological analysis?**

## Chemistry-climate models:

**Ozone forecast error →  
Temperature analysis error**

- **Without** ozone data assimilation (only met. data are assimilated)  
→ Large T errors of the models still exists in upper stratosphere in both models.
- Need to correct ozone/radiation.

**Fig: Temperature error (bias:shaded and RMSE:contour) compared to (assimilated) JCDAS.**

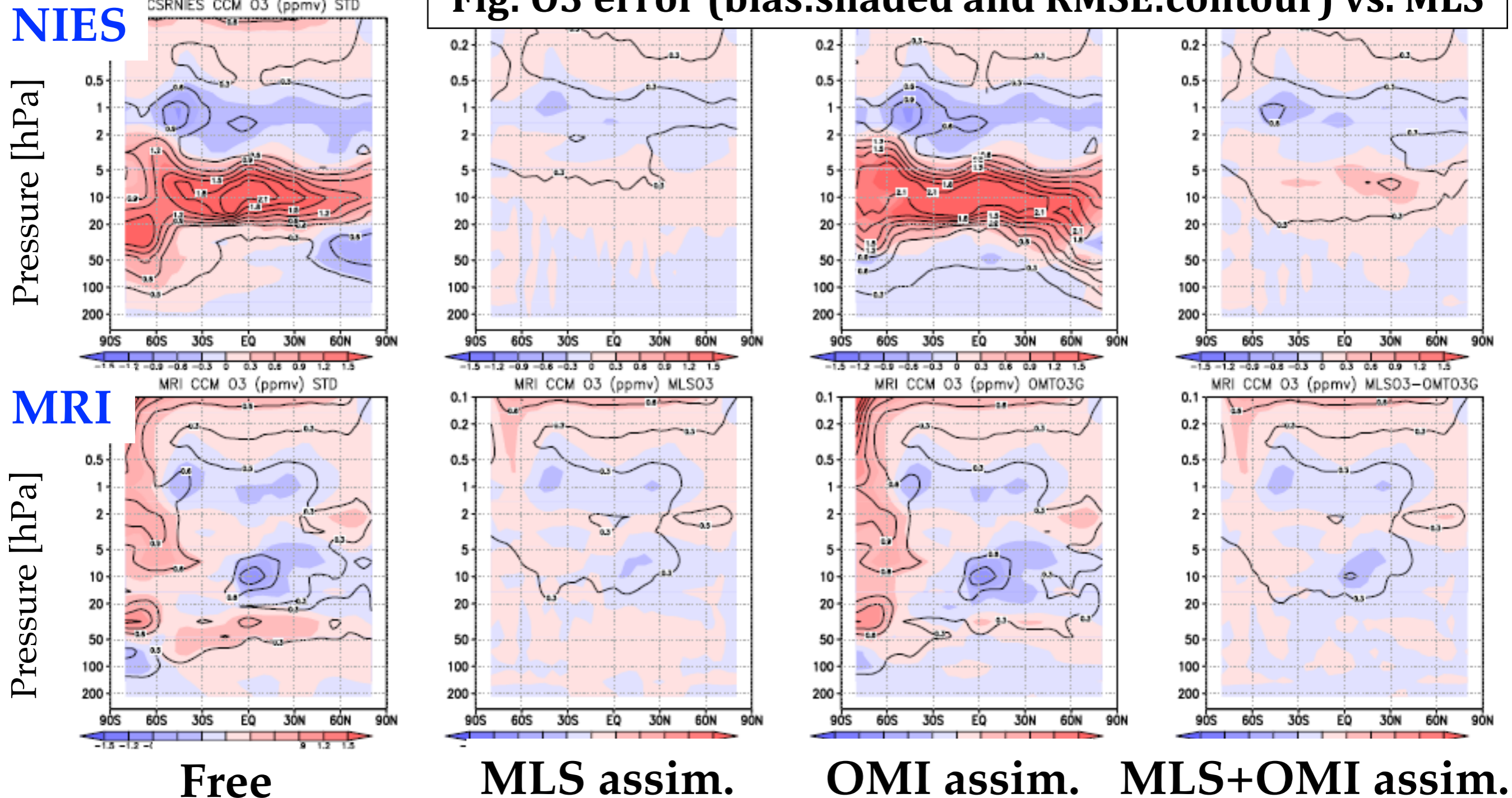




# Ozone data assimilation

- **Improvements by MLS O3 assimilation:** throughout the stratosphere.
- **Improvements by OMI-T03 assimilation:** only in the lower stratosphere.
- **No improvement in the mesosphere** due to too small ensemble spread.

Fig: O3 error (bias:shaded and RMSE:contour) vs. MLS

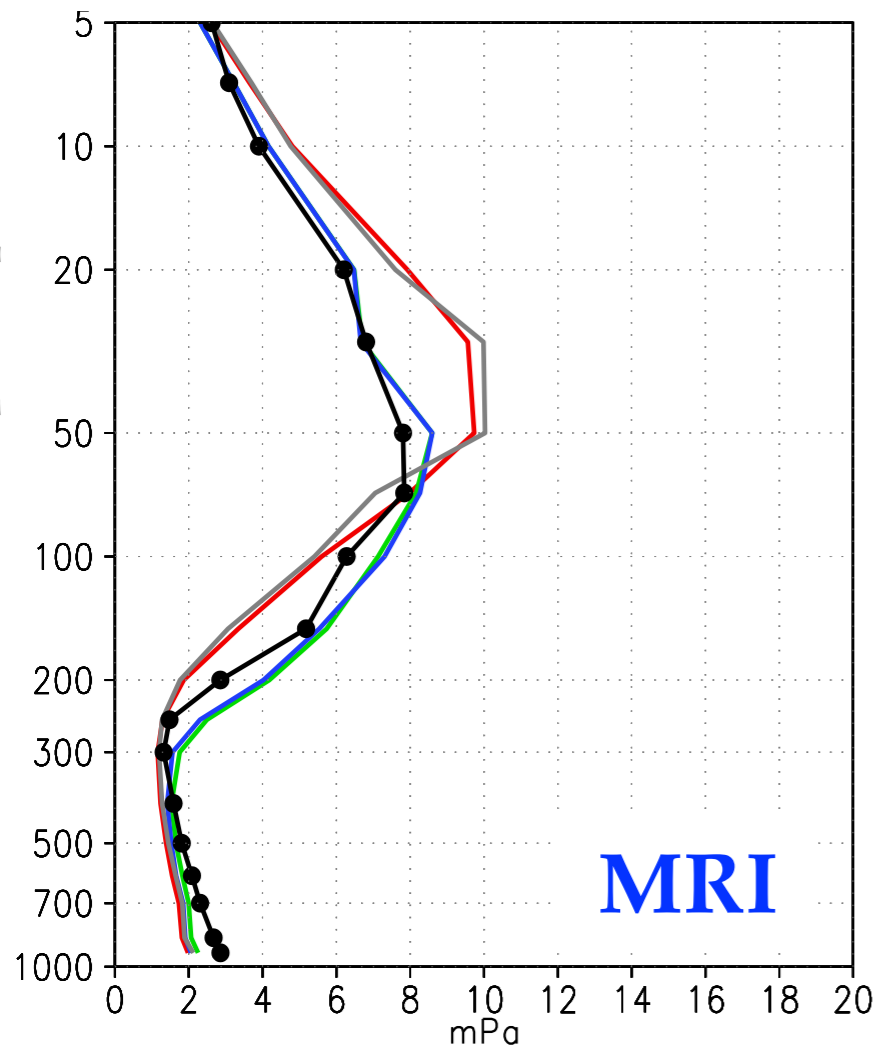


# Ozone data assimilation

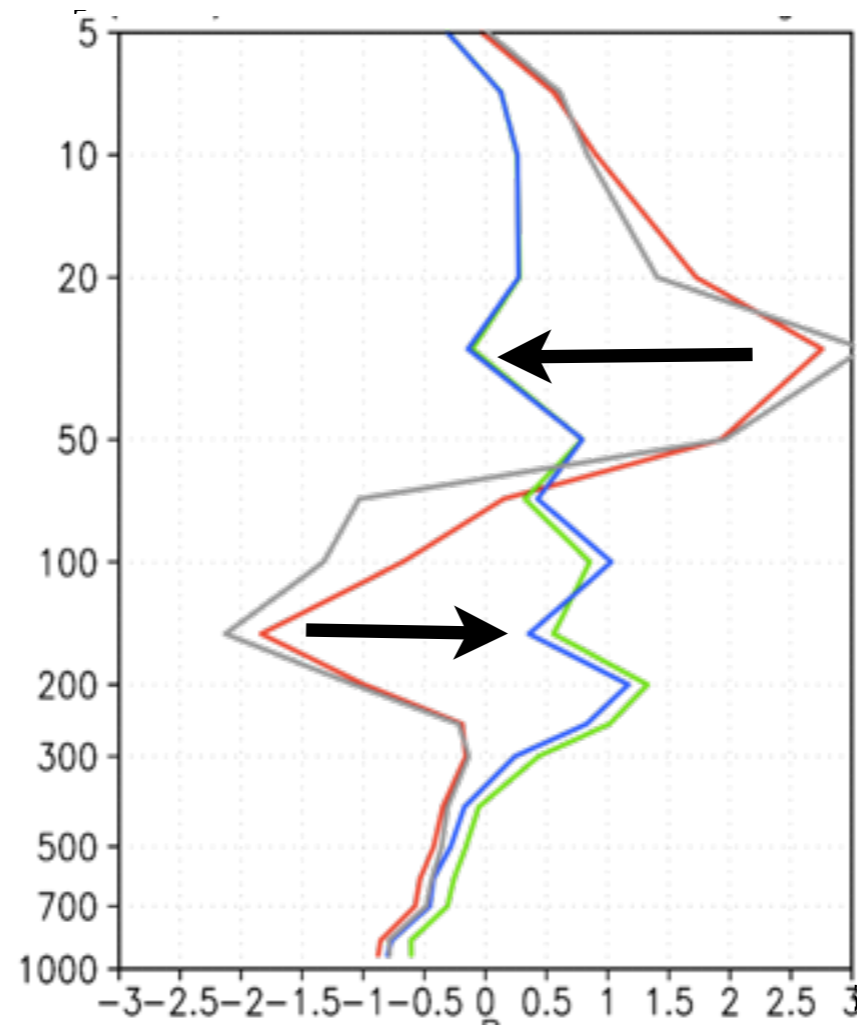
(vs. Sonde, 60S-90S)

August-September, 2006

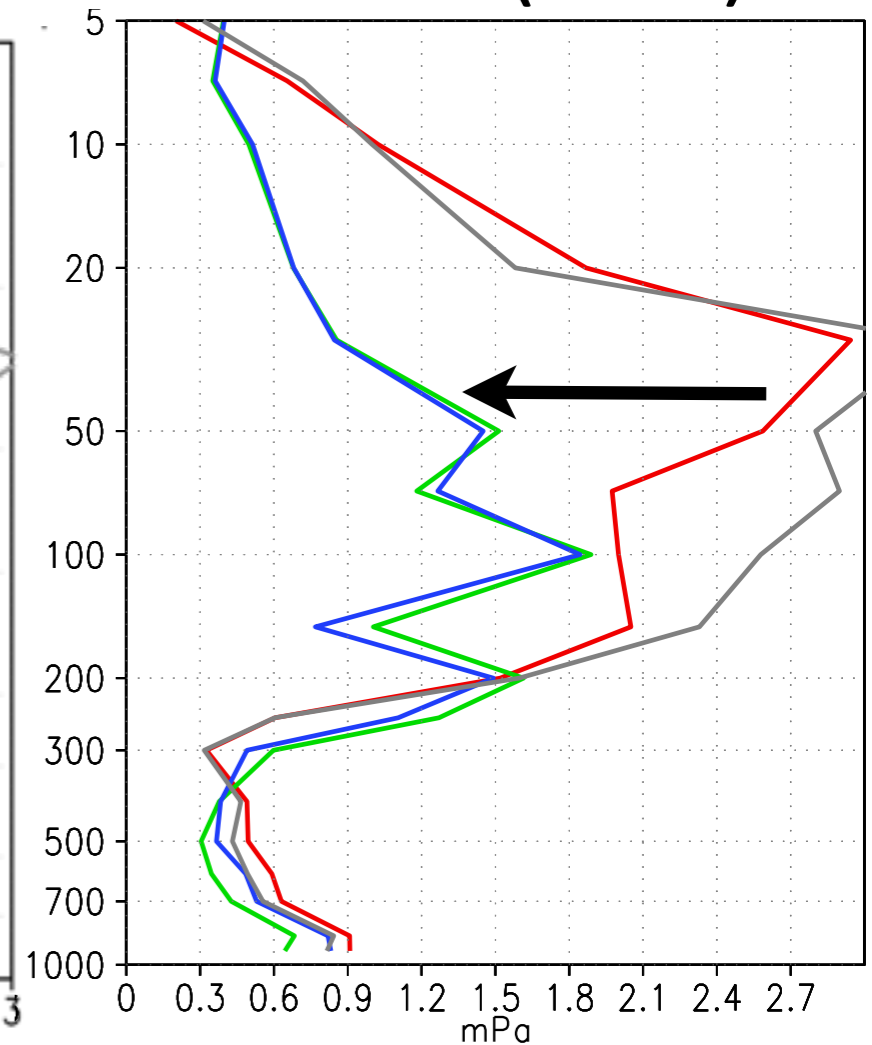
### Ozone(mPa)



### BIAS (mPa)



### RMSE (mPa)



**OBS**

**OMI+JCDAS**

**JCDAS**

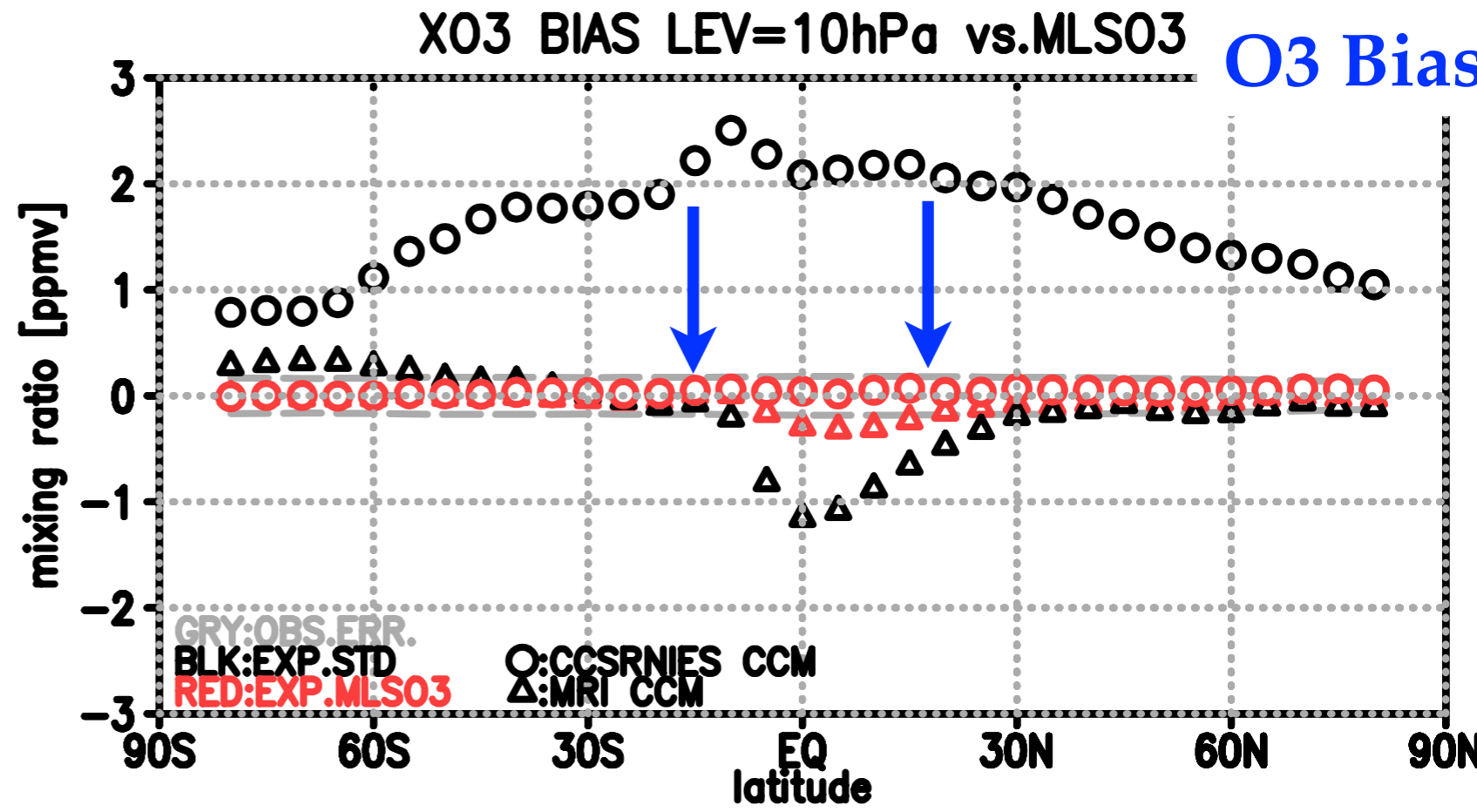
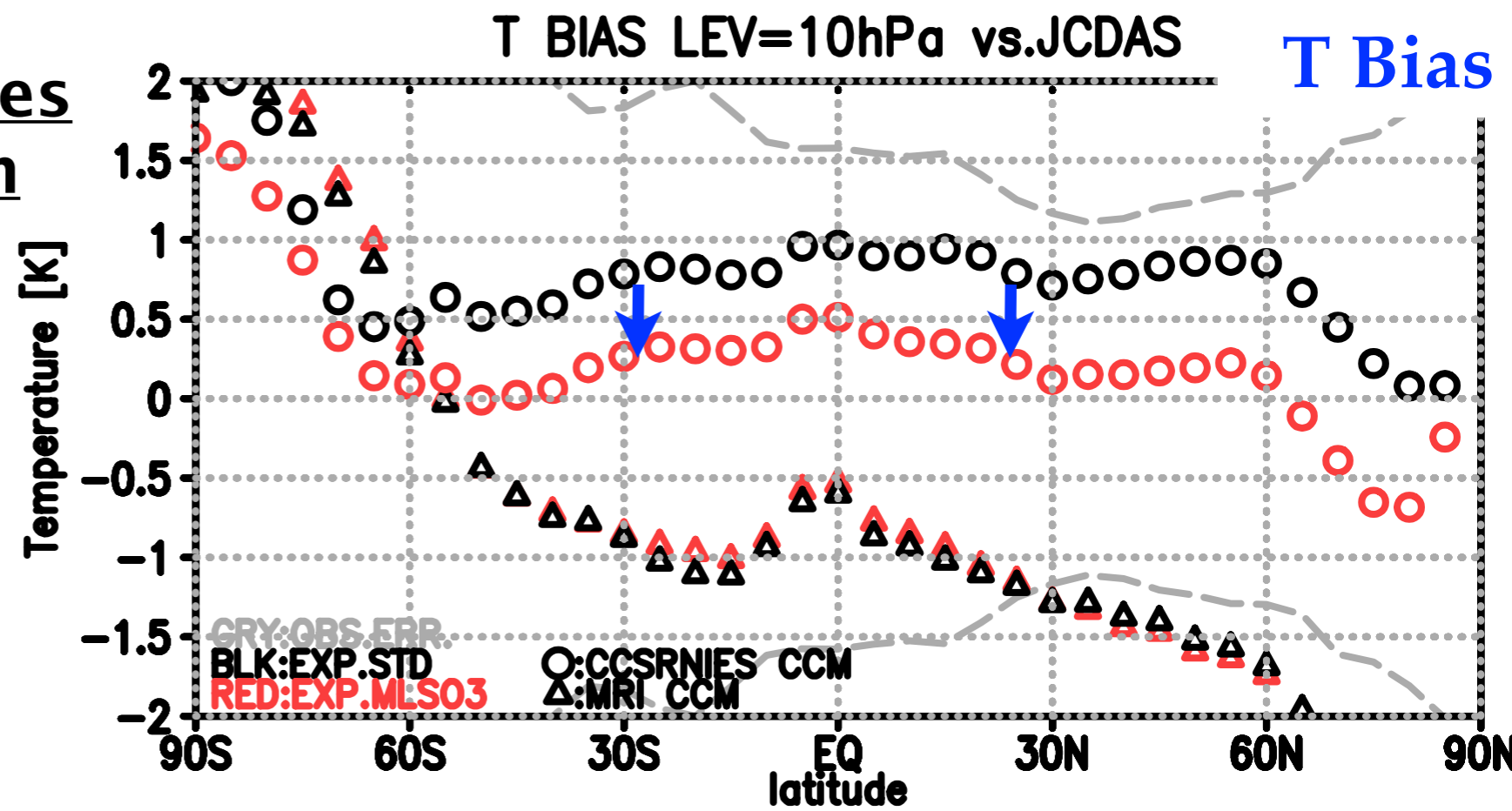
**OMI+MLS+JCDAS**

**MLS+JCDAS**

# Improvements of temperature and o3 biases by O3 data assimilation

- NIES: simulated o3
- NIES: w/ o3 assim.
- △ MRI: simulated o3
- △ MRI: w/ o3 assim.

- The temperature bias of the NIES model has been mostly (about 50 %) removed by ozone data assimilation.
- The impact is not obvious in MRI model, since the MRI model has very small bias in the forecasted ozone fields.

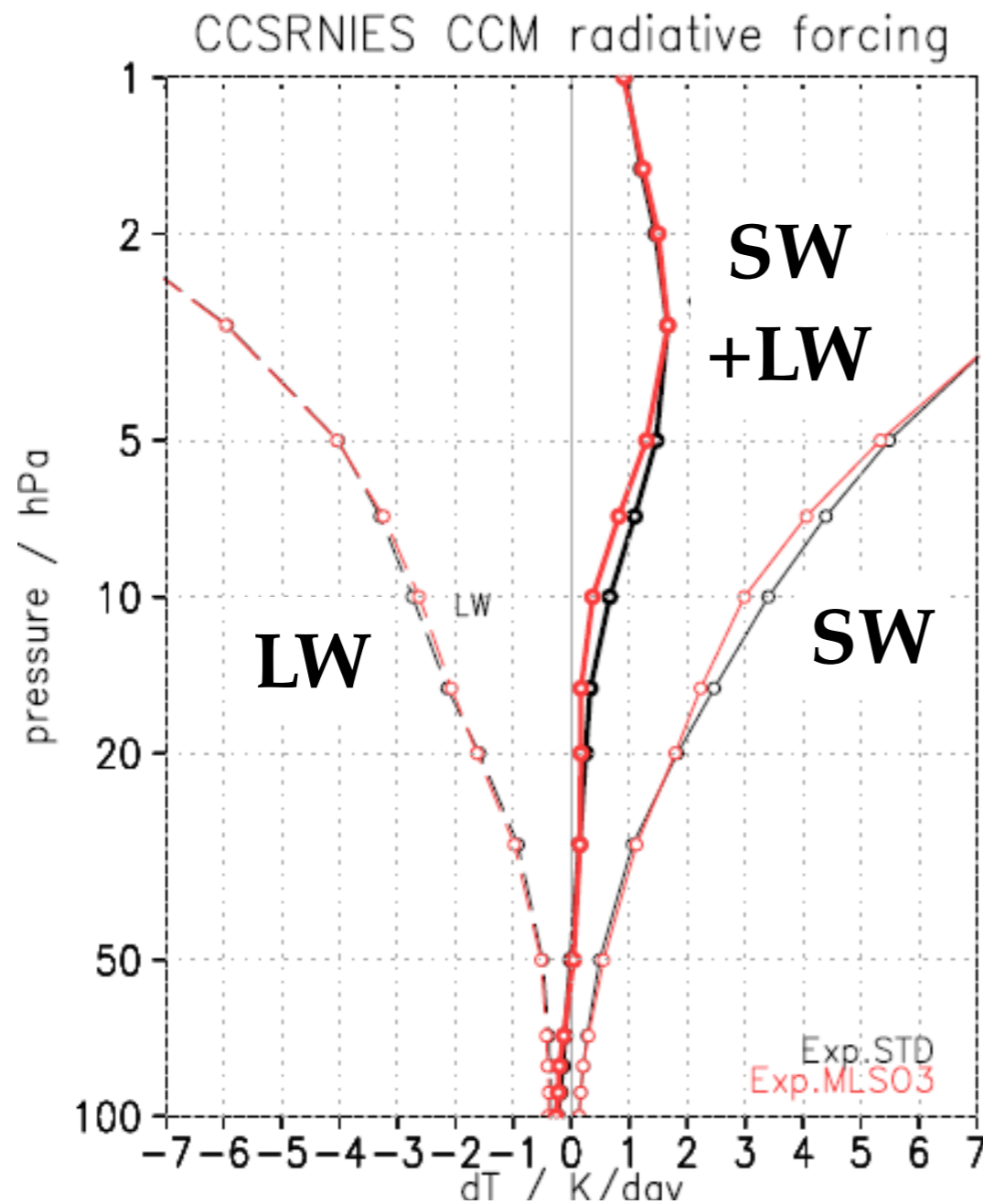




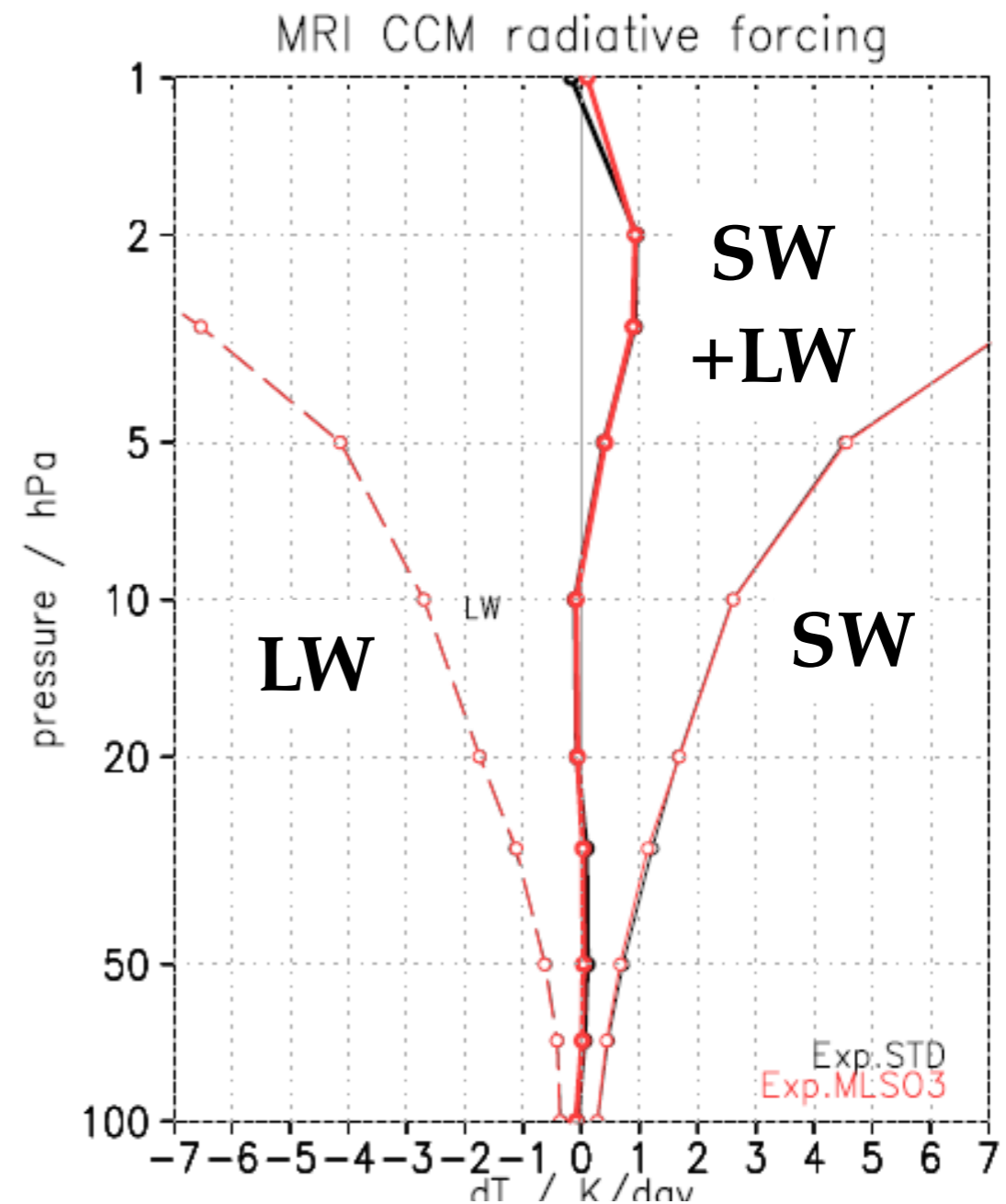
- **NIES in the middle stratosphere:** O<sub>3</sub> data assimilation → less positive O<sub>3</sub> bias → 10 % reduction in SW heating → 40% reduction in net radiative heating
- **MRI:** Almost no impact on the heat budget. The radiative scheme needs to be improved to remove the cold bias.

**Fig: Radiative forcing by SW & LW**

**Simulated o3  
w/ O3 assim.**



**NIES**



**MRI**

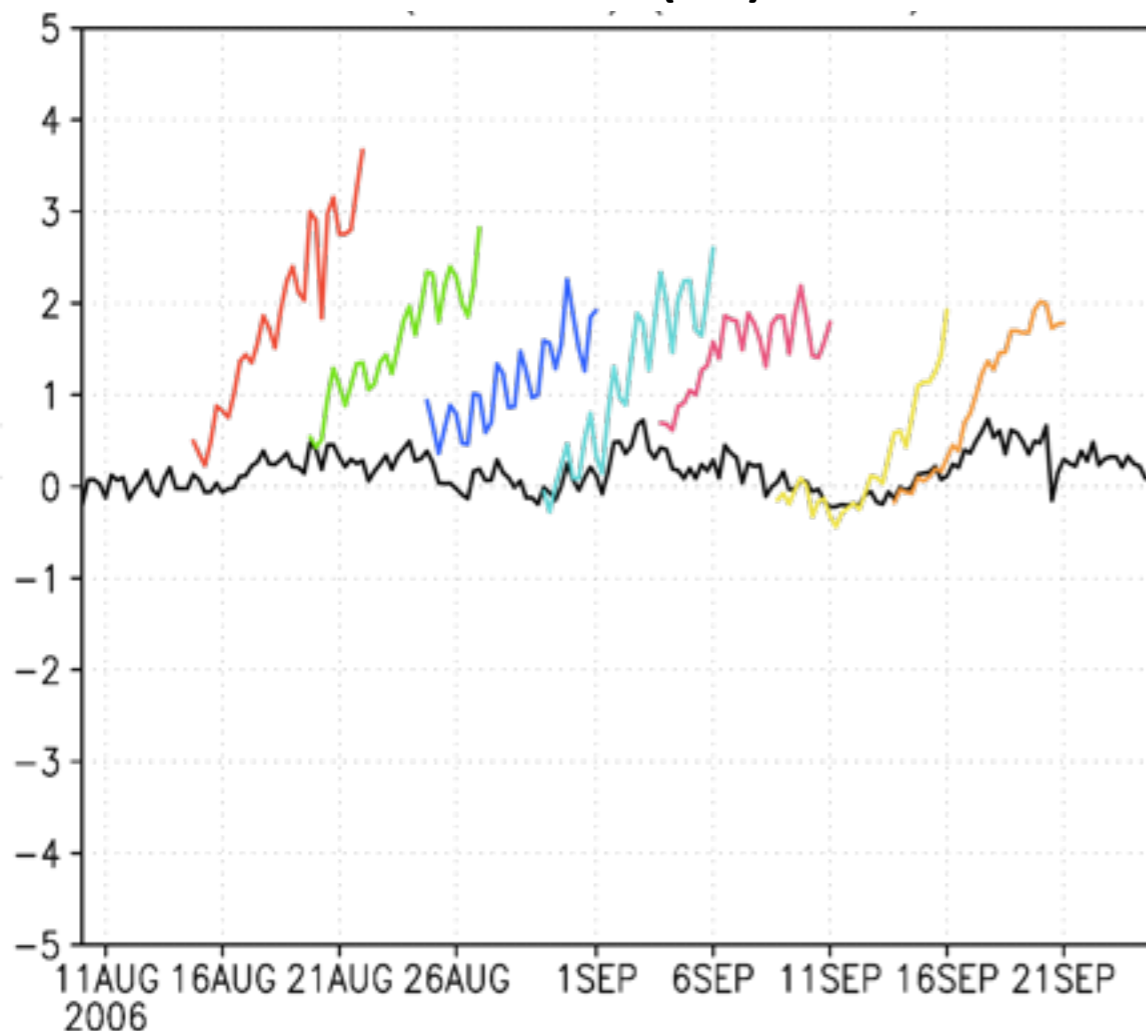
# 7-days Hindcast experiments using the assimilated field

- Initialization with assimilated fields.

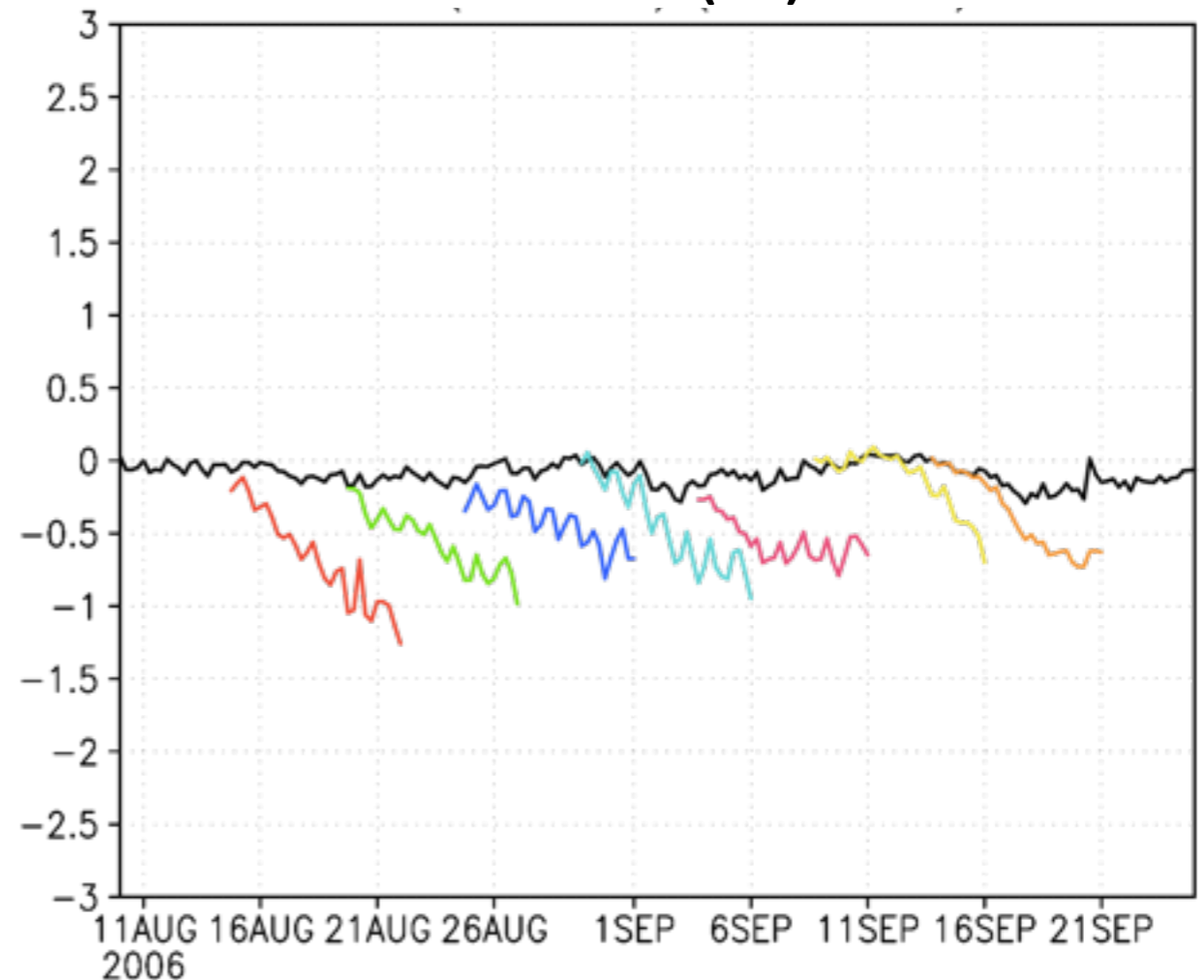
→ High quality forecast ( $< 3\%$  RMSE,  $< 1\%$  bias)

Performance of the total ozone hindcast runs ( vs. OMI, 30N-60N)  
2006 08.10 – 2006 09.25

RMSE(%)



BIAS (%)



## 2. Aerosols

under development by JMA (T. Sekiyama)

- **Asian Dust**

- seasonal phenomenon sporadically affecting East Asian countries during the springtime,
- causes health and aviation problems,
- originates in the deserts of Mongolia and China.

**Forecast models:** MASINGAR

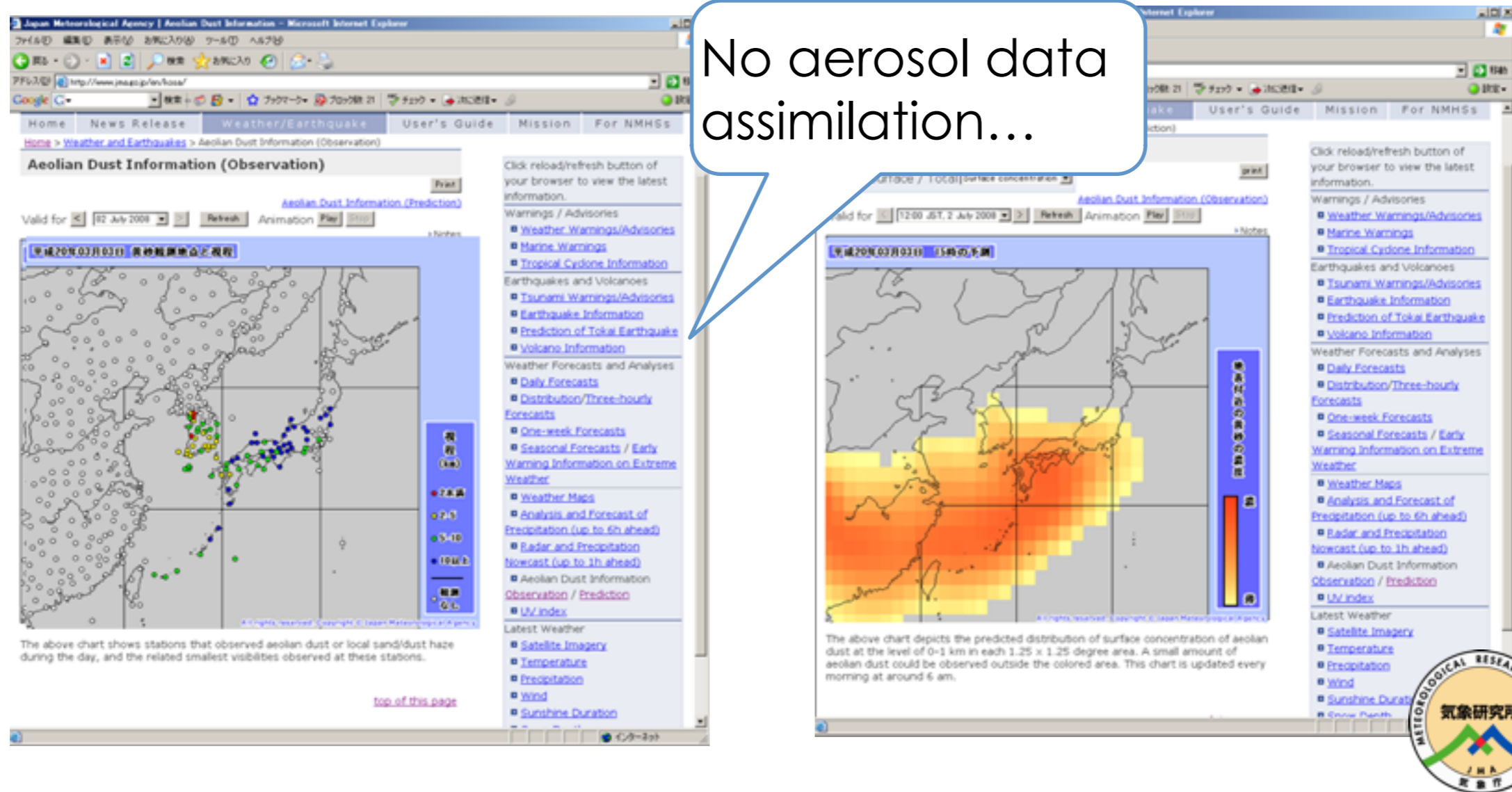
**Assimilated data:** Satellite (CALIPSO/CALIOP) and ground-based lidar

**Control variables:** dust (partitioned into 10-size bins), dust flux, sea-salt, OC, BC, and sulfate aerosols

**Assimilation setting:** 4D analysis with 48-h time window



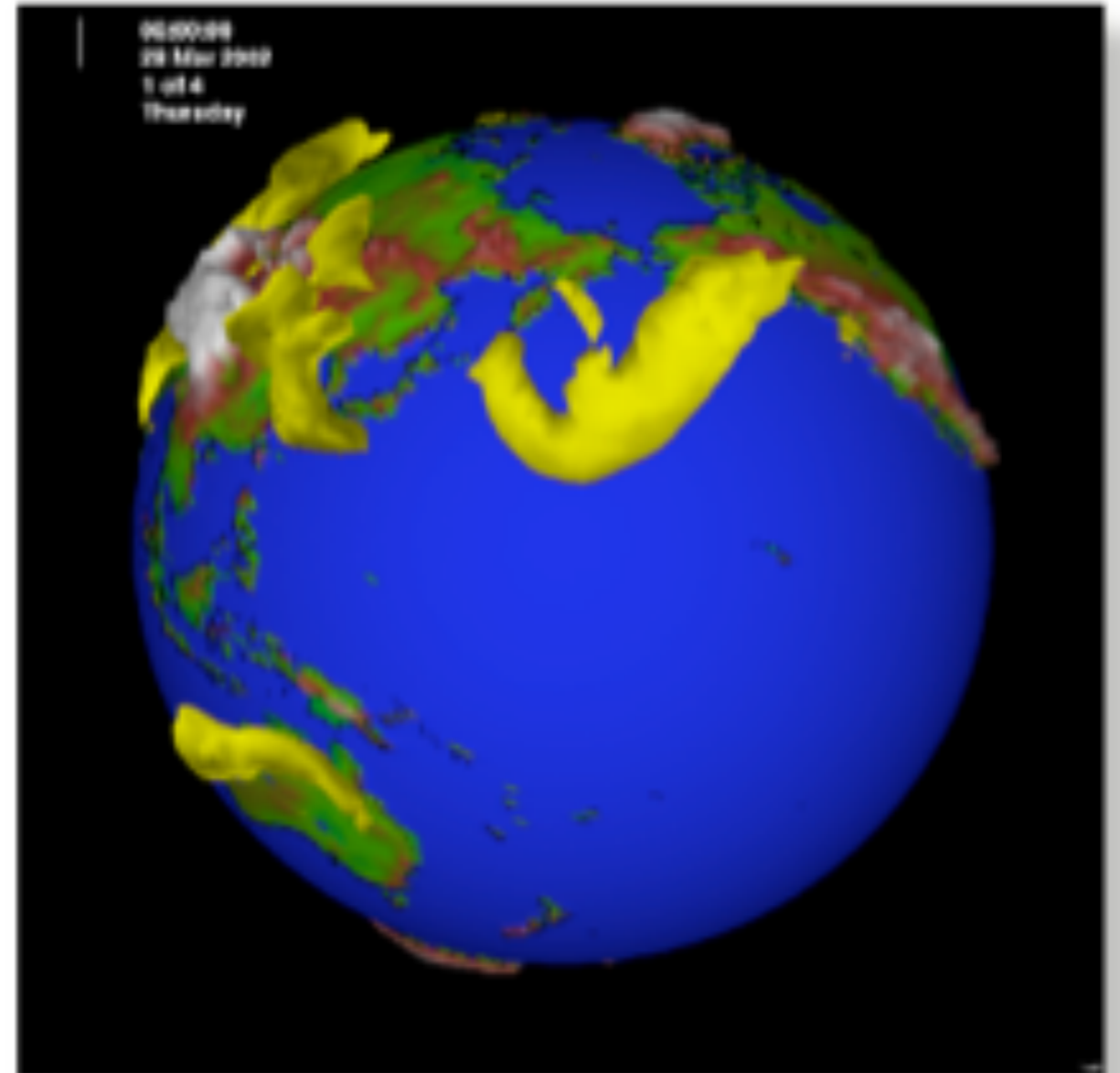
# Operational dust prediction



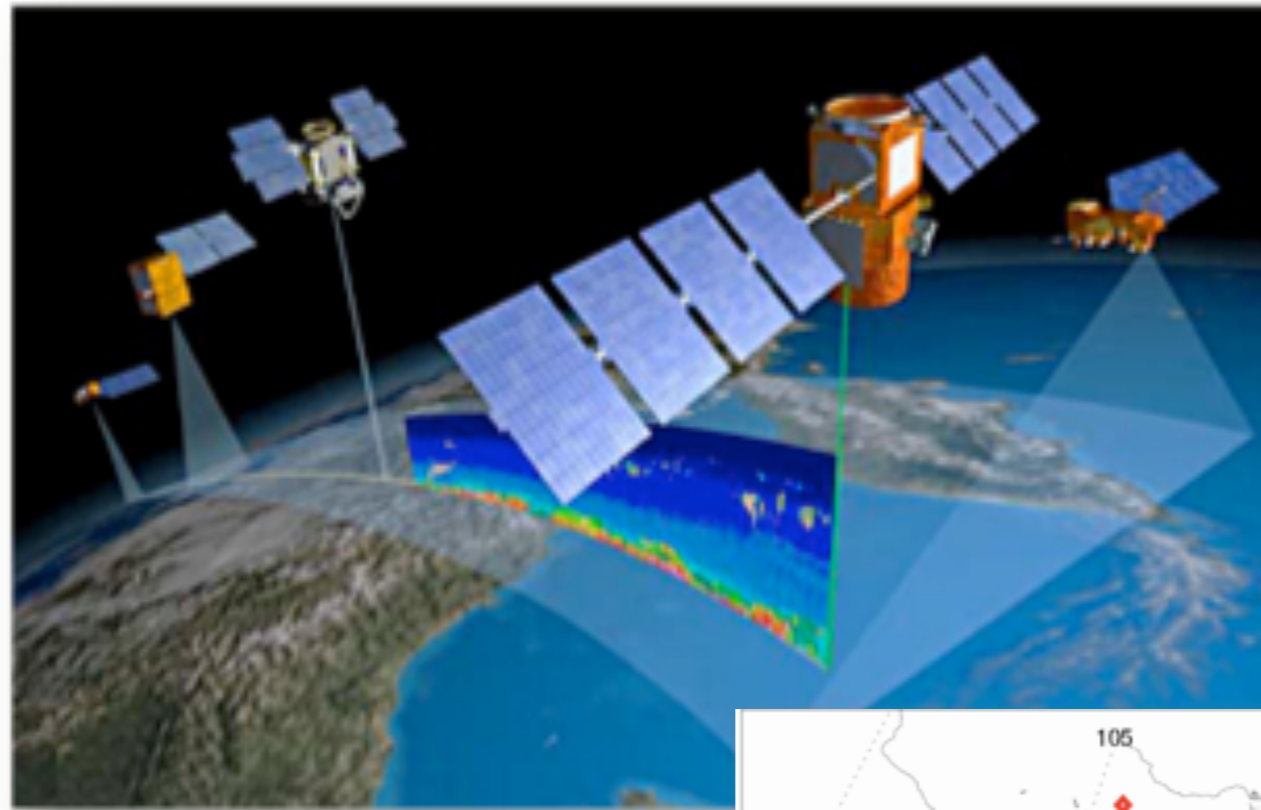
- JMA wants to utilize aerosol data assimilation for improving their operational dust prediction.
- If possible, they want to use the aerosol analysis for their NWP and climate simulations.

# EnKF for aerosol analysis

- The Model of Aerosol Species in the Global Atmosphere (**MASINGAR**) of MRI/JMA simulates...
- **dust** (partitioned into 10-size bins), sea-salt, OC, BC, and **sulfate** aerosols



# EnKF for aerosol analysis



**Satellite Lidar observation (CALIPSO/CALIOP):**  
NASA launched the polar-orbit satellite in 2006.



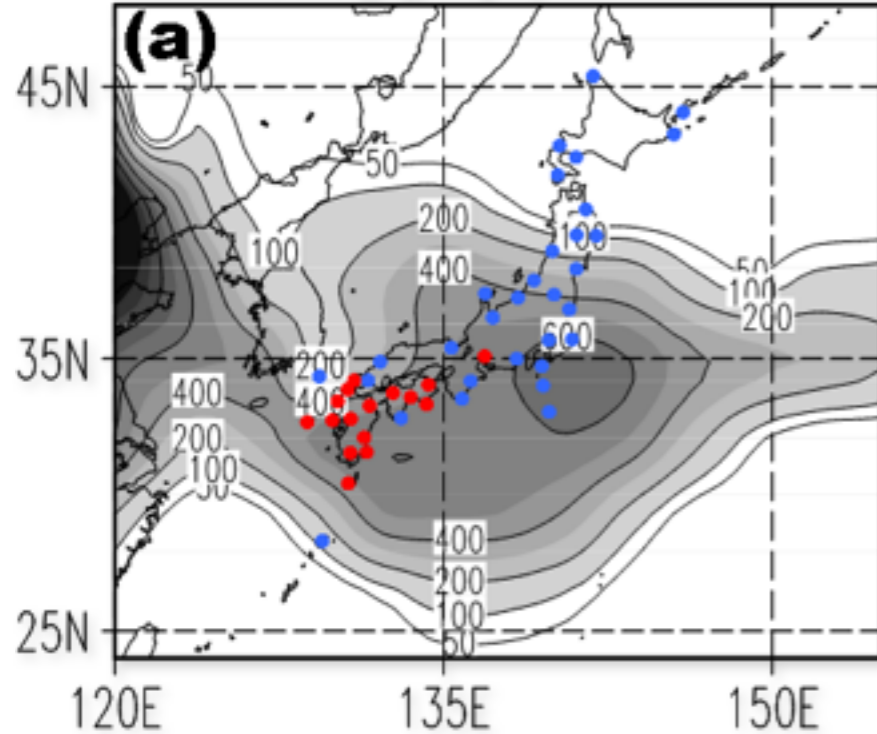
**Ground-based lidar network (NIES AD-Net):**  
NIES Japan is operating more than 20 lidar stations in East Asia.



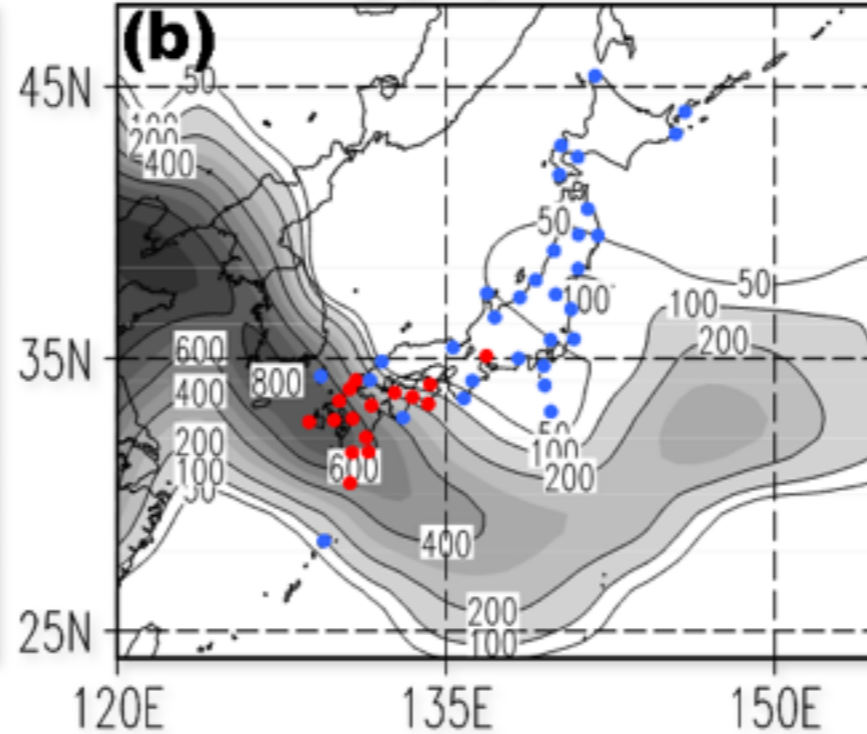


# EnKF for aerosol analysis

Surface Dust [ $\mu\text{g}/\text{m}^3$ ] w/o EnKF 28MAY2007



Surface Dust [ $\mu\text{g}/\text{m}^3$ ] with EnKF 28MAY2007

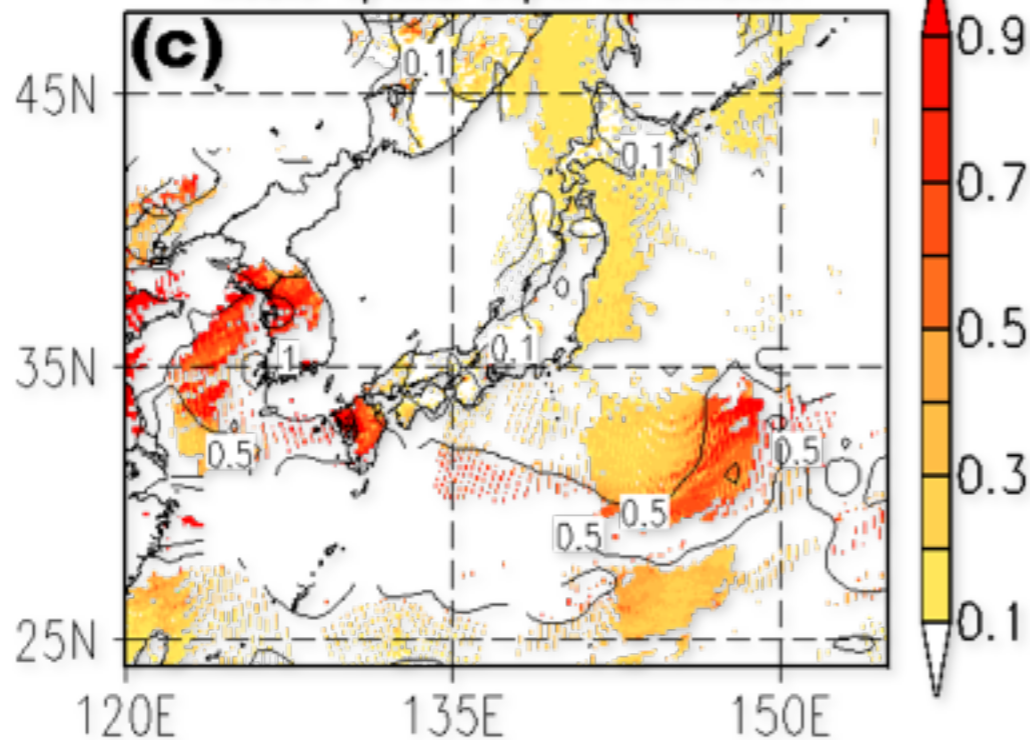


Contours and gray shades are **surface dust concentrations**.

**(a)** Free model-run result without data assimilation.

**(b)** CALIPSO data assimilation result.

MODIS Optical Depth 28MAY2007



*Red and blue circles are weather stations.*

*Red ones observed aeolian dust.*

*Blue ones did not observe any dust events.*

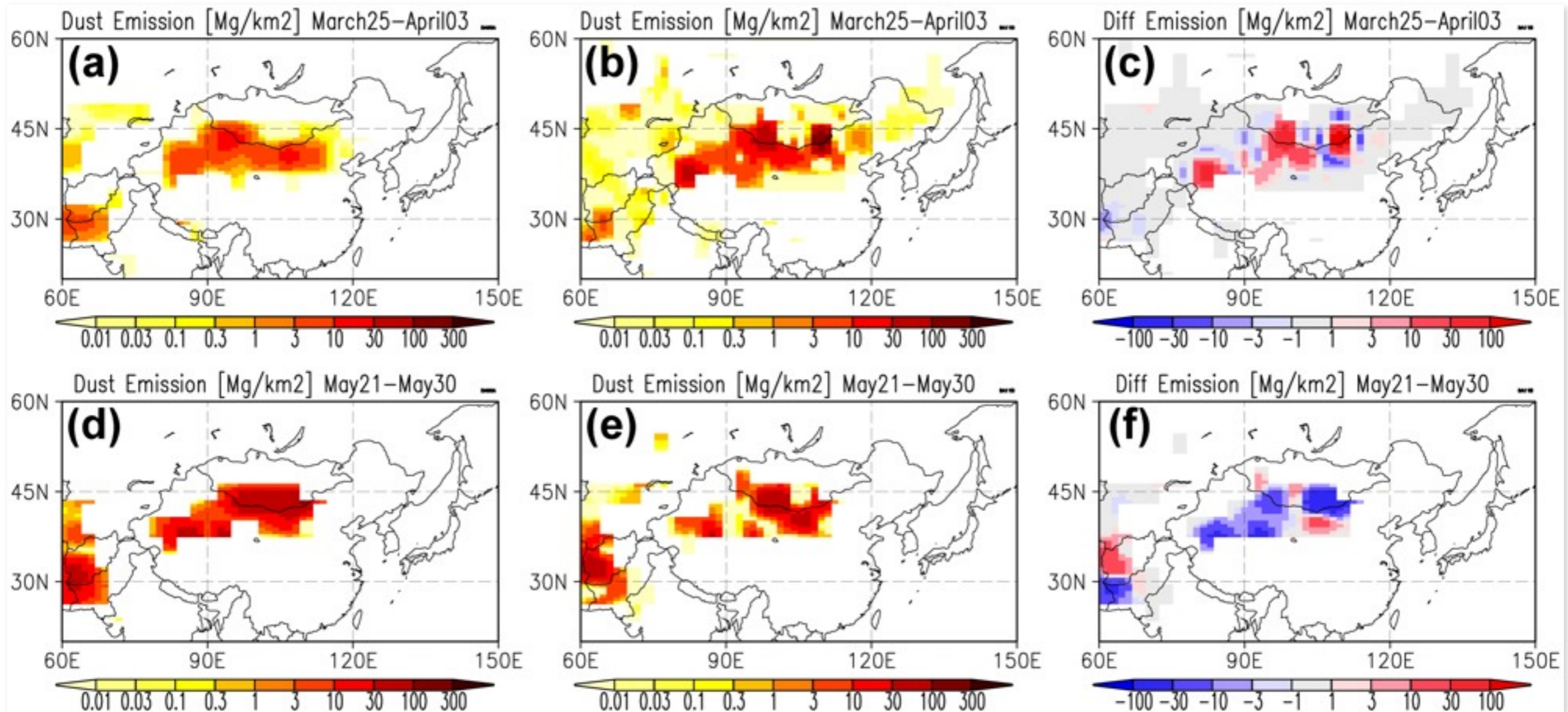
Sekiyama et al.,  
ACP (2010)

**The data assimilation result makes the dust plume mostly limited to the area of the red weather stations, in contrast to the free model-run result in which the dust plume covers both red and blue stations.**



# EnKF for aerosol analysis

- Dust emission inverse analysis by EnKF



Sekiyama et al., SOLA (2011)

**The dust concentrations in the downwind region are evidently improved when this dust emission analysis is installed to the model simulation.**

# JMA's plan for aerosol prediction

- **The EnKF aerosol analyses as initial conditions of aerosol prediction.**  
(hopefully, in practical use by 2014...)
- **Aerosol reanalysis:**  
available for climate modeling?
- **Aerosol climatology (detailed):**  
available for NWP?
- **Ideally, weather-chemistry coupled DA...**



# 3. Surface CO<sub>2</sub> flux

- establish a 4D-EnKF data assimilation system to estimate global surface CO<sub>2</sub> fluxes from various data.
- evaluate the potential impacts of various data obtained from the surface network measurements, GOSAT measurements, and CONTRAIL aircraft measurements (OSSEs).
- Real data assimilation with a bias-corrected GOSAT data.

**Forecast models:** MJ98-CDTM, FRCGC ACTM

**Assimilated data:** Satellite (GOSAT), Aircraft (CONTRAIL),  
Ground-based network

**Control variables:** Surface CO<sub>2</sub> flux, Atmospheric CO<sub>2</sub> concentration

**Assimilation setting:** 4D analysis with 72-h time window



# 4D data assimilation system for carbon cycle

- Simultaneously estimate atmospheric concentrations and surface fluxes of CO<sub>2</sub> at high spatial (2.8°) and temporal (1.5 days) resolution.

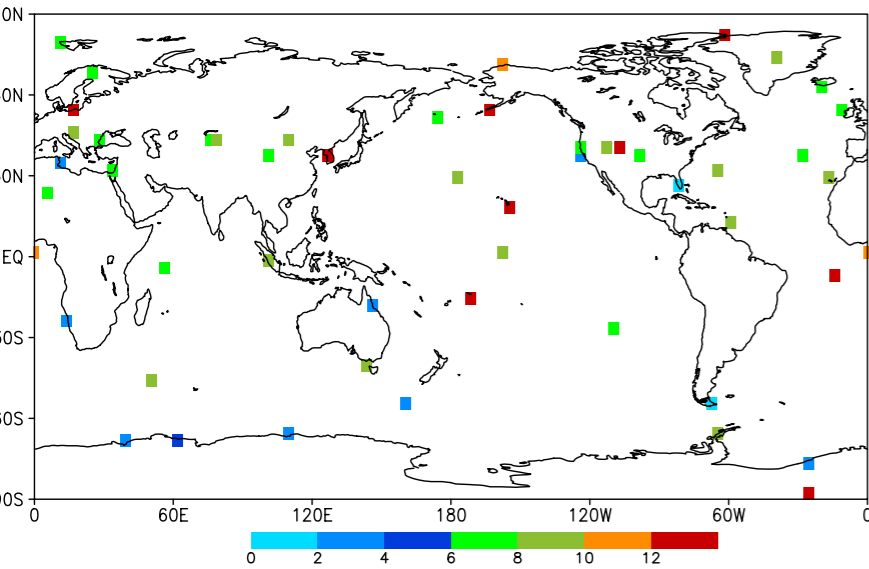
**Forecast models:** (1) FRCGC ACTM (Miyazaki et al., 2008)  
(2) MJ98-CDTM

**Data assimilation:** 4D-EnKF with localization (LETKF, Hunt et al., 2007)

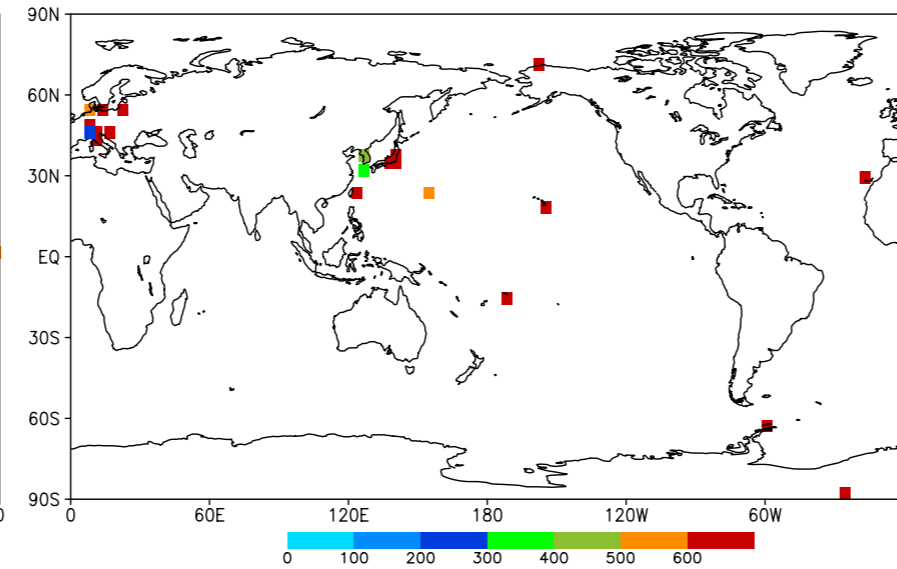
- State augmentation approach
- Conditional inflation for surface flux
- Data assimilation window: 3-day
- Super observation for CONTRAIL data
- Long vertical localization length for CONTRAIL
- 48 ensemble members

# Number of obs per month

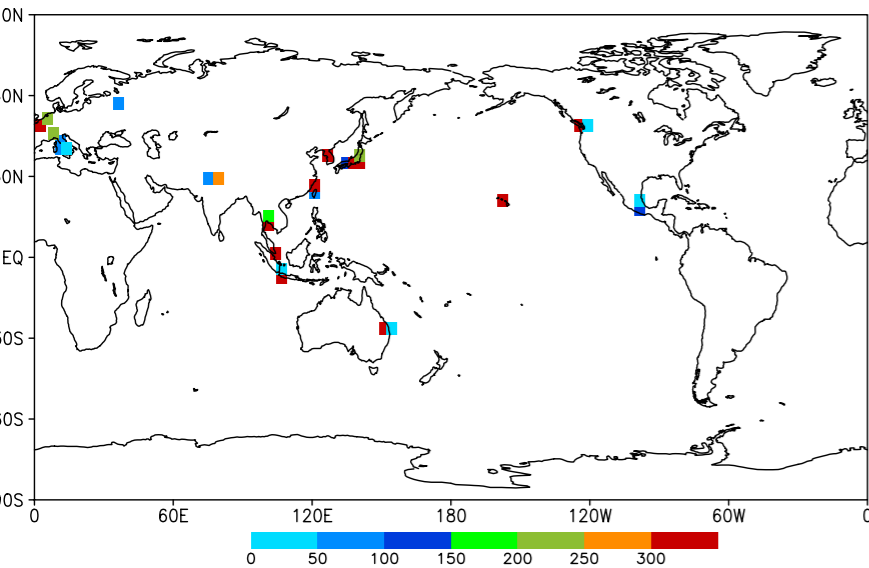
(a) Surface: flask



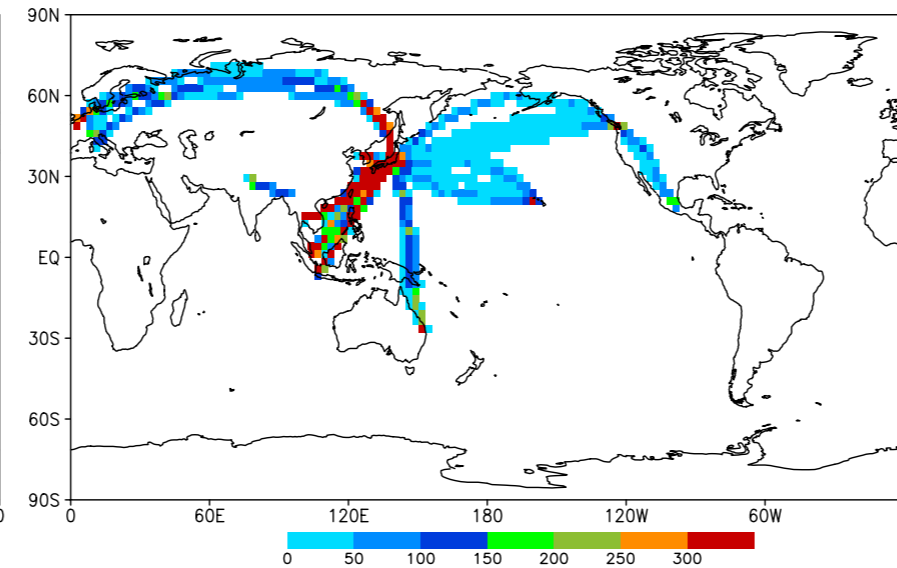
(b) Surface: continuous



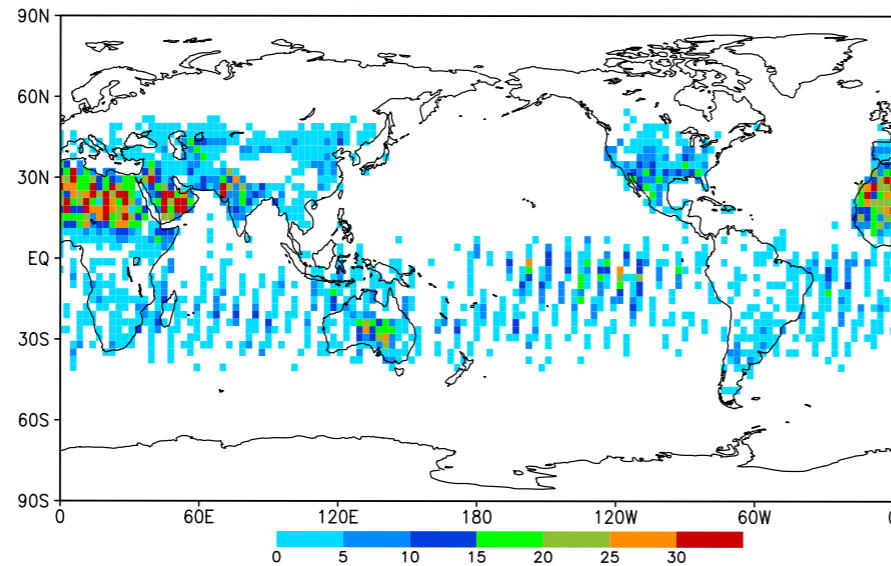
(c) CONTRAIL: vertical profile



(d) CONTRAIL: upper air



(e) GOSAT

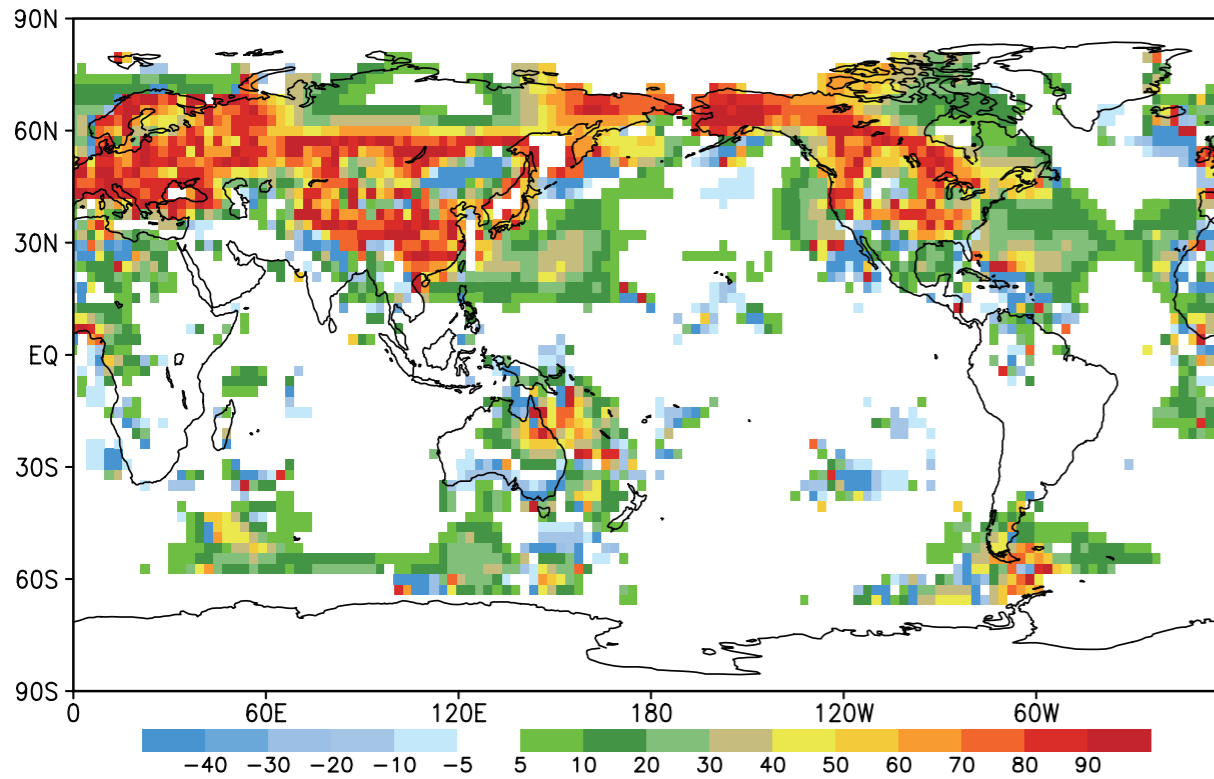


Observation  
system  
simulation  
experiments  
(OSSEs)

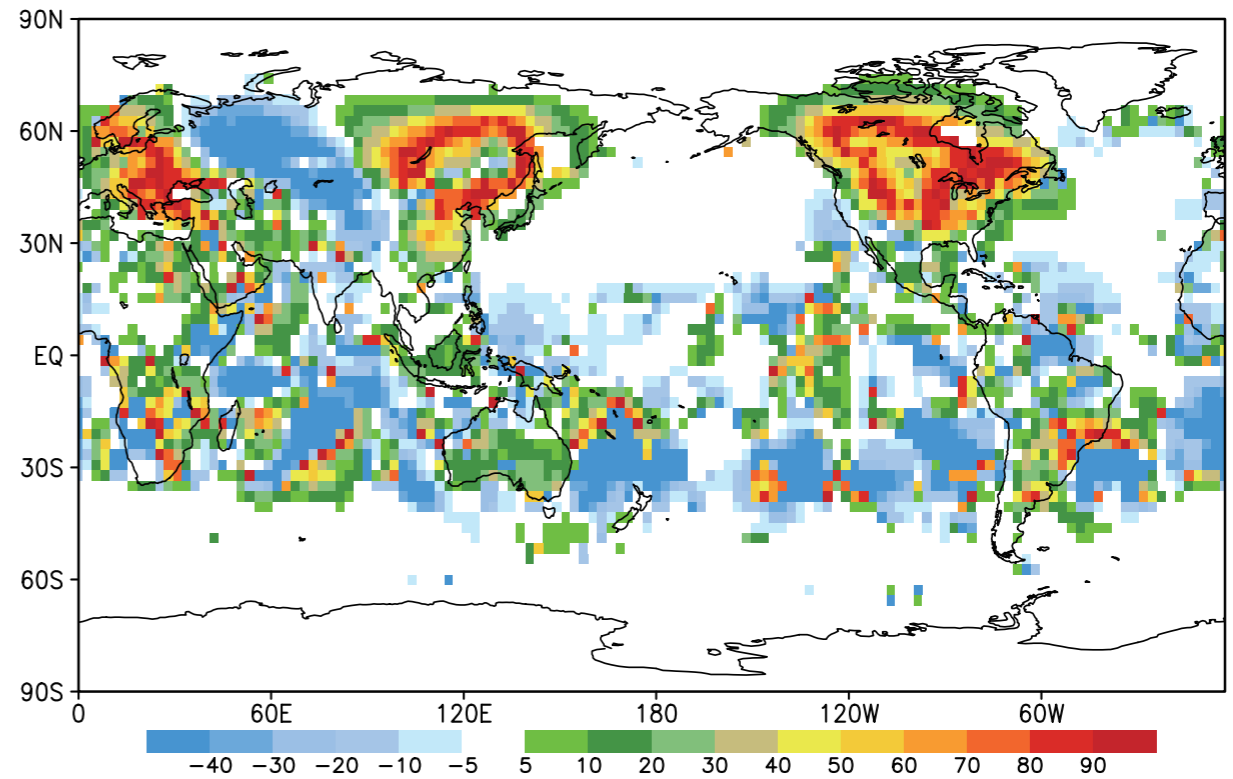
- demonstrate the performance of the DA scheme
- tell us how much error reductions can be expected by each dataset

# Flux error reduction rate [%]: grid-scale

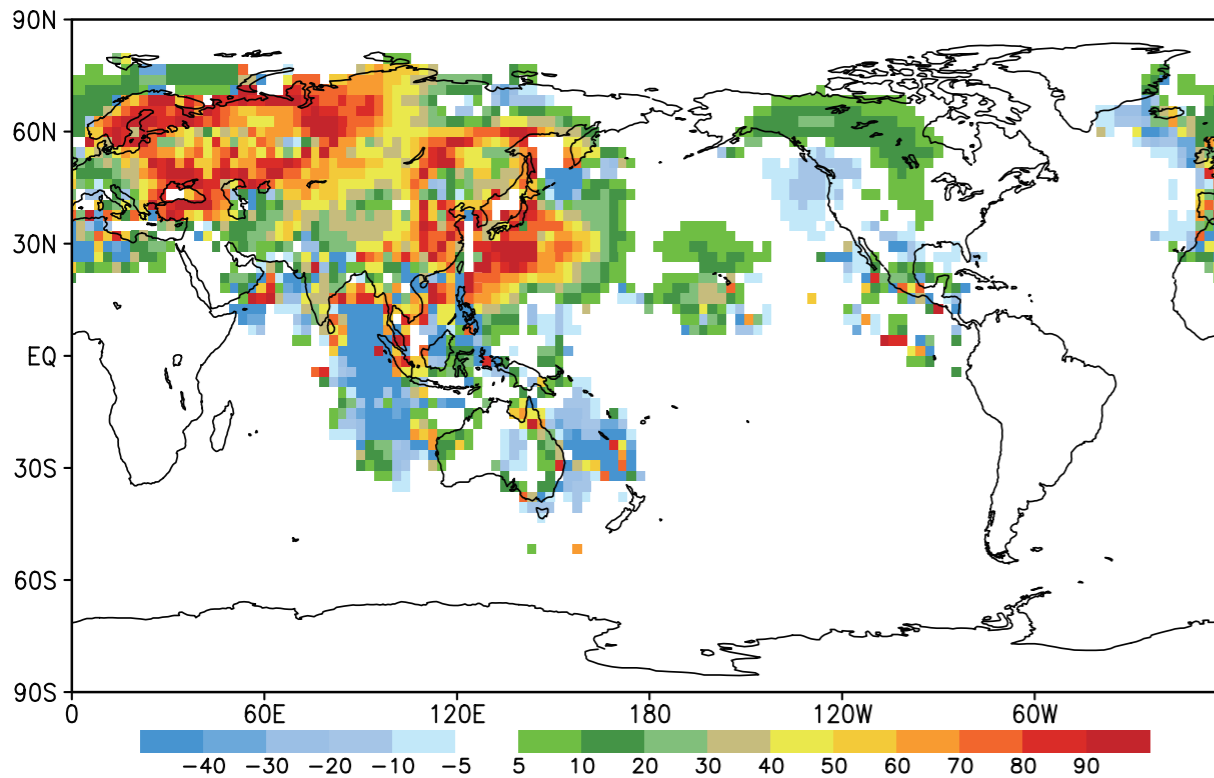
(a) Surface network



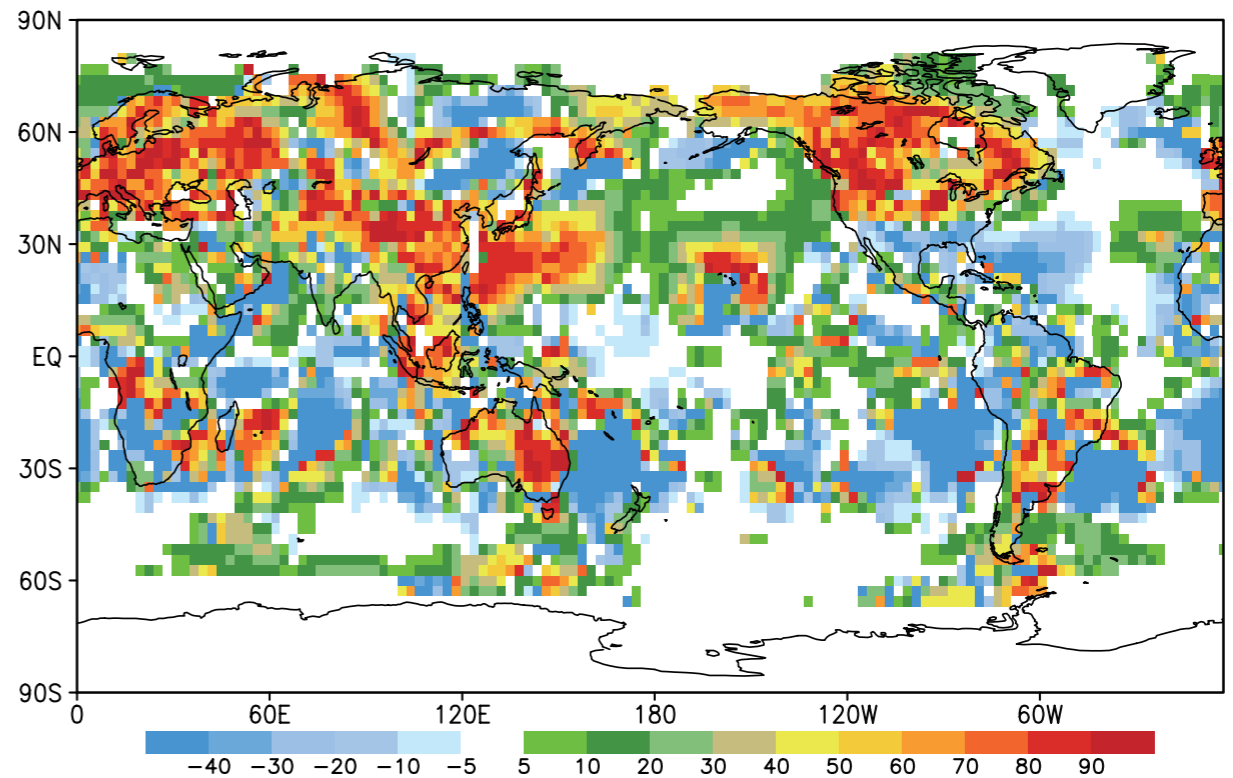
(b) GOSAT



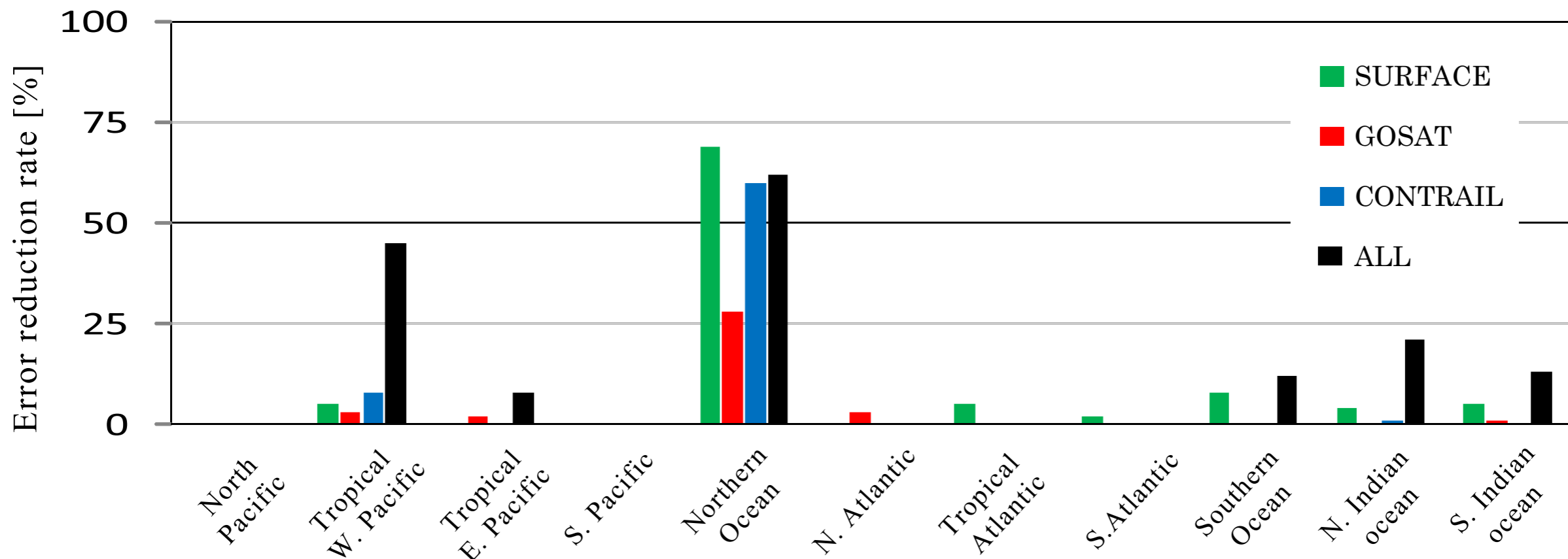
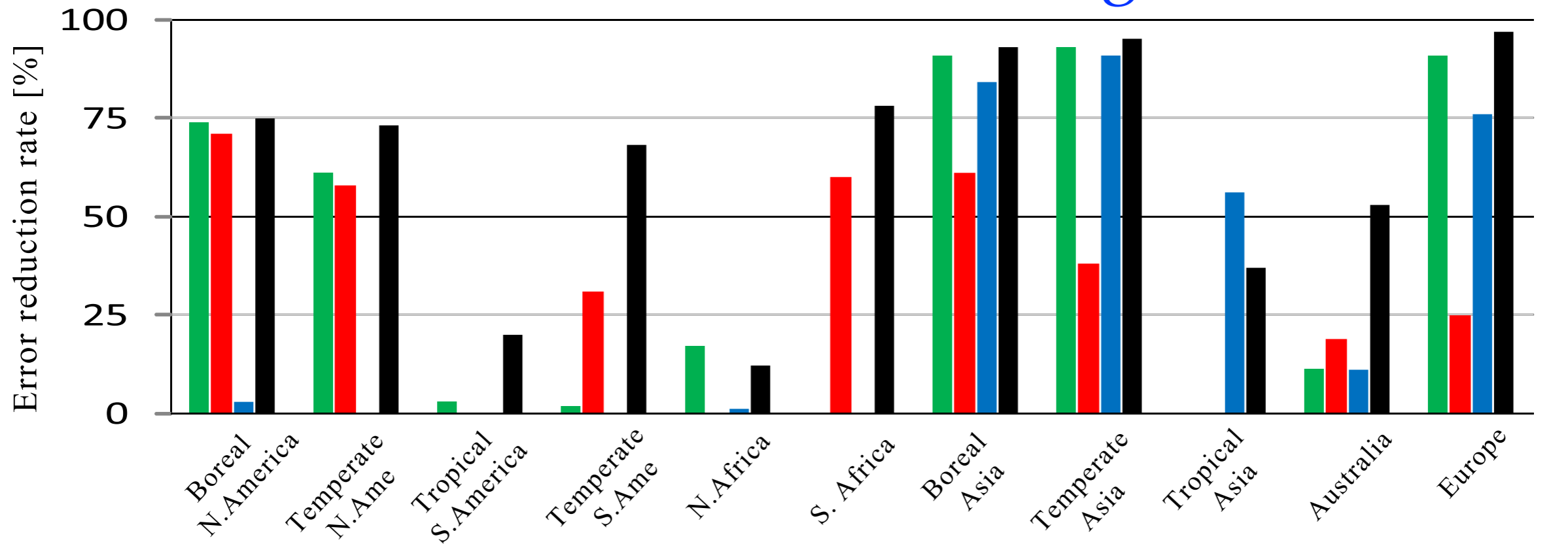
(c) CONTRAIL



(d) All



# Flux error reduction rate [%]: regional-fluxes

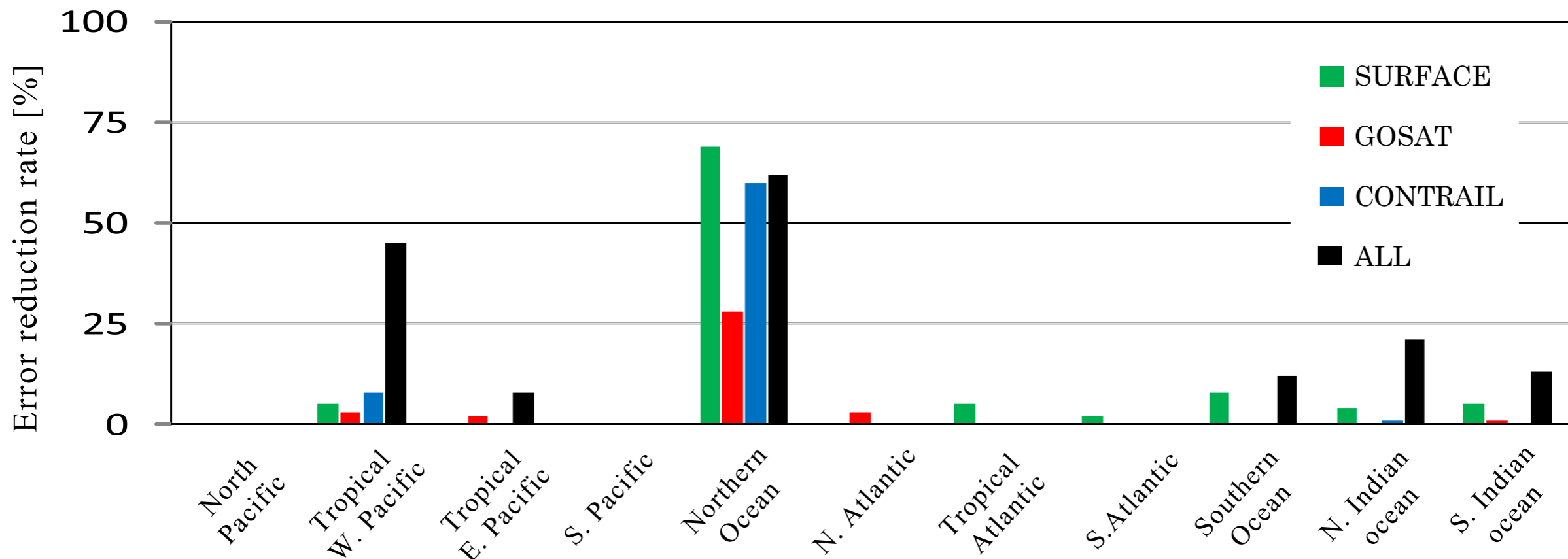
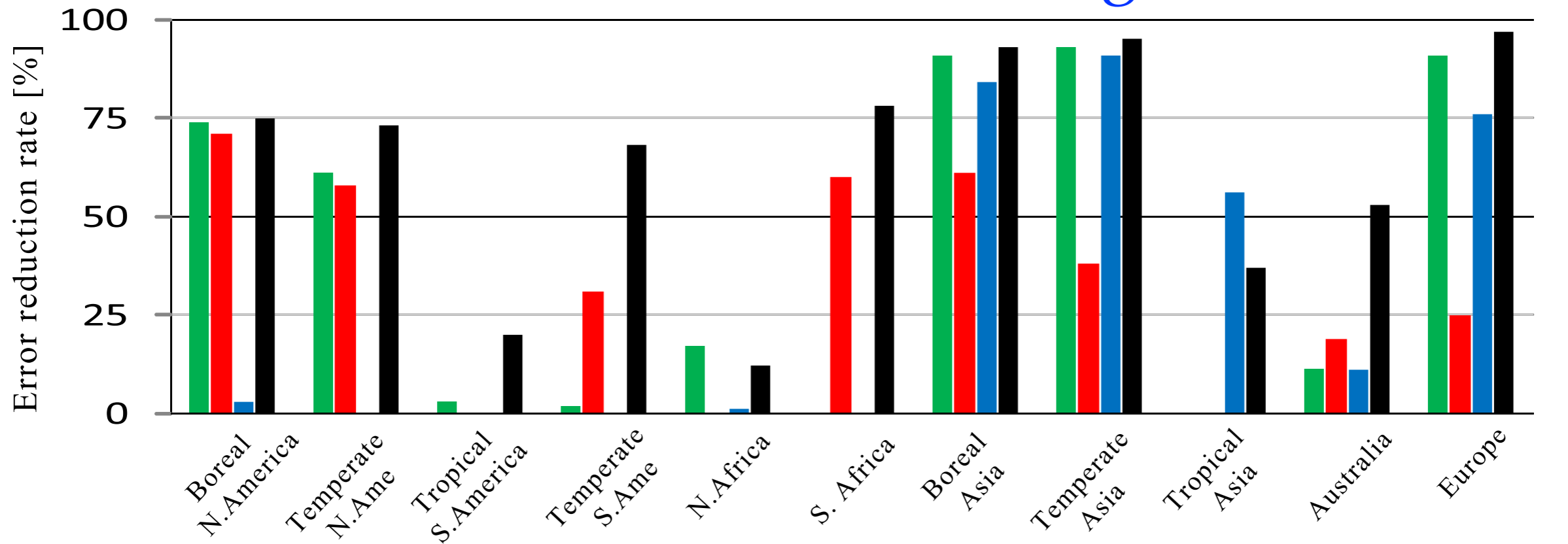


**CONTRAIL data: Europe and Asia.**

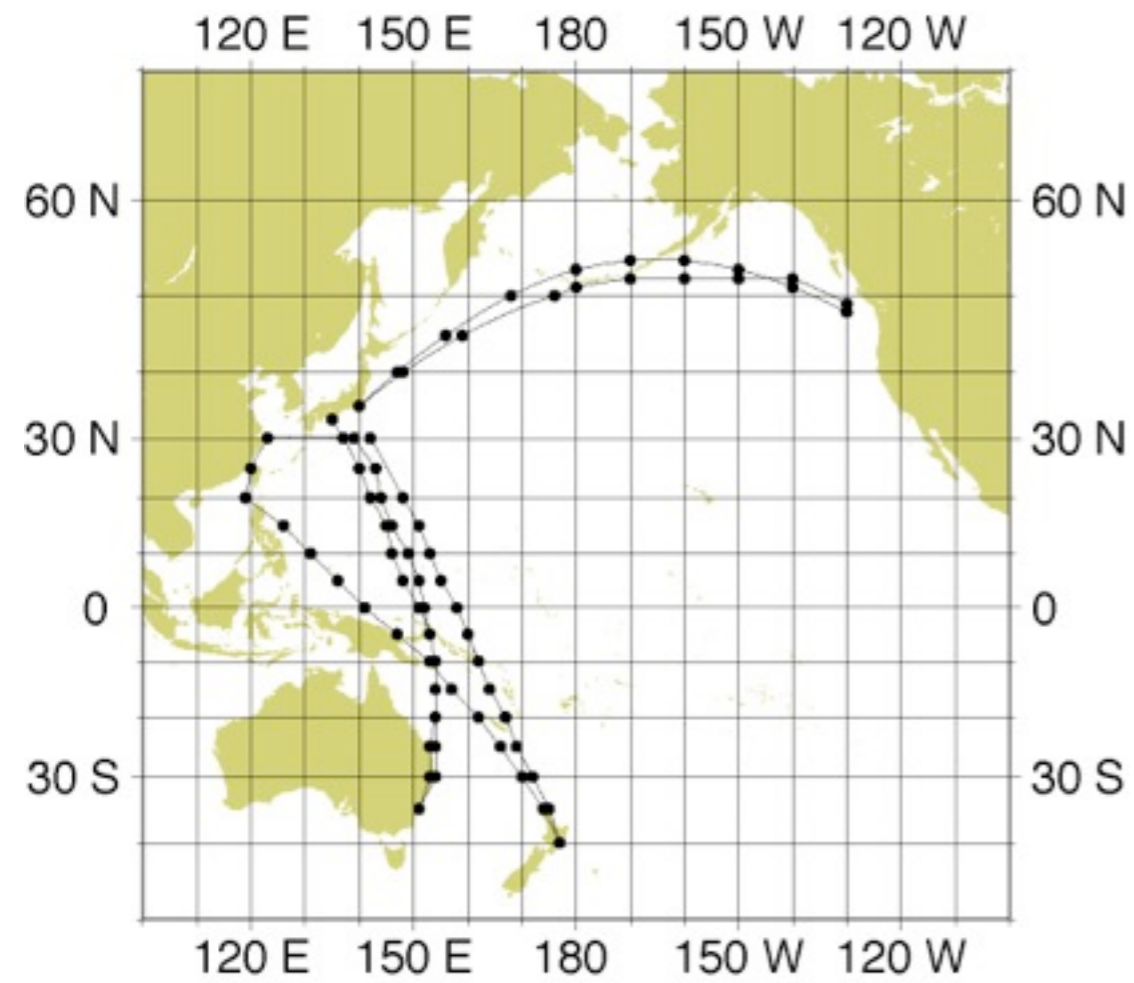
**GOSAT data: North and South America, South Africa, Asia, and Europe**



# Flux error reduction rate [%]: regional-fluxes



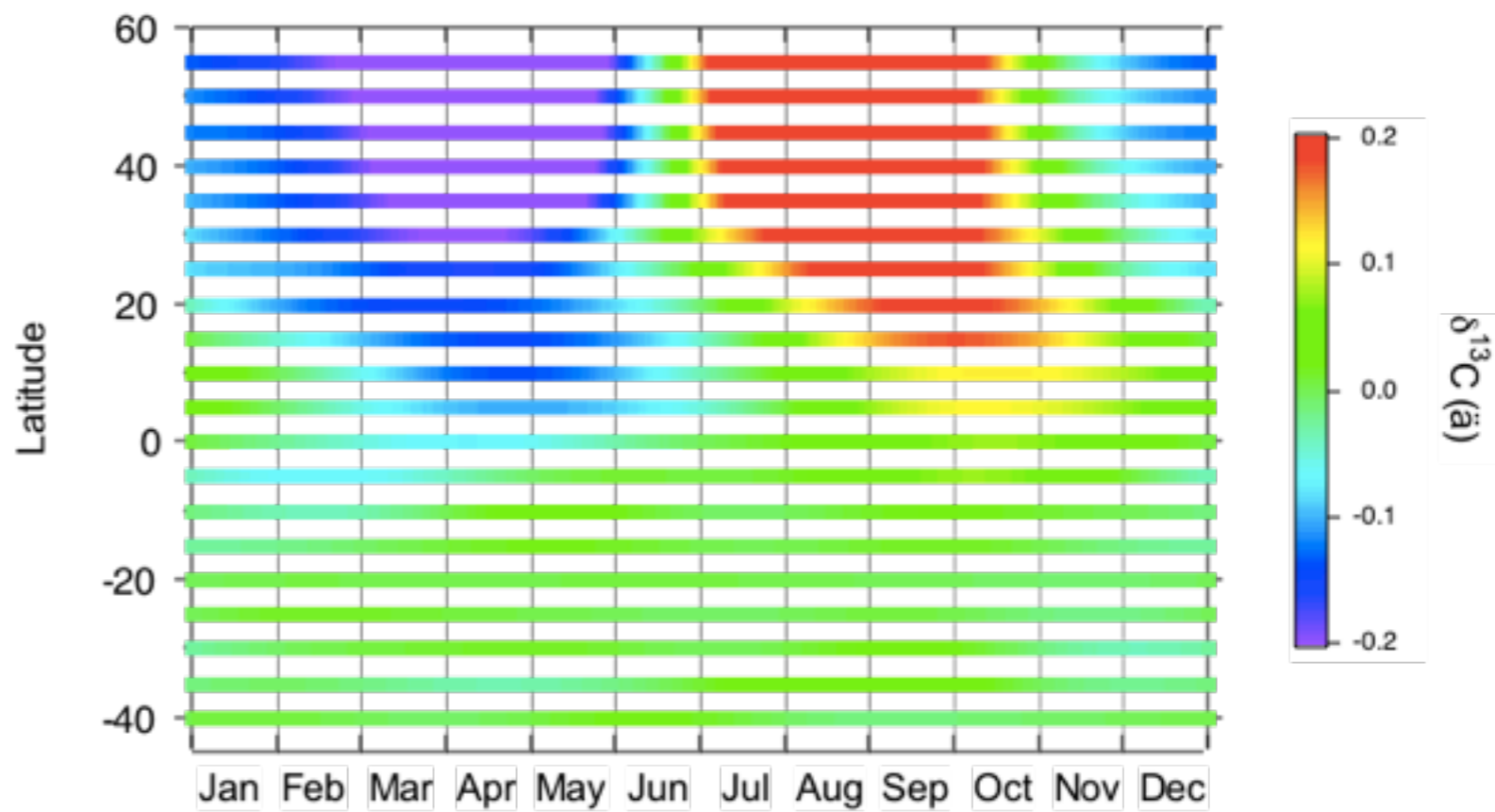
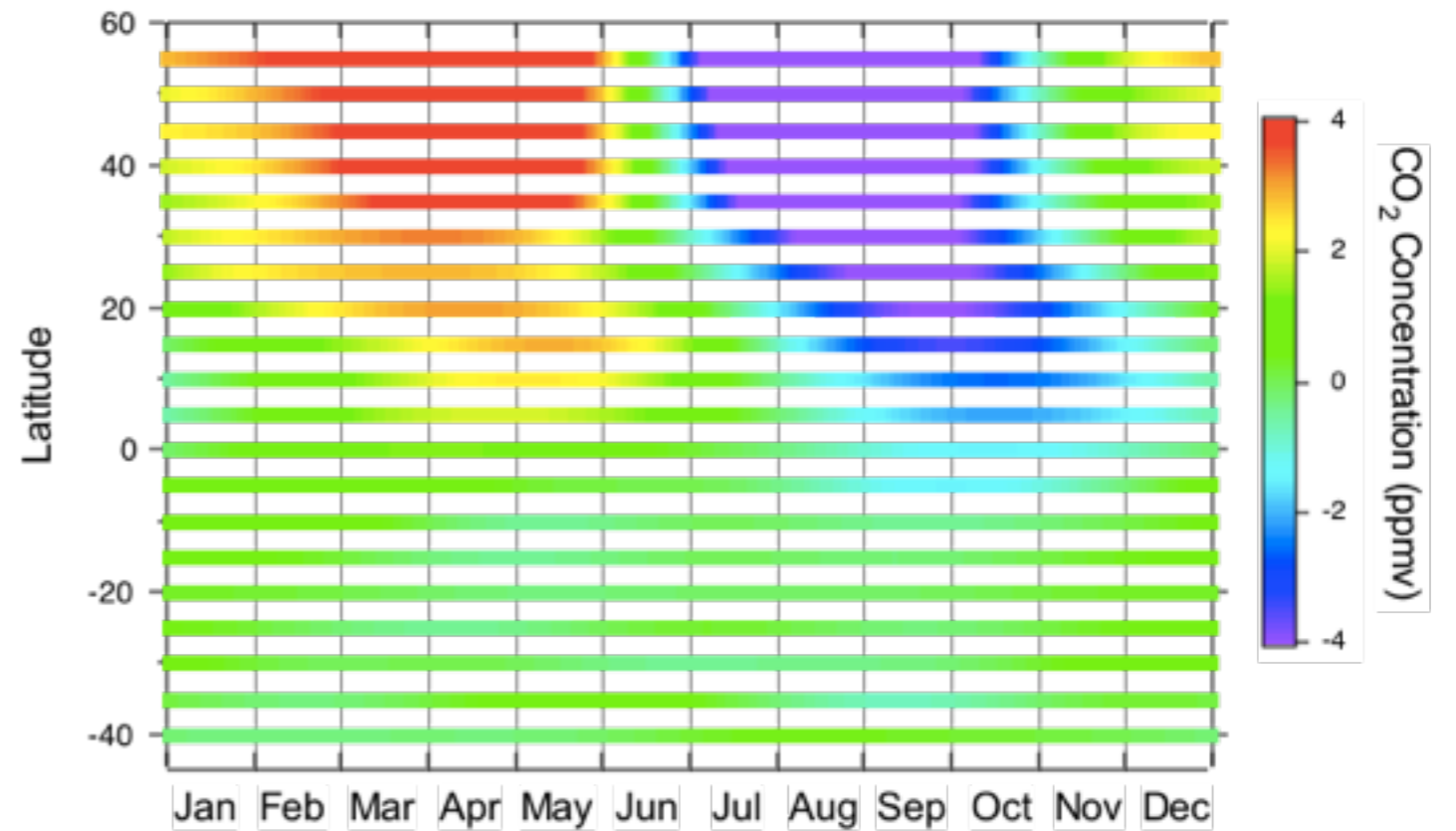
**Additional constraints are required especially over North Africa, tropical South America, southern North America, and the oceans.**



**Air sampling on board commercial container ships since 1984.**

**Further constraints will be added...**

**Fig: Mean seasonal cycles of CO<sub>2</sub> concentration and δ<sup>13</sup>C at each latitude band.**

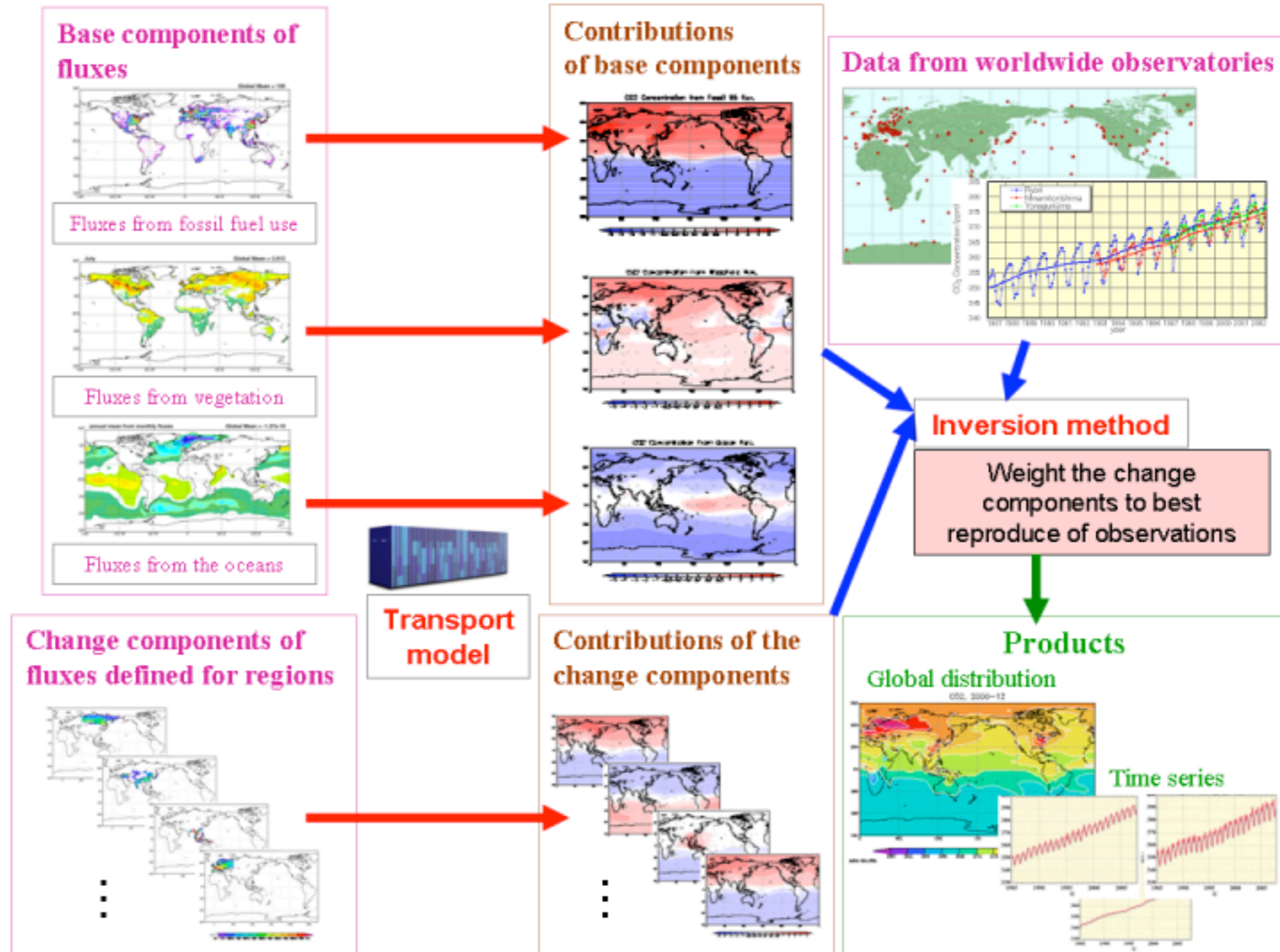


# Sensitivity to OSSE settings and model/obs errors

- **The OSSE results are sensitive to its settings (e.g., initial and true fluxes, and observation errors).**
- **Many sources of error associated with the observations and the transport model will strongly decrease the usefulness of each observation; this could become a limiting factor in the data assimilation that involves real data (Miyazaki et al., 2011).**
- **E.g., realistic systematic errors in the GOSAT data can reduce the usefulness of the observations by a factor of 2.**

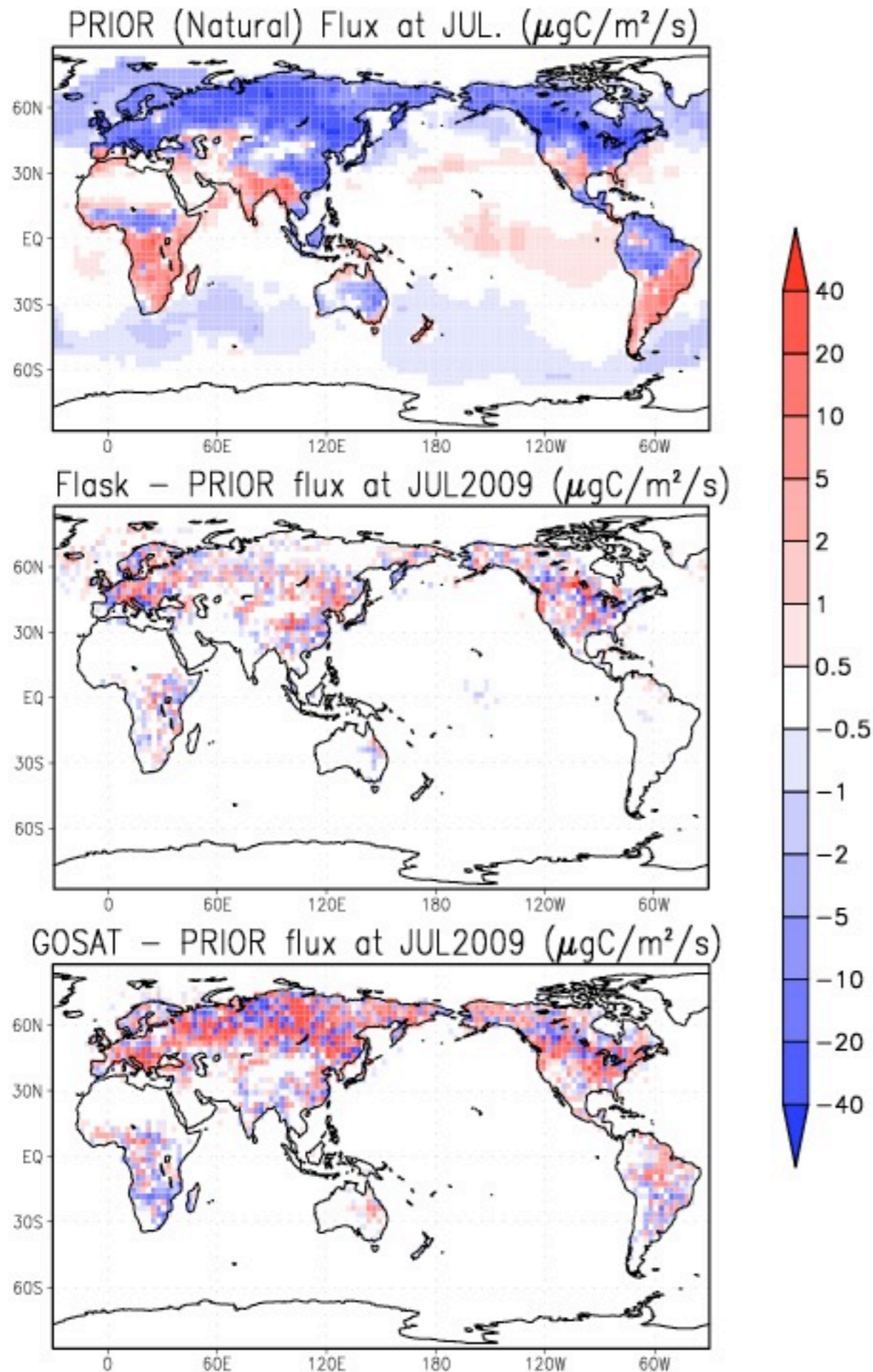
# A bias correction scheme for GOSAT

- Monthly mean bias of GOSAT is estimated by comparing GOSAT XCO<sub>2</sub> (L2SWIR) with JMA CO<sub>2</sub> analysis (based on surface observations).
- Hot spot fluxes are further adjusted using surrounding data.





# Real data assimilation



- **Bias-corrected GOSAT data provide additional corrections and improve the agreement with independent data.**

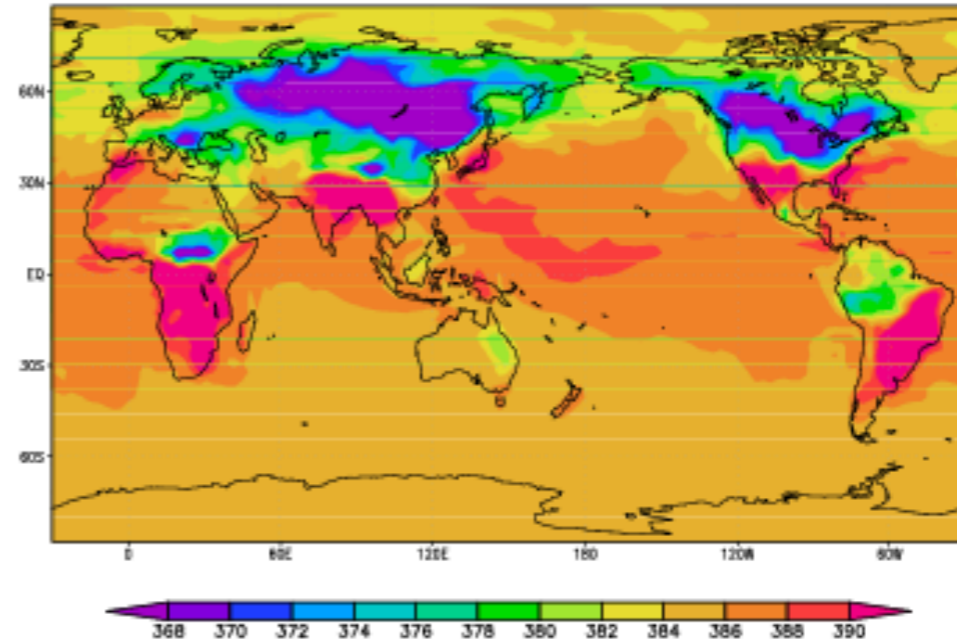
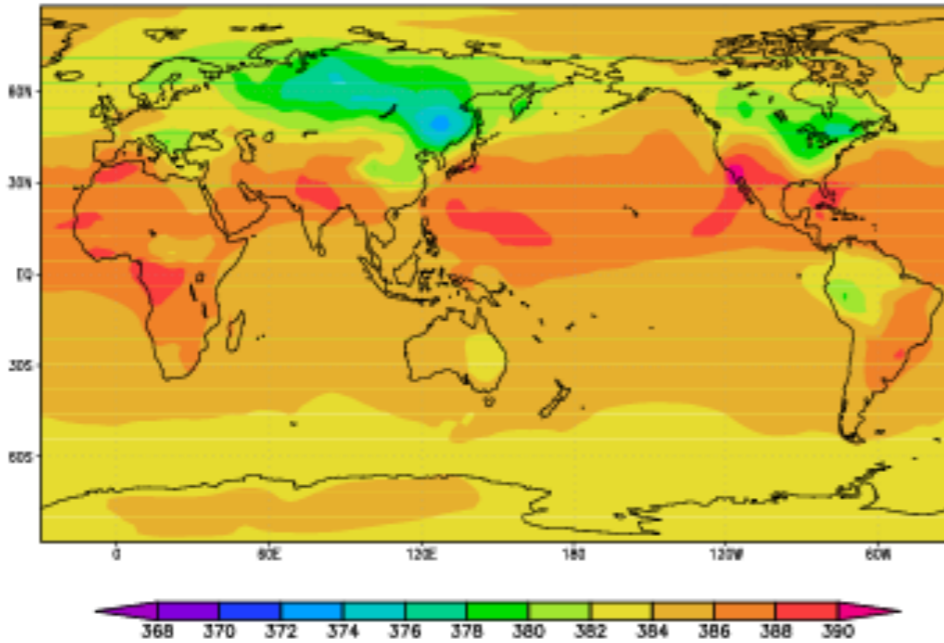
# CO<sub>2</sub> Analysis Results (Jul 2009)

Surface CO<sub>2</sub> concentrations

RMSE=3.96ppm

JMA Analysis (Jul. 2009)

MJ98-CDTM w/o data Assimilation (Jul. 2009)

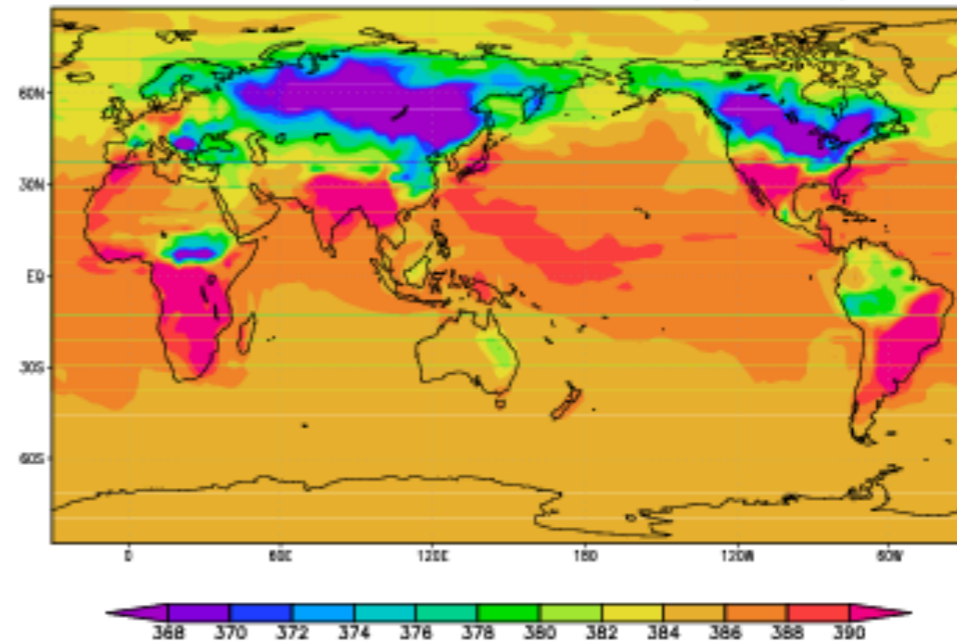
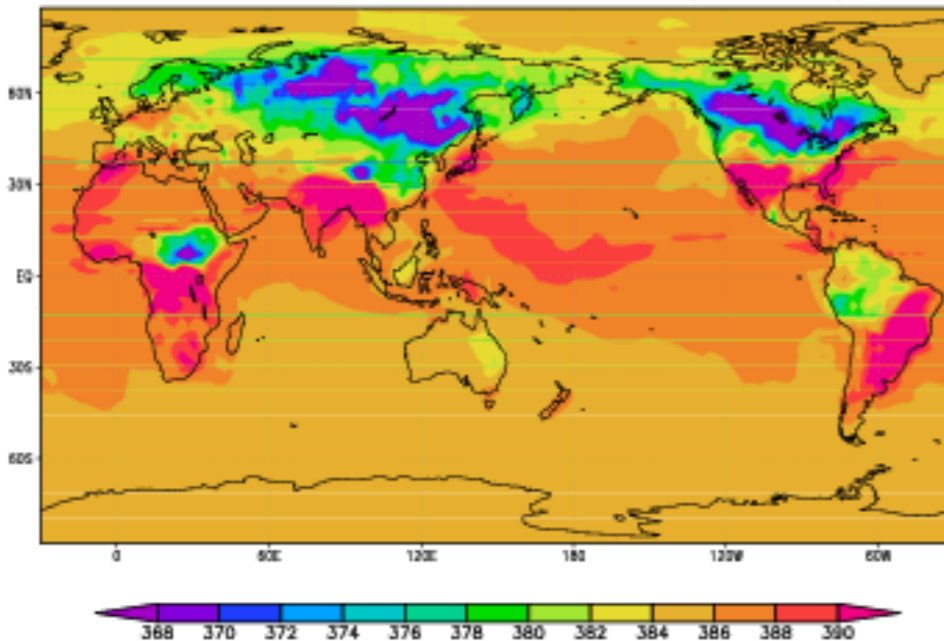


JMA  
Analysis

w/o assim.

Assimilation result with GOSAT Data (Jul. 2009)

Assimilation result with Flask Data (Jul. 2009)



GOSAT  
assim.

Flask  
assim.

RMSE=3.12ppm

RMSE=3.83ppm



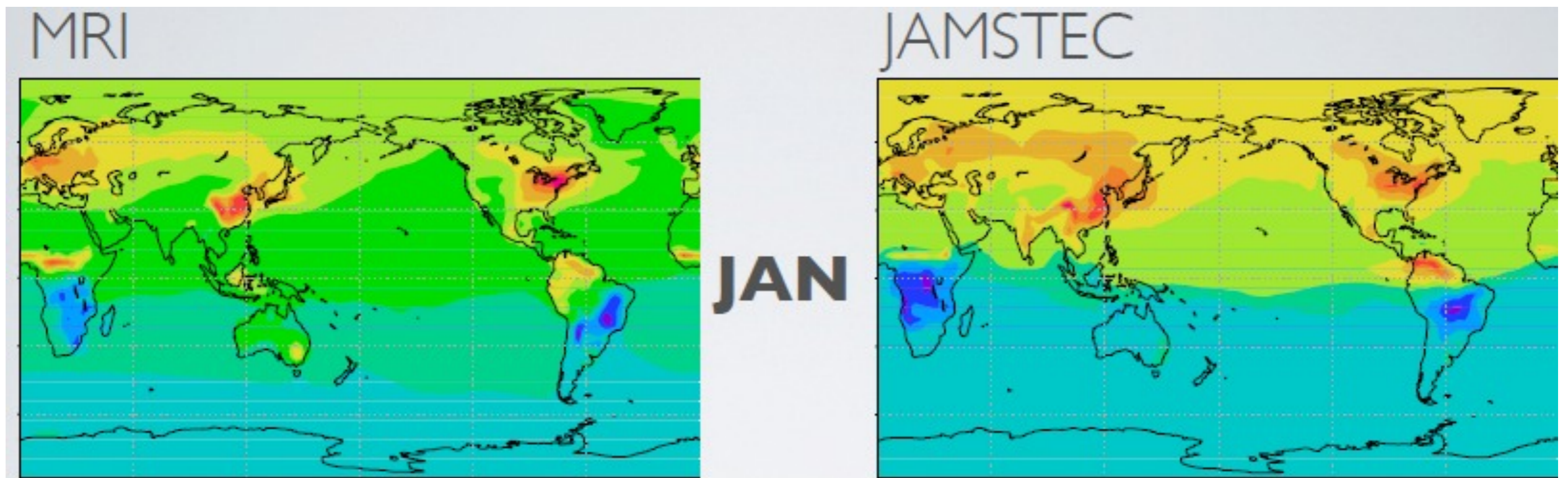
# Multi-model comparison of surface CO<sub>2</sub> flux estimates

Forecast models:

(1) **MRI CDTM** (Maki et al., 2010)

(2) **JAMSTEC ACTM** (Miyazaki et al, 2008)

Fig: CO<sub>2</sub> Mixing Ratio Anomaly in the lower troposphere



*e.g., choice of vertical diffusion scheme largely affects simulation/assimilation results.*



# 4. Air quality

## Forecast models:

(1) **CHASER** (Sudo et al., 2002)

T42L32 p-top=3 hPa

(2) **MRI CCM** (Shibata and Deushi, 2008)

T42L68 p-top=0.01 hPa

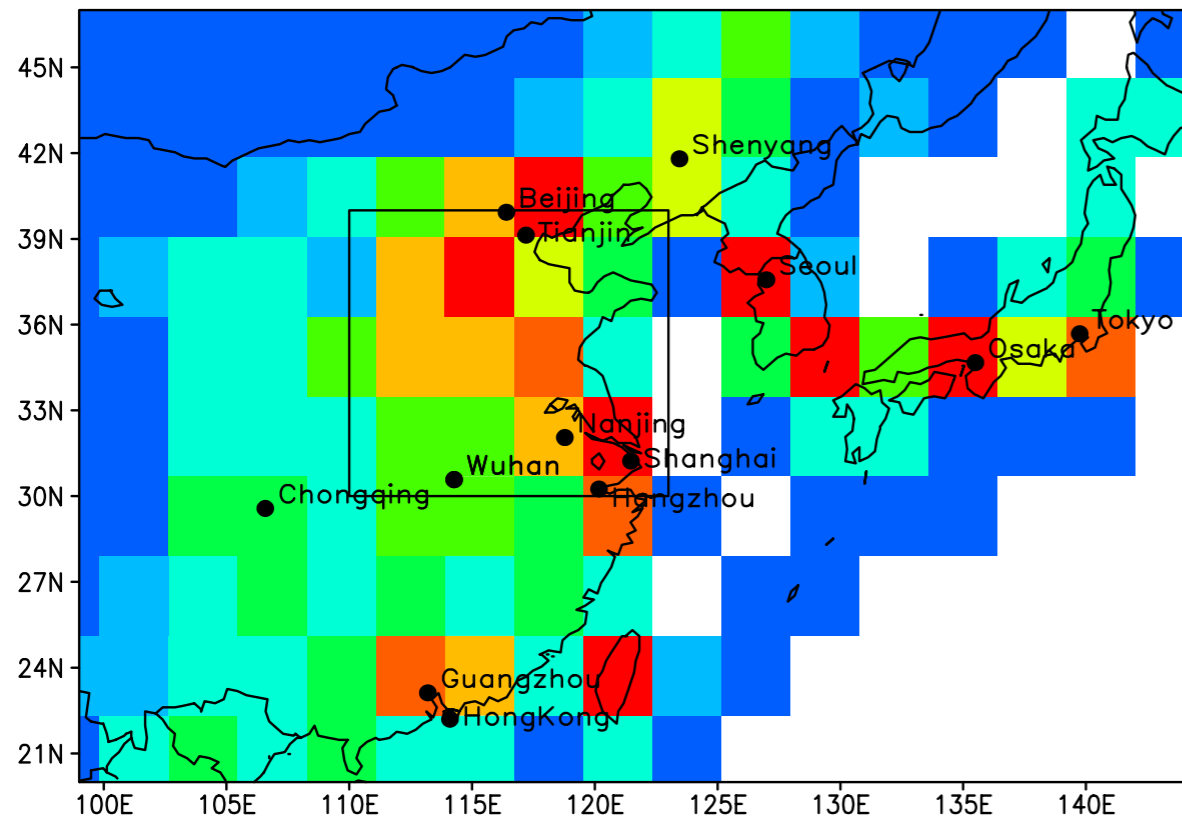
- **for reanalysis/monitoring of Asian/global atmospheric environment**

Assimilated data: OMI NO<sub>2</sub>, SCIAMACHY NO<sub>2</sub>, TES O<sub>3</sub>, etc...

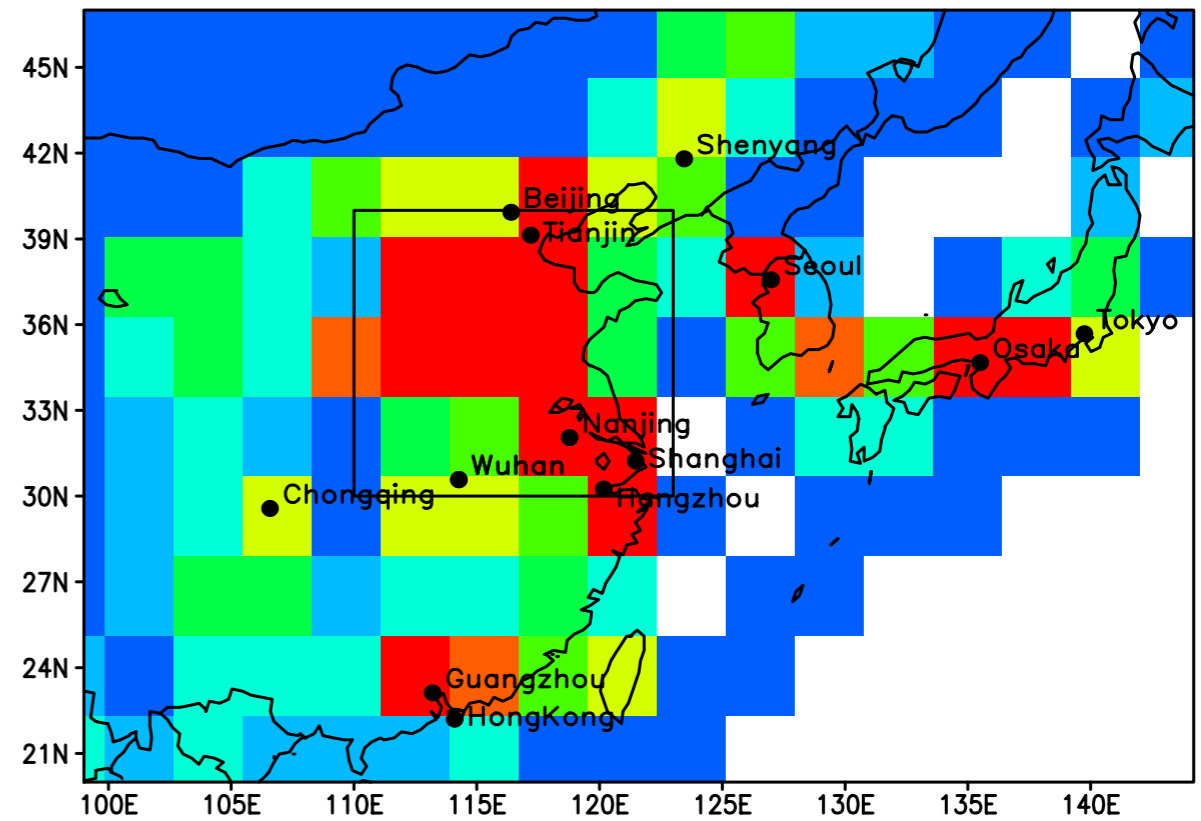
Control variables: NO<sub>x</sub> emission, NO<sub>2</sub>, O<sub>3</sub>, HNO<sub>3</sub>, etc...

Assimilation settings: 3D-analysis

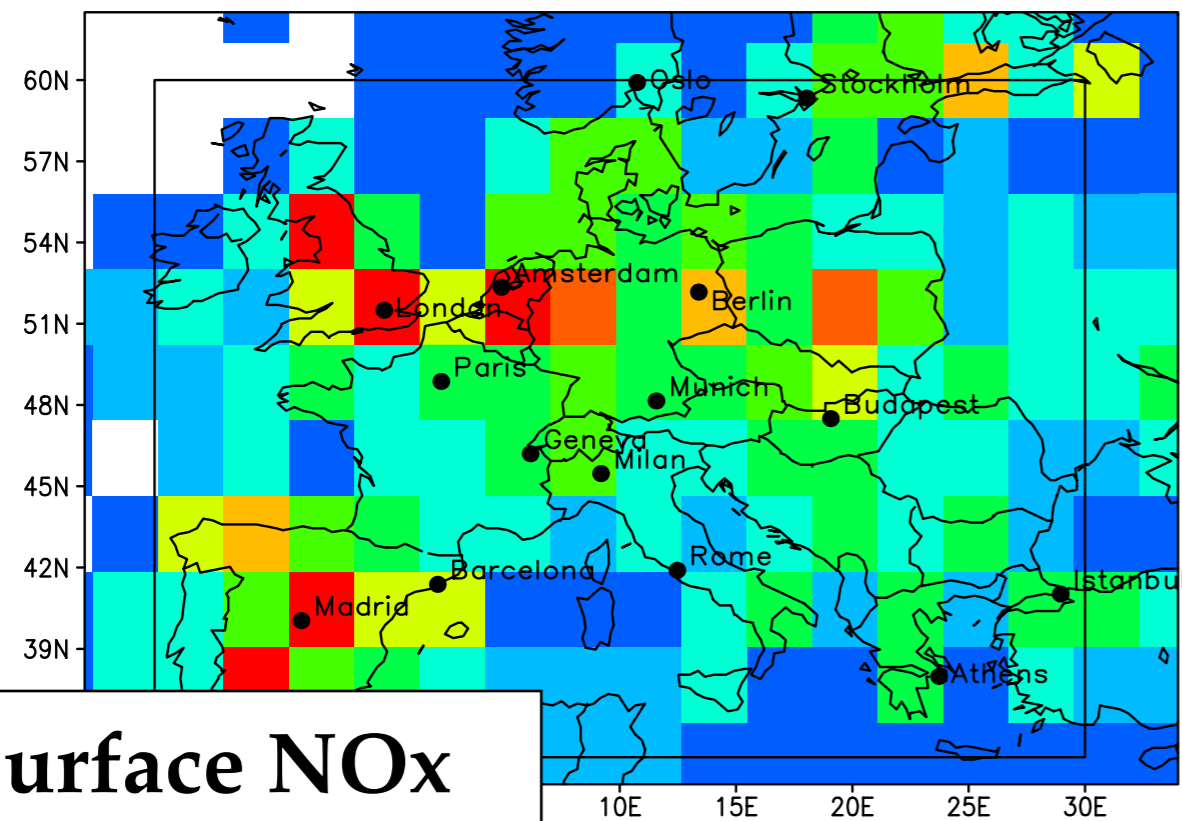
### A priori: east Asia



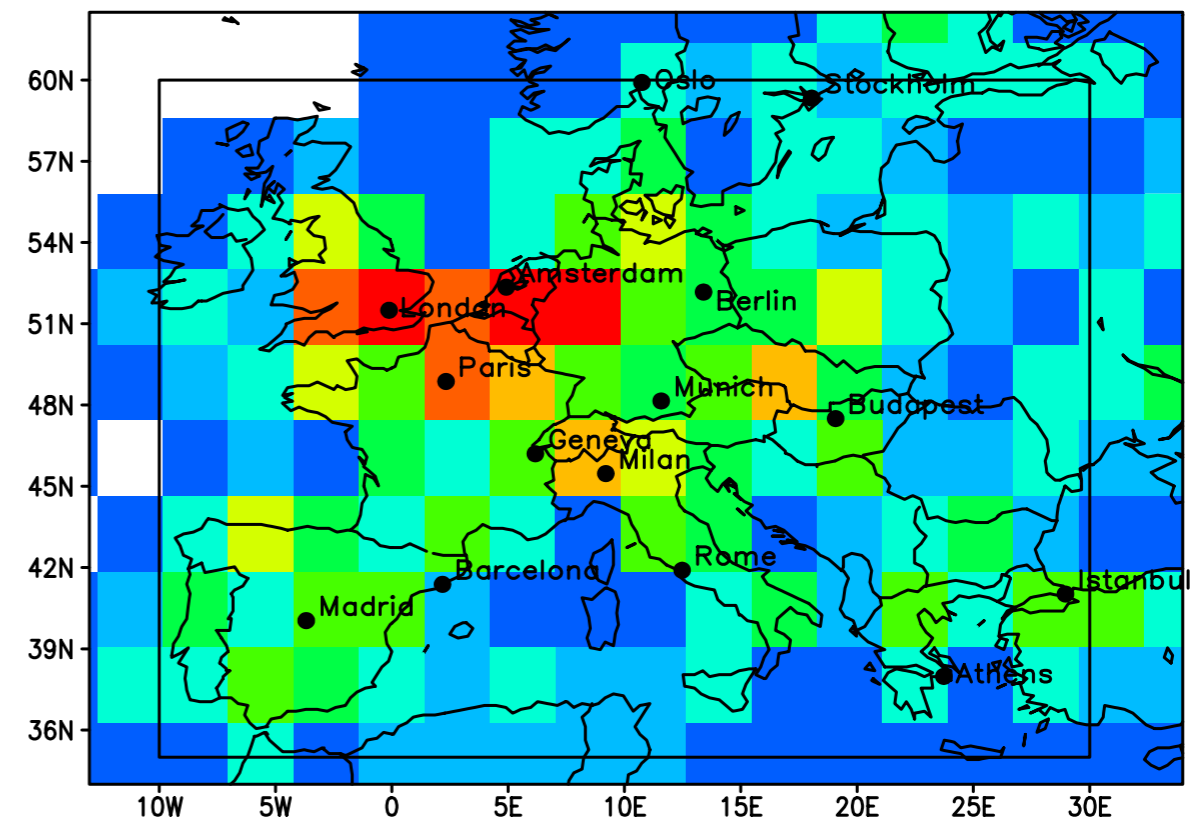
### A posteriori: east Asia



### A priori: Europe



### A posteriori: Europe



**Surface NOx  
emission**



# Summary

**We have developed chemical data assimilation systems to analyze Asian/global atmospheric environment, using a same scheme.**

- **Meteorology-chemistry coupling data assimilation**
  - **for better understanding stratospheric processes/stratospheric reanalysis??**
- **Aerosols analysis/forecast**
  - **for operational use at JMA...?**
- **High resolution surface CO<sub>2</sub> flux estimates**
  - **(the knowledge obtained from the OSSEs will help to interpret the real data assimilation results)**
- **atmospheric concentrations and emissions of polluted gasses**
  - **for monitoring Asian/global atmospheric environment.**

*... more data will be included ...*

- Miyazaki et al., Assessing the impact of satellite, aircraft, and surface observations on CO<sub>2</sub> flux estimation using an ensemble-based 4D data assimilation system, JGR, 2011. **(CO<sub>2</sub> DA system, OSSE study)**
- Miyazaki, Performance of a local ensemble transform Kalman filter for the analysis of atmospheric circulation and distribution of long-live tracers under idealized conditions, JGR, 2009. **(CO<sub>2</sub> DA system, OSSE study)**
- Miyazaki et al., Formation mechanisms of latitudinal CO<sub>2</sub> gradient in the upper troposphere over the subtropics and tropics, JGR., 2009 **(CO<sub>2</sub> transport/CONTRAIL analysis)**
- Miyazaki, et al., Global-scale transport of carbon dioxide in the troposphere, JGR, 2008. **(CO<sub>2</sub> transport/modeling)**
- Miyazaki et al., Global NO<sub>x</sub> emission estimates from data assimilation of OMI tropospheric NO<sub>2</sub> columns, to be submitted **(air quality DA)**
- Maki et al., New techniques to analyze global distributions of CO<sub>2</sub> concentrations and fluxes from non-processed observational data, Tellus, 2010. **(QC processes)**
- Maki et al., The Impact of Ground-Based Observations on the Inverse Technique of Aeolian Dust Aerosol, SOLA, 2011. **(Dust inversion)**
- Sekiyama et al., Data assimilation of CALIPSO aerosol observations. ACP, 2010. **(Aerosols assimilation)**
- Sekiyama et al., The Effects of Snow Cover and Soil Moisture on Asian Dust: II. Emission Estimation by Lidar Data Assimilation, SOLA, 2011. **(Aerosols assimilation)**
- Iwasaki et al., Comparisons of Brewer-Dobson Circulations diagnosed from Reanalyses, JSMJ, 2009. **(BD inter-comparison among reanalyses)**
- Presentation at IUGG: Nakamura et al., Data Assimilation session (JM02). **(Strat. O<sub>3</sub>)**
- **and more soon... (hopefully!!)**