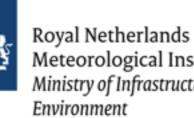
大気組成データ同化システム の開発と長期再解析

宮崎 和幸 独立行政法人海洋研究開発機構





Meteorological Institute Ministry of Infrastructure and the

第4回データ同化ワークショップ、気象庁、2014年1月8日

1. 大気組成データ同化とは

2. システムの開発

3. 解析結果の検証

4. 長期再解析の実施

5. 今後の課題

<u>Miyazaki</u> et al., Global lightning NOx production estimated by an assimilation of multiple satellite datasets, *ACPD*, 2013.

<u>Miyazaki</u> et al., Constraints on surface NOx emissions by assimilating satellite observations for multiple species, *GRL*, 2013.

Nakamura, <u>Miyazaki</u> et al., A multi-model comparison of stratospheric ozone data assimilation based on an ensemble Kalman filter approach, *JGR*, 2013.

<u>Miyazaki</u> et al., Simultaneous assimilation of satellite NO2, O3, CO, and HNO3 data for the analysis of tropospheric chemical composition and emissions, ACP, 2012b.

<u>Miyazaki</u> et al., Global NOx emission estimates derived from an assimilation of OMI tropospheric NO2 columns, ACP, 2012a.

<u>Miyazaki</u> et al., Assessing the impact of satellite, aircraft, and surface observations on CO2 flux estimation using an ensemble-based 4D data assimilation system, *JGR*, 2011.

<u>Miyazaki</u>, 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.

with thanks to Henk Eskes (KNMI), Kengo Sudo (Nagoya Univ.), Folkert Boersma (Einthovohen Univ.), Michiel van Weele (KNMI)

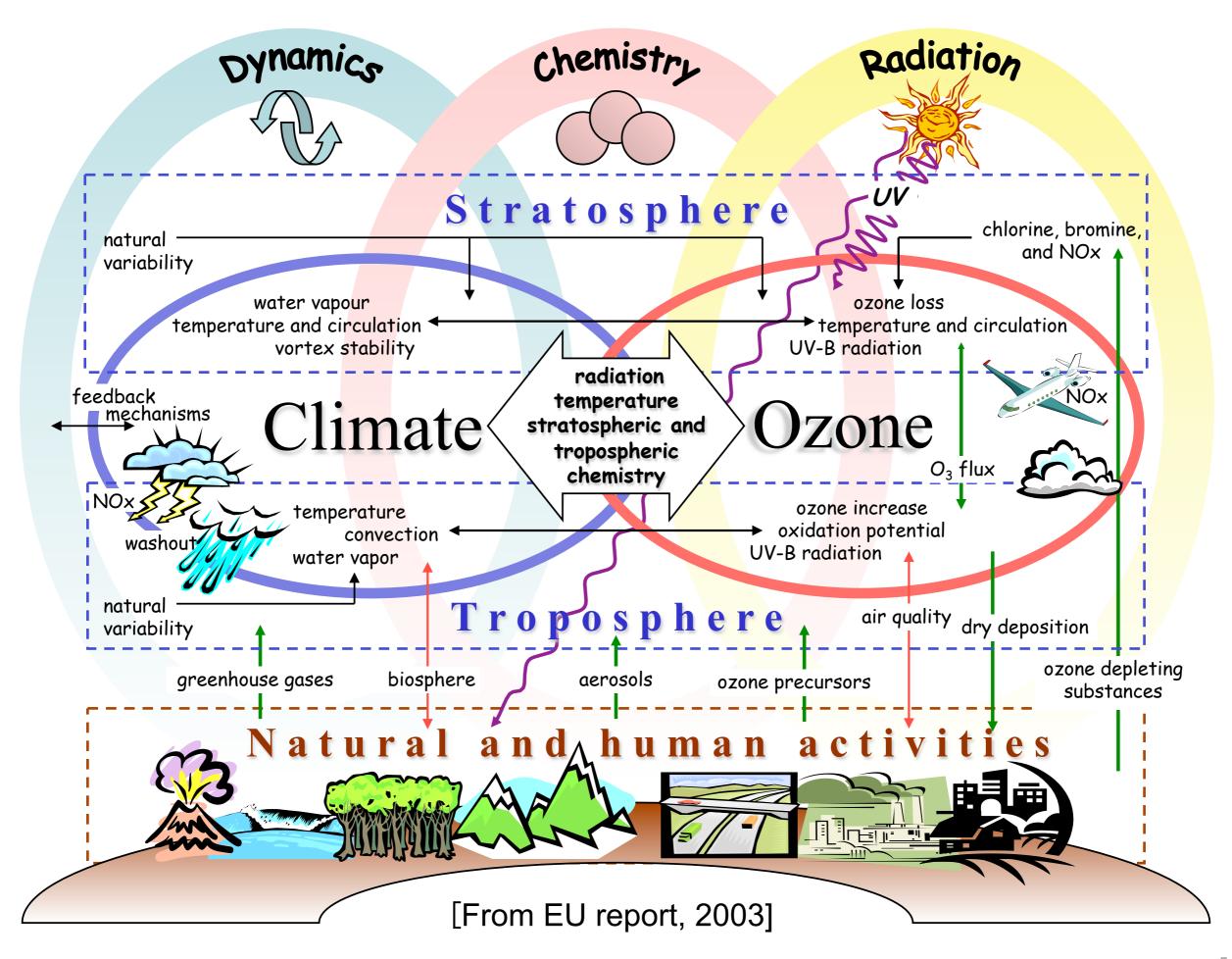
1. 大気組成データ同化とは

2. システムの開発

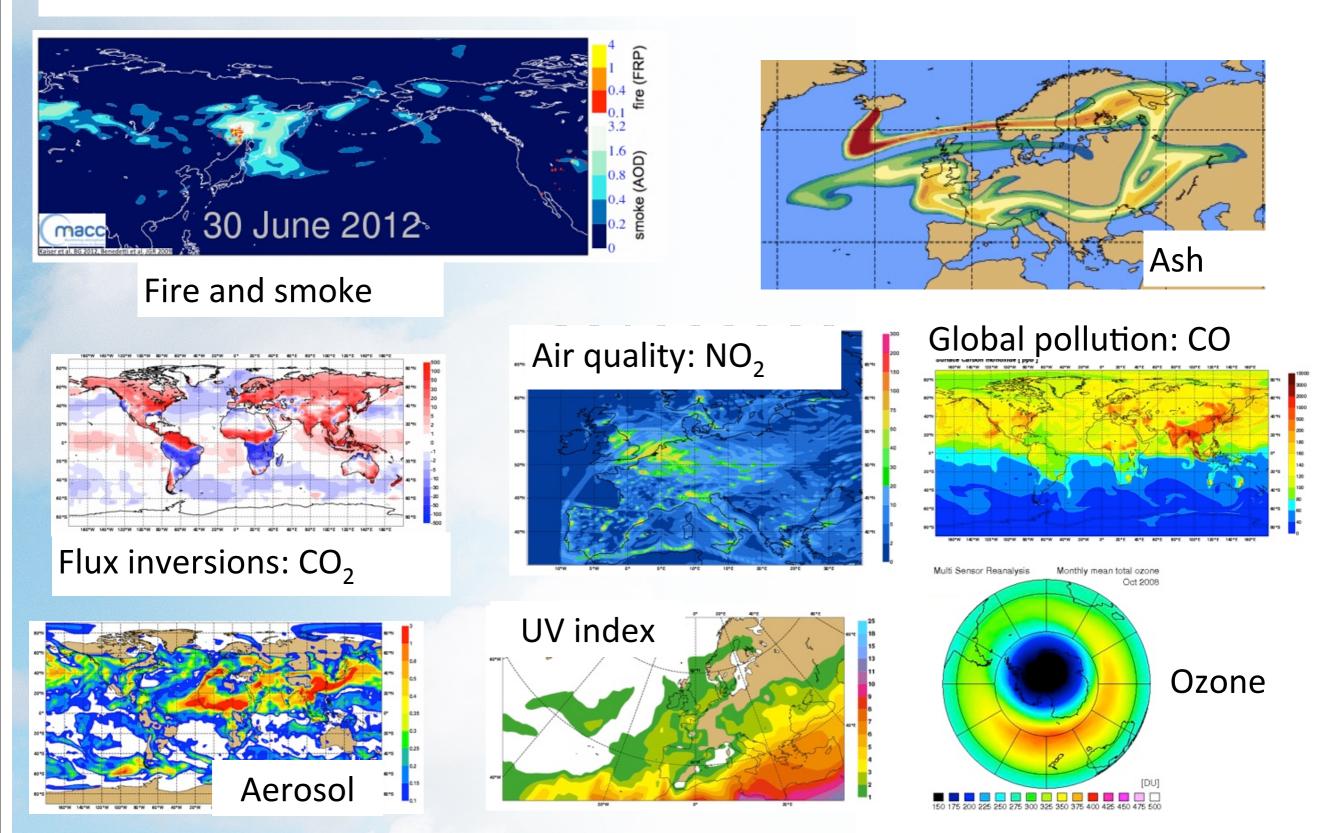
3. 解析結果の検証

4. 長期再解析の実施

5. 今後の課題



大気組成 解析・予報の必要性



(A. Thorpe, ECMWF DG, AMS Presidential Forum address)

大気組成データ同化の特徴

- 様々なスケール(数秒から数10年)の現象が内在
- 化学システムは頑固(Stiff)、局所平衡濃度へ
- •初期値に加えて、排出量や化学反応係数の修正が重要

大気組成データ同化の必要性

- 初期値の高精度化:大気汚染・UV・オゾンホール予報
- 放射過程・背景誤差共分散を考慮した気象解析の向上
- 再解析データ:人間活動と大気組成変動、放射伝達計算、気候モデル・気象再解析へのインプット

大気組成データ同化システム

NWPベース(現業センター)

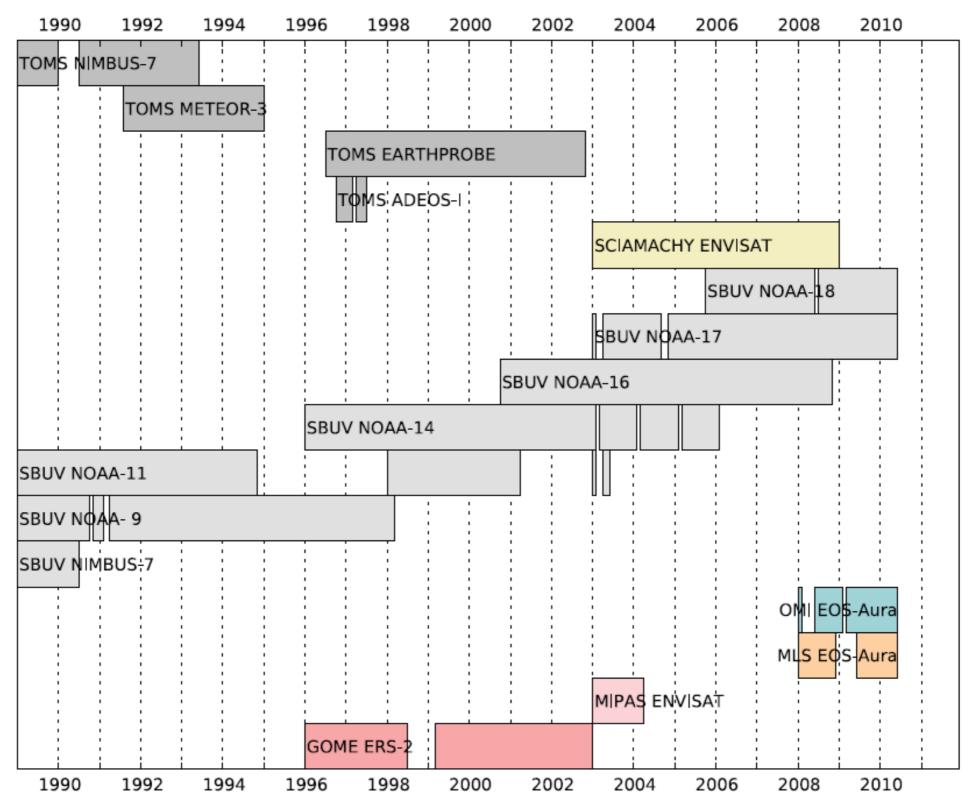
- 化学過程は簡略化して表現。主に成層圏オゾンのみを対象。
- 放射過程を介して気象解析を改善することが目的。

CTMベース(主に研究機関)

- 複雑な化学・輸送過程を含み、様々な物質を対象。
- •大気組成変動要因の理解、化学天気予報などのため。
- 気象場は外部データ。排出量推定にも応用可能。

NWP

ERA-Interim Sources of Profile and Total Ozone



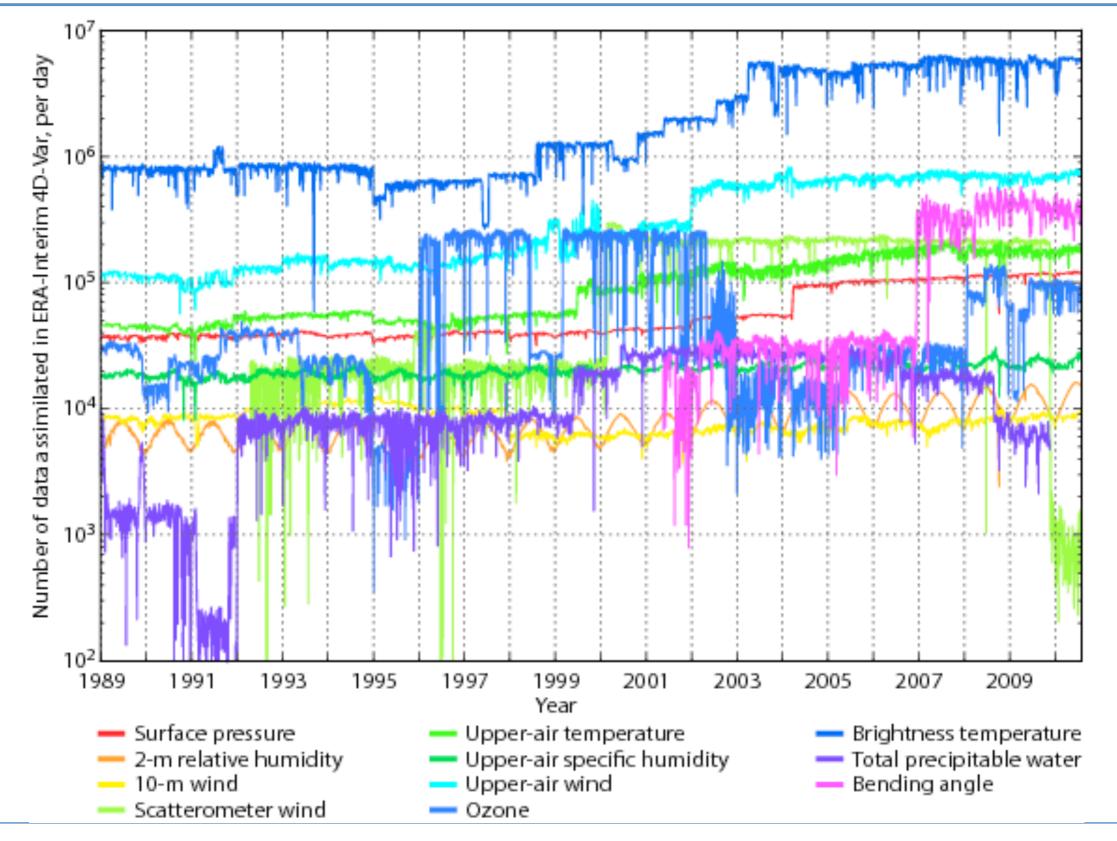
gure 15. Timeline of ozone data assimilated in ERA-Interim.

SPARC – DA Workshop

Brussels, Belgium

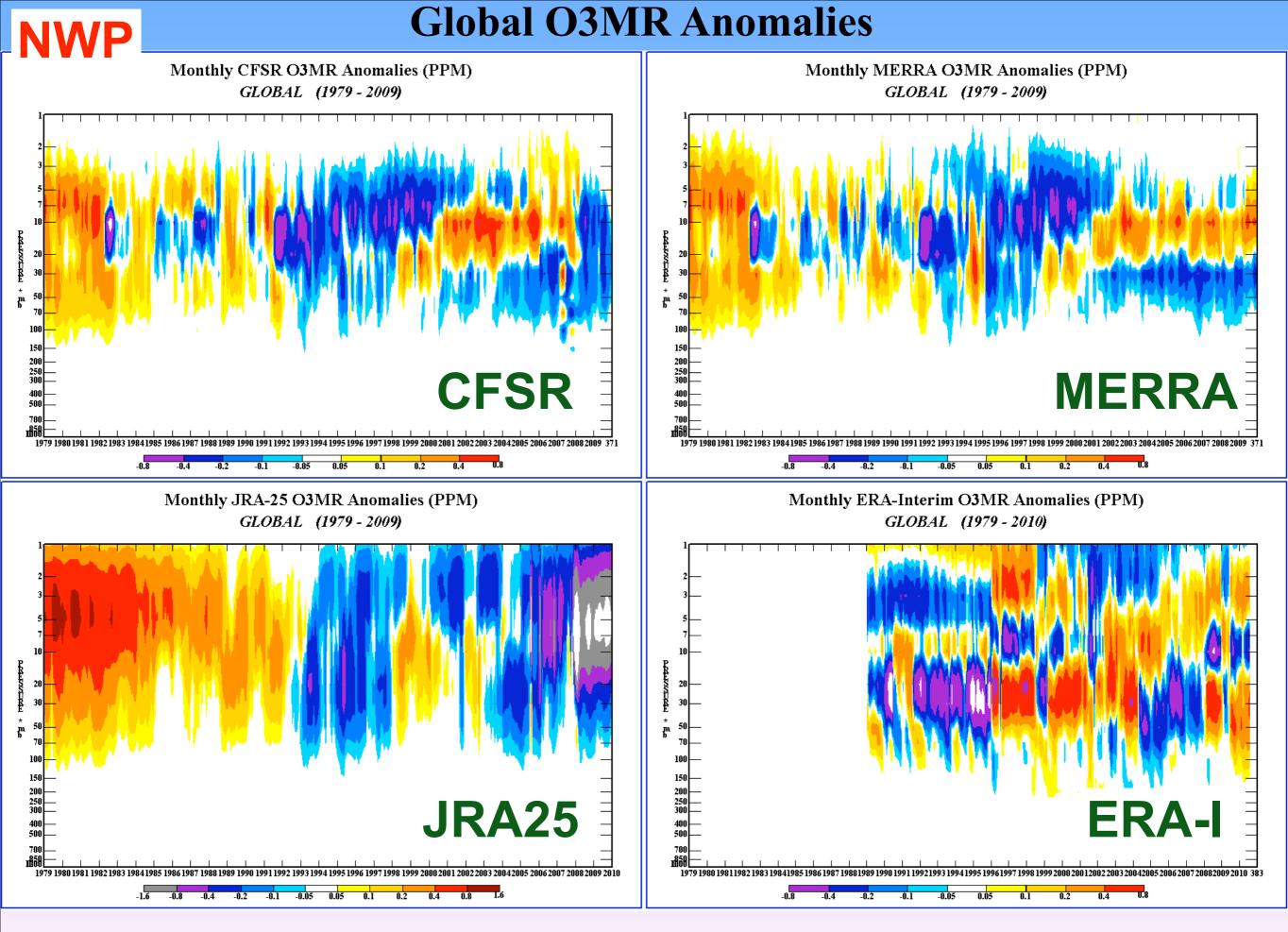
June 20-22, 2011

NWP Observations used in ERA-Interim: Data counts









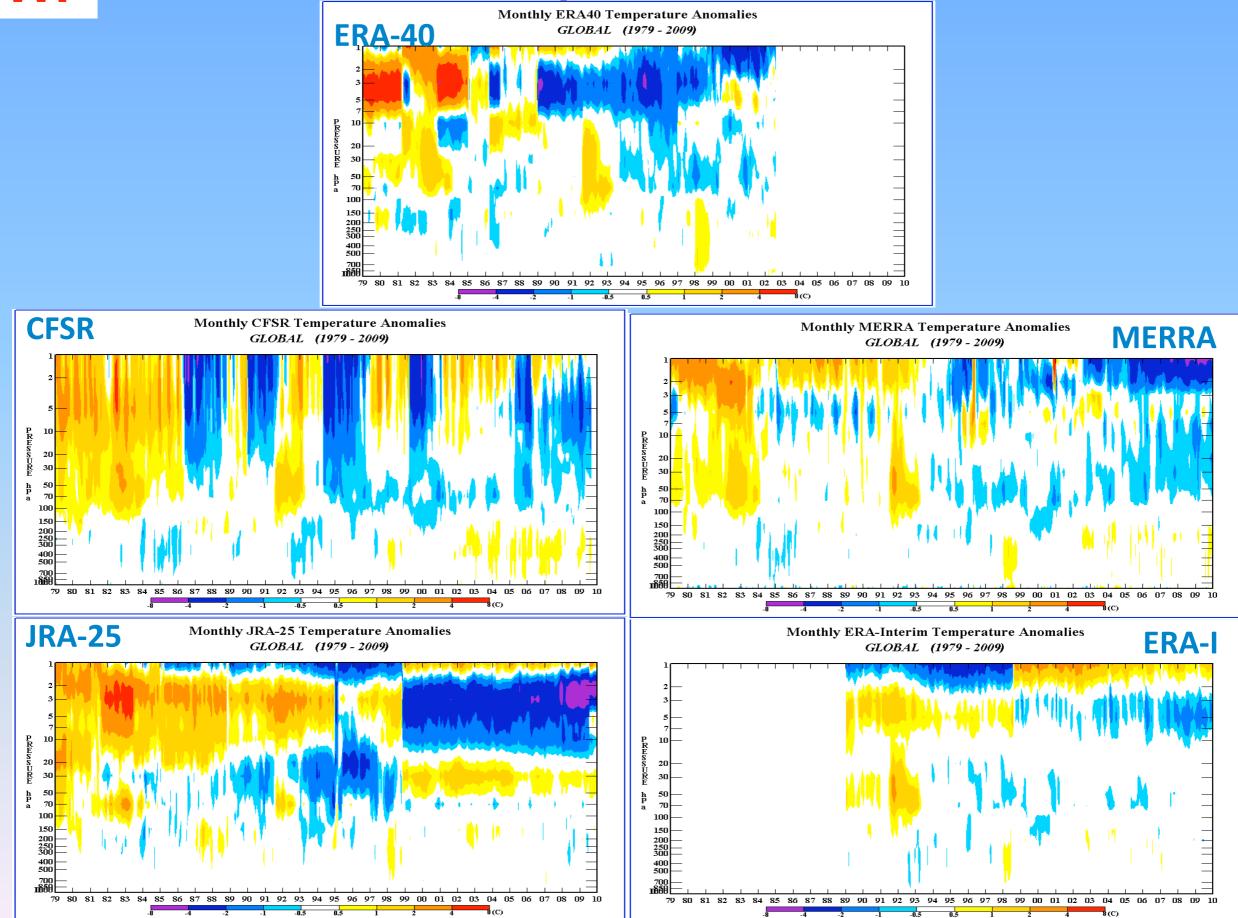
SPARC – DA Workshop

Brussels, Belgium

June 20-22, 2011

NWP

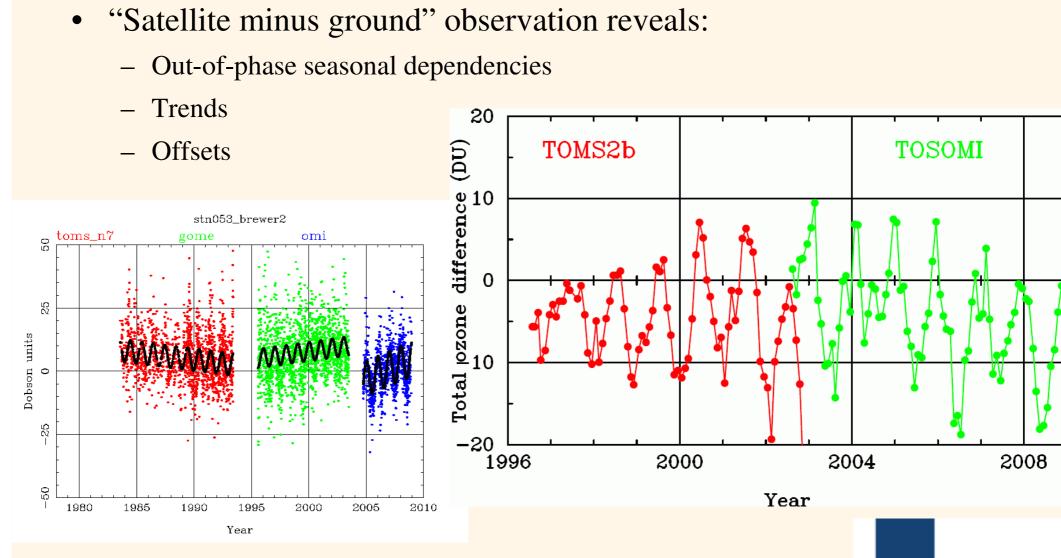
Global Temperature Anomalies



SPARC – DA Workshop

Brussels, Belgium

June 20-22, 2011



Available level 2 ozone data (UV-VIS)

TOMS Nimbus 7:	1978-1993	TOMS v.8	NASA
TOMS EarthProbe:	1996-2002	TOMS v.8	NASA
SBUV 7, 9a, 9d, 11, 16:	1978-2004	SBUV v.8	NOAA
GOME :	1995-2008	GDP v.4	ESA/DLR
GOME :	1995-2008	TOGOMI v1.2	KNMI
SCIAMACHY :	2002-2008	SGP v.3	ESA/DLR
SCIAMACHY :	2002-2008	TOSOMI v.0.43	KNMI
OMI :	2004-2008	TOMS v.3	NASA
OMI :	2004-2008	DOAS v.3	KNMI
GOME-2 :	2007-2008	GDP v.4.2	EUMETSAT/DLR

1978-2008

WOUDC:

CTM

Brewer(3,4), Dobson, Filter

Expected dependencies of satellite data

• Solar zenith angle (DOAS-AMF, O3 cross-section)

Royal Netherlands

Environment

Meteorological Institute

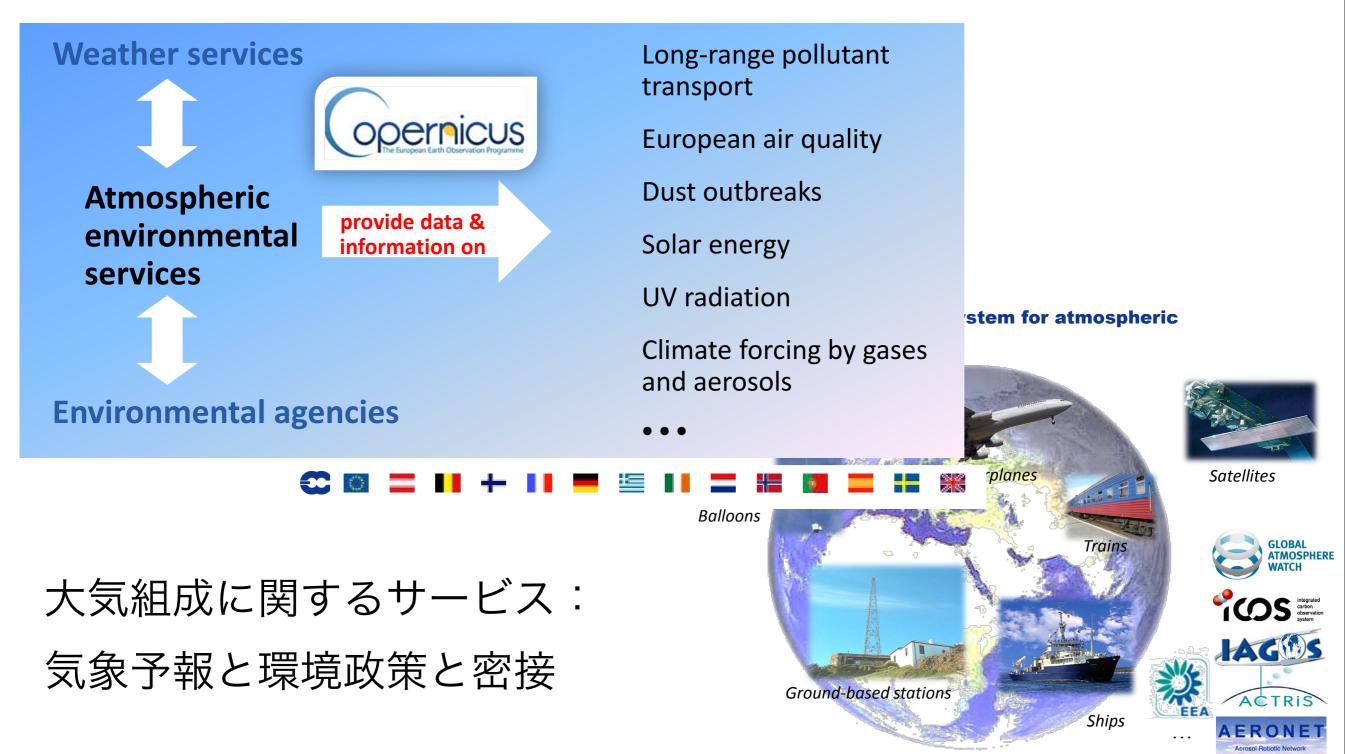
Ministry of Infrastructure and the

- Viewing zenith angle (scan mirror)
- Effective temperature (O3 cross-section)
- Time (instrument degradation)
- Offset (calibration)

–KNMI 30-year multi sensor reanalysis of total ozone ¹³

Monitoring Atmospheric Composition and Climate – Interim Implementation

MACC-II is the third in a series of FP6 & 7 EU projects (since 2005), benefiting also from earlier ESA/GSE projects. It is coordinated by ECMWF and the consortium comprises 36 partners from 13 countries. MACC-II runs until end of July 2014, when the operational Copernicus Atmosphere Service starts.

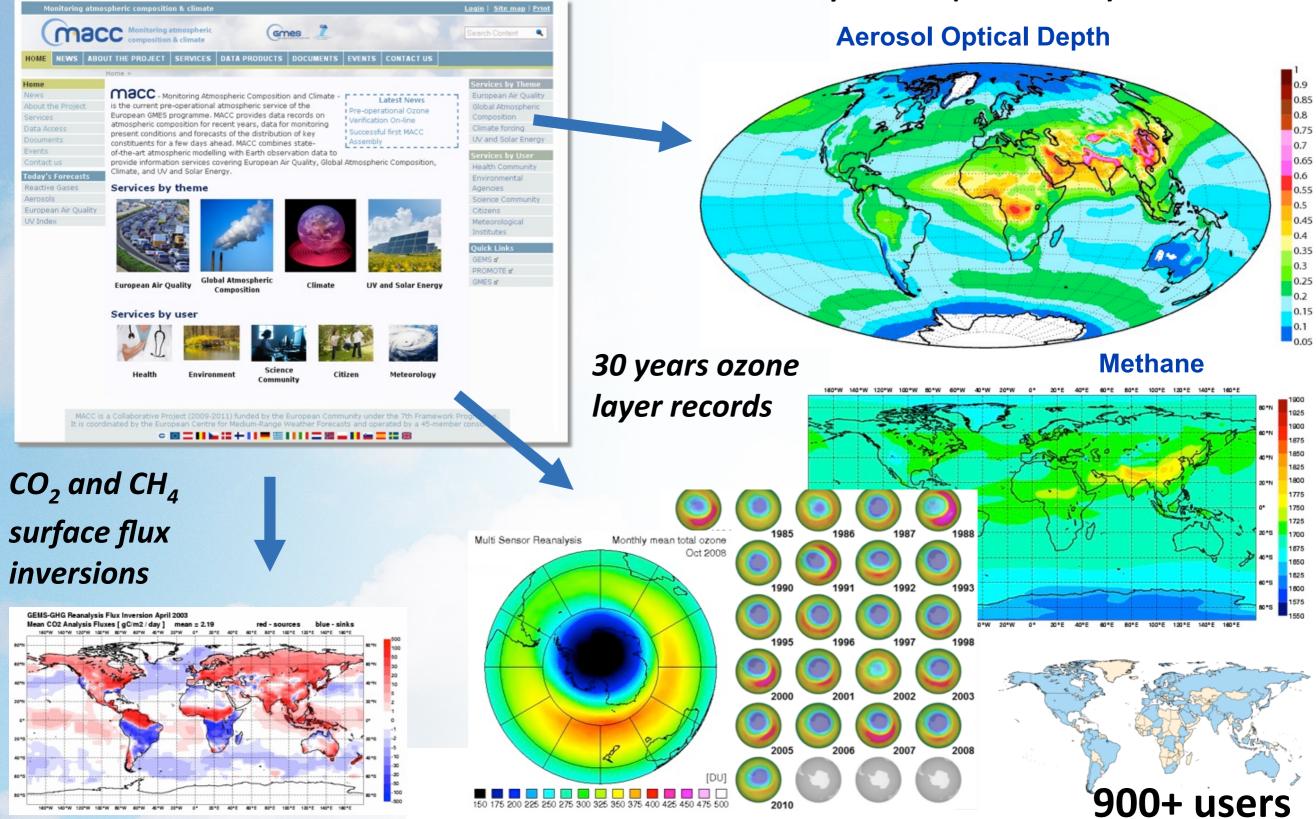


NWP&CTM

http://www.gmes-atmosphere.eu Retrospective Service Provision

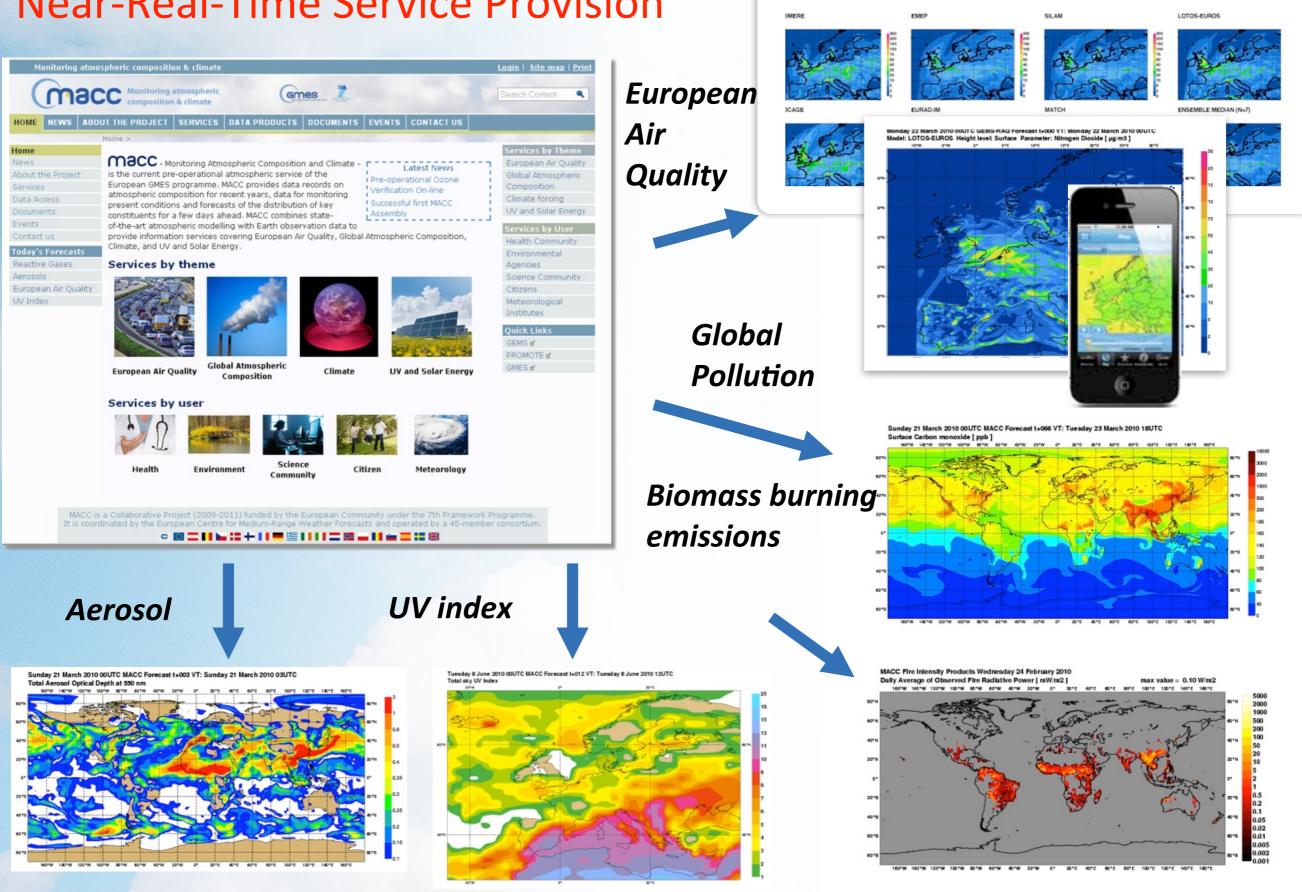
NWP&CTM

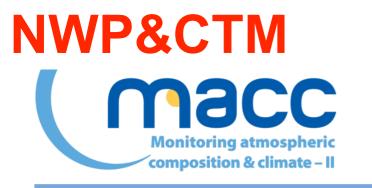
Reanalysis of Atmospheric Composition (2003-2011)



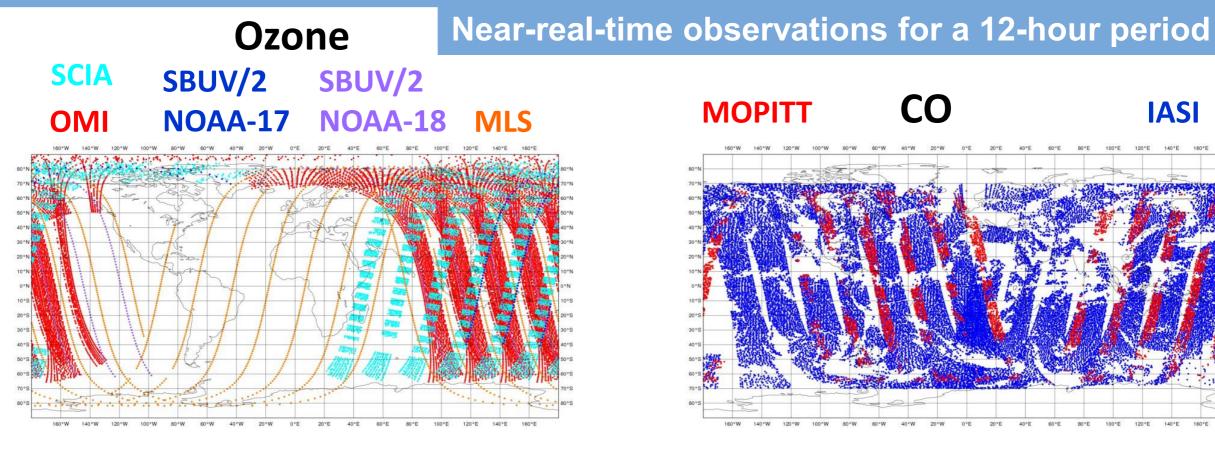
http://www.gmes-atmosphere.eu Near-Real-Time Service Provision

100+ users a NWP&CTM

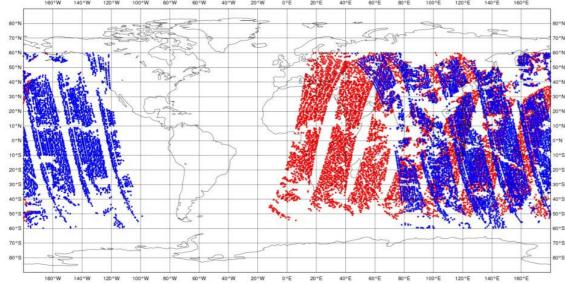


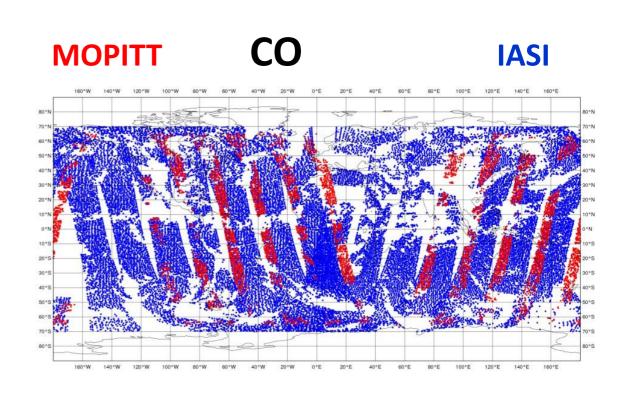


Combining many observations

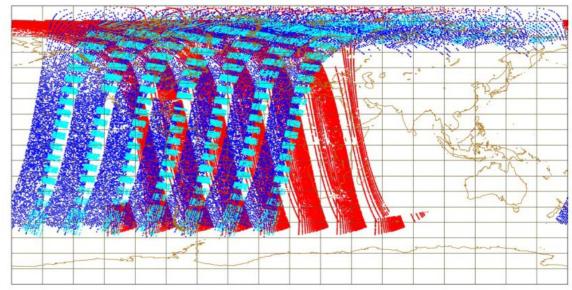


NO2 OMI **GOME-2**





SO2 OMI SCIA **GOME-2**

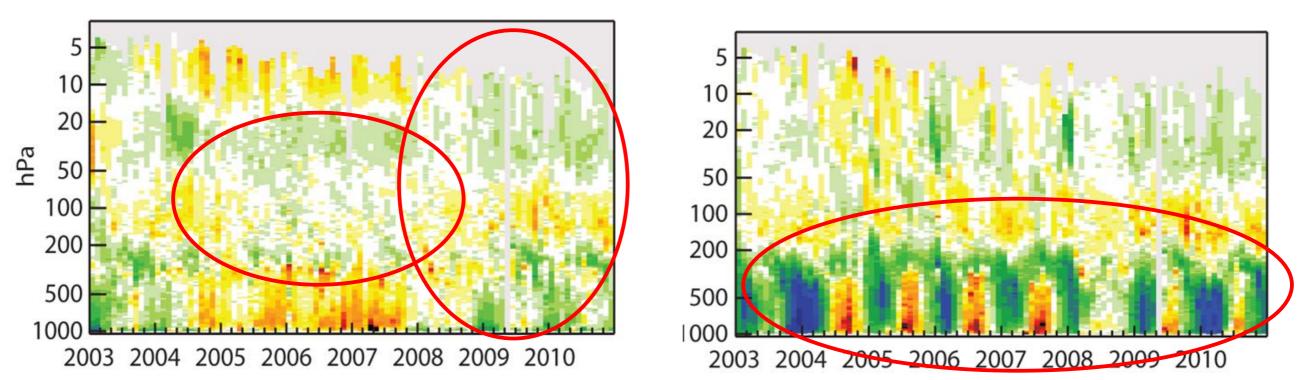




Balance of model and observations

ERA-Interim Reanalysis

MACC Reanalysis



Limb-sounding ozone data assimilated from August 2004 (MLS) are clearly improving stratospheric ozone.

Switch to near-real-time version of MLS observations, which misses lowest layers.

Chemical modelling is needed for correct representation of tropospheric ozone.



Global chemical data assimilation systems

Institute/Project	Species	Region	Assimilation	Notes
NWP operational centers	O ₃	Stratosphere –	mainly 4D-VAR	Simplified chemistry
C-IFS (ECMWF MACC)	Various	Troposphere/ Stratosphere –	coupled to IFS 4D- VAR	Multi-models, w/o emission inversion
NASA GMAO	Various (EOS-Aura)	Troposphere/ Stratosphere –	Incremental 3D- VAR	Simplified chemistry
NASA JPL/Harvard Univ.	Mainly O _{3,} CO	Troposphere/ Stratosphere –	3D-VAR	
NCAR	Mainly CO	Troposphere	Ensemble Kalman filter	w/ emission inversion
KNMI	O ₃	Troposphere/ Stratosphere –	Sub-optimal Kalman filter	30 years, Simplified chemistry
DARC/Reading	Mainly O₃ (MIPAS)	Stratosphere –	3D-VAR	
BASCOE (BIRA-IASB)	Various	Stratosphere –	4D-VAR	
JAMSTEC	Various	Troposphere/LS	Ensemble Kalman filter	w/ emission inversion

1. 大気組成データ同化とは

2. システムの開発

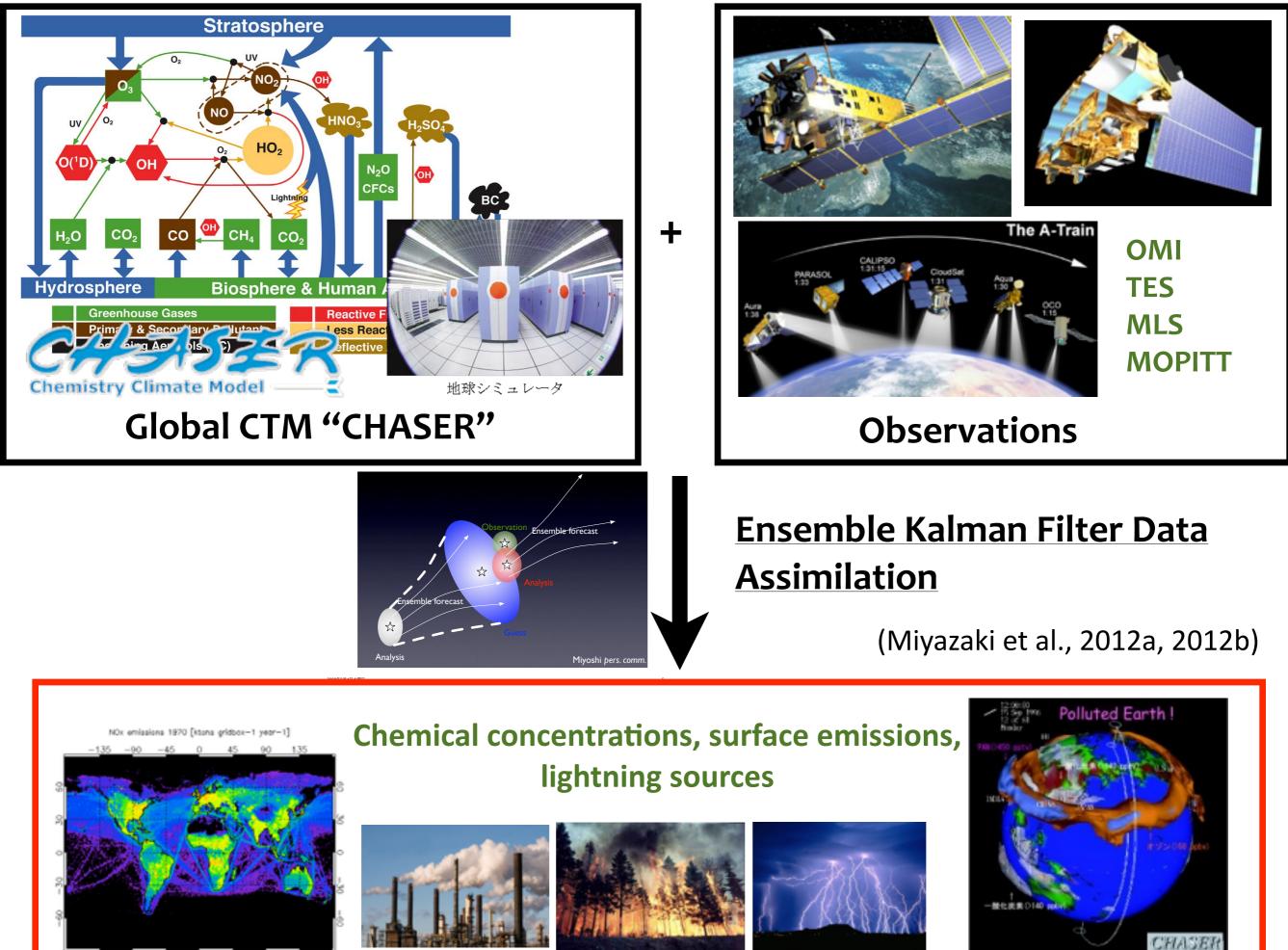
3. 解析結果の検証

4. 長期再解析の実施

5. 今後の課題

Tropospheric chemistry data assimilation

- ✓ The use of data assimilation for atmospheric chemistry, especially for short-lived chemical species, is still challenging (e.g., MACC).
- ✓ A large part of the chemical system is not sensitive to initial conditions, but is sensitive to the model parameters (e.g., reaction rates, emissions).
- \checkmark \rightarrow Simultaneous adjustment of model parameters and concentrations is a powerful framework.
- ✓ The advantage of Ensemble Kalman filter (EnKF) is its easy implementation for complicated systems and parameter estimations.



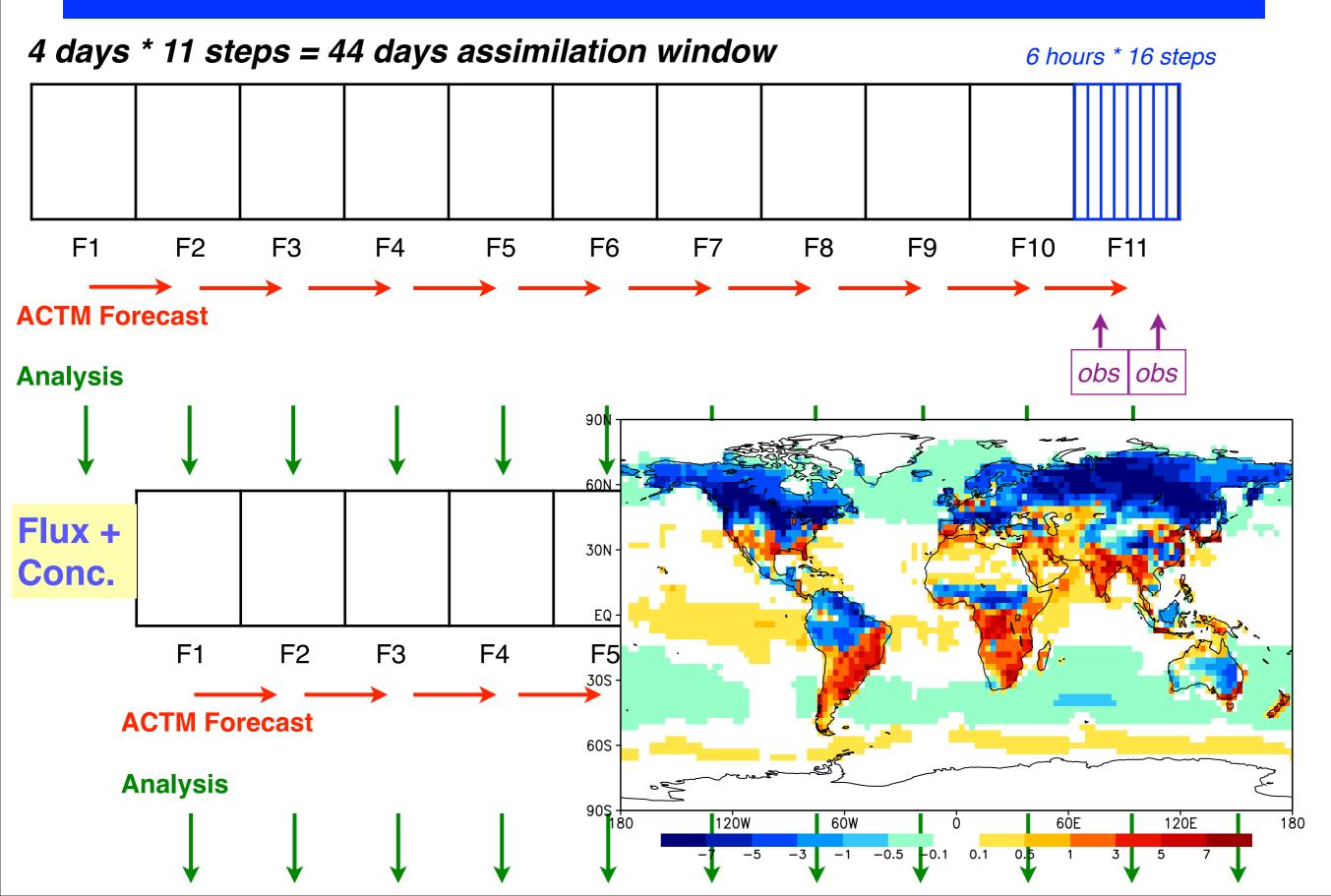
-135 -90 -45 0 45 90 13

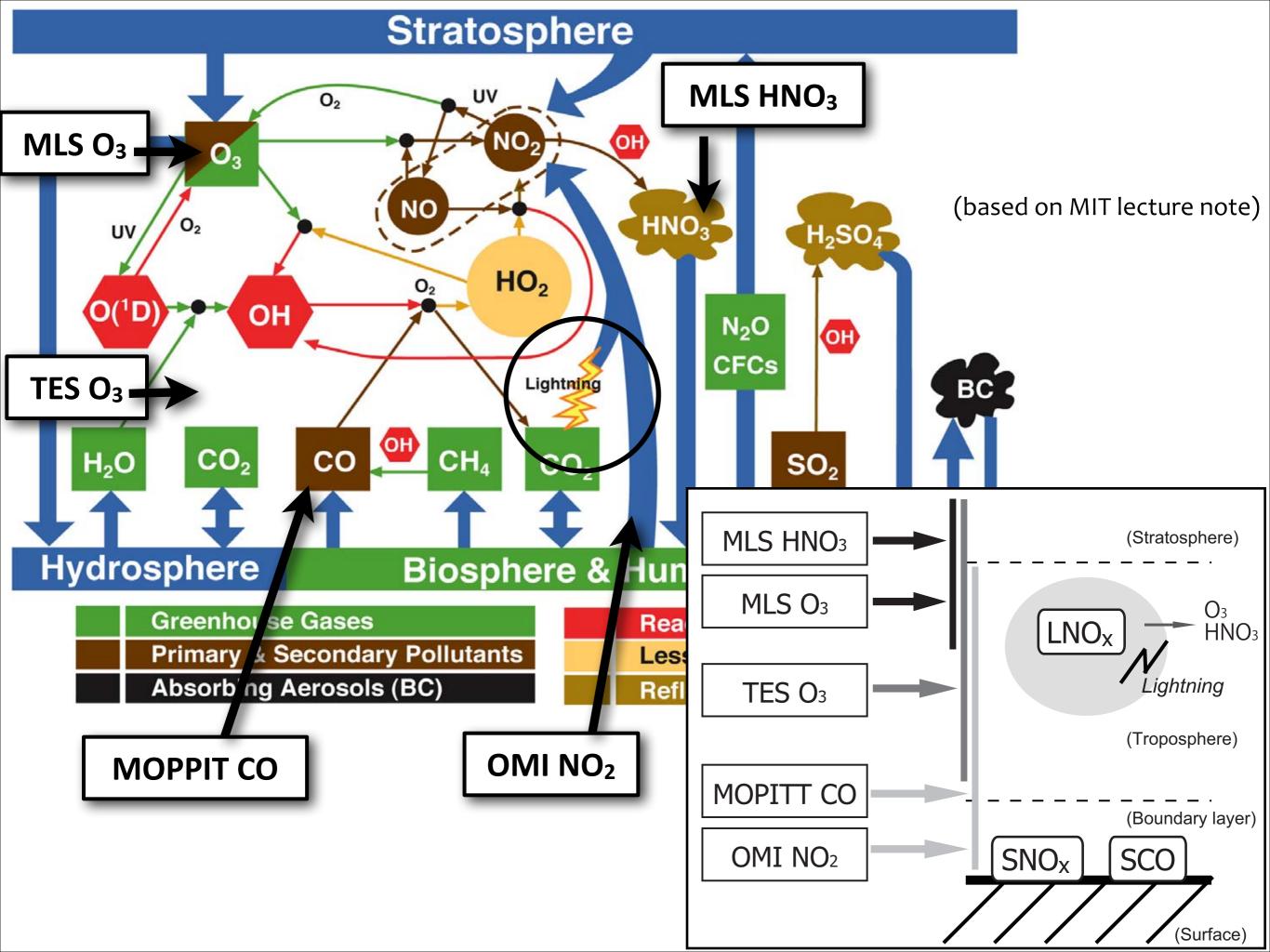
0 135

CHASER-DAS (Miyazaki et al., 2012a, 2012b, 2013a, 2013b)

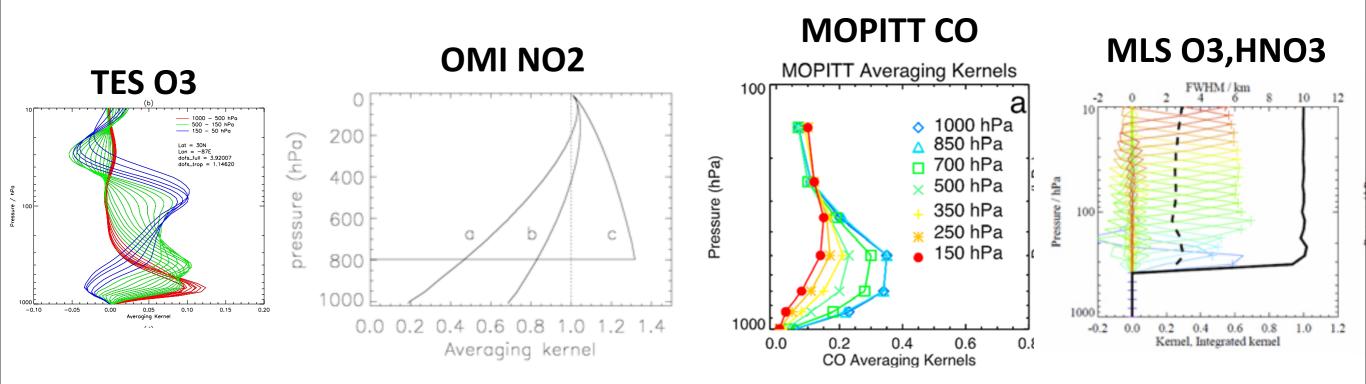
Assimilation scheme	LETKF (Hunt et. al., 2007), 48 members	
Forecast model	CHASER (Sudo et al., 2002), 47 species & 88 reactions, T42L32	
A priori emissions	EDGAR4.2 + GFED3.1 + GEIA	
State vector	NOx & CO emissions, lightning NOx, 35 chemical species	
Obs operator	Averaging kernel and a priori information	
Super Obs	applied for OMI NO ₂ and MOPPIT CO data	
Cycle	100 min.	
Techniques	Spatial & variable covariance localization, covariance inflation	
Assimilated data	OMI NO ₂ (DOMINO2), TES O ₃ (ver. 4), MOPITT CO (ver. 5), MLS O ₃ & HNO ₃ (ver. 3.3)	
Validation data	SCIAMACHY NO ₂ , GOME-2 NO ₂ , TES CO, Ozonesonde, Aircraft (IAGOS, NASA, HIPPO) etc	

JAMSTEC carbon DA system ver.2





Observation operators



• The observation operator (H) converts the model profiles to the profile that would be retrieved from satellite measurements.

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

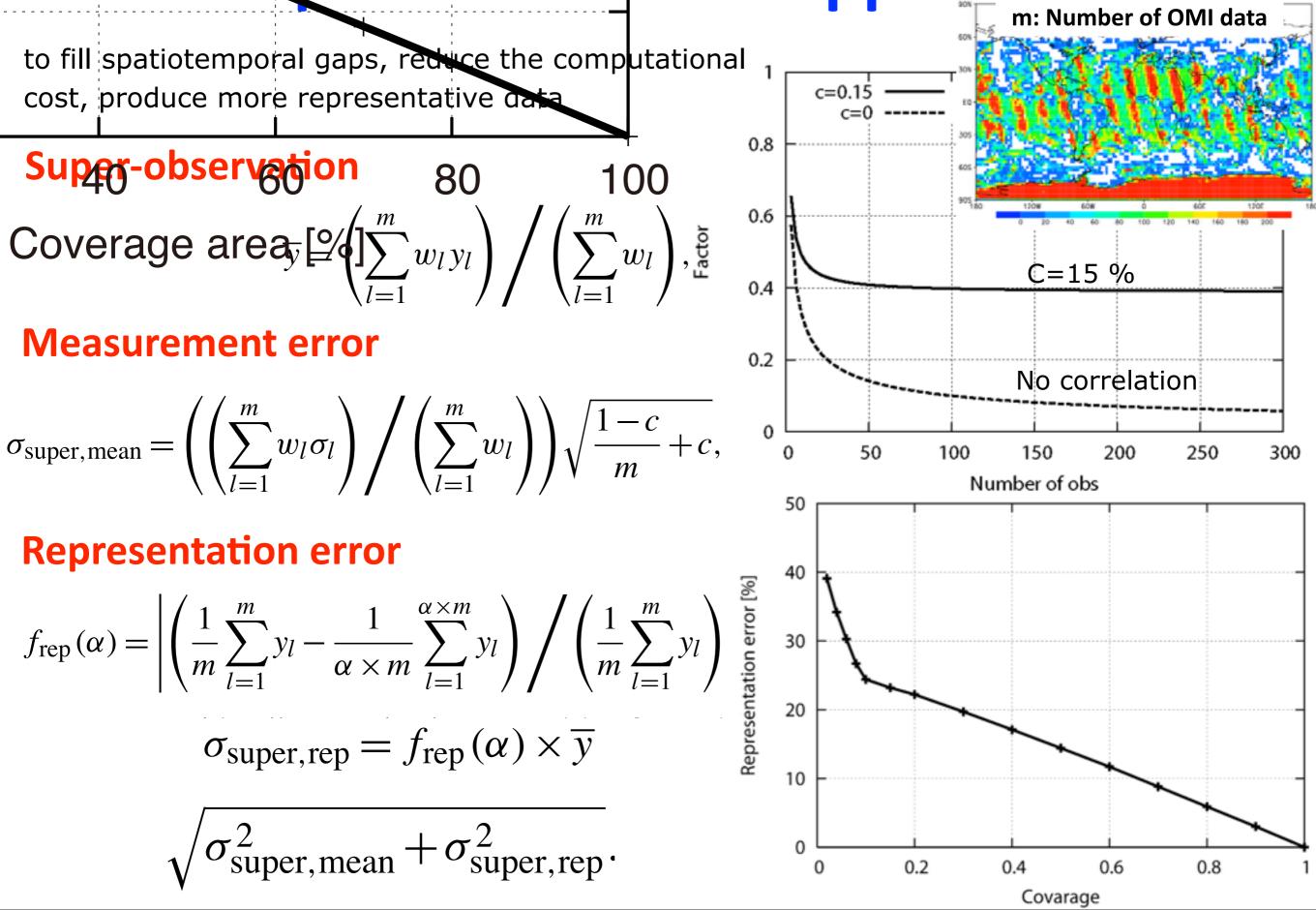
• The model-satellite difference (the innovation) is not biased by the a priori profile

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

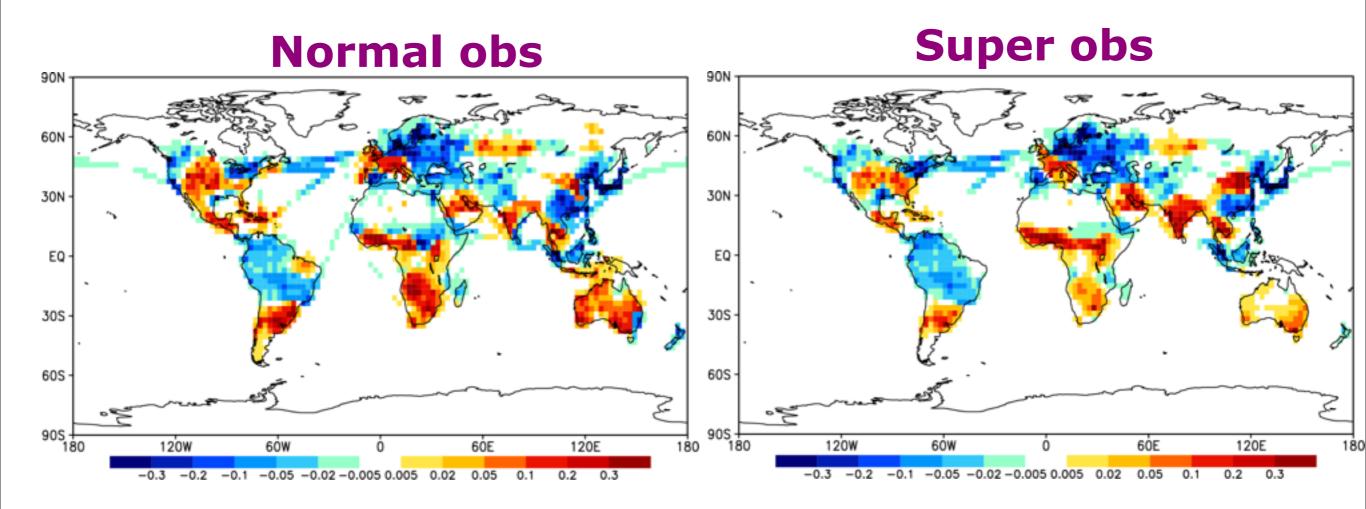
(Rodgers, 2000; Eskes and Boersma, 2003)

• The observational error matrix (R) in each retrieval includes smoothing error, systematic error, measurement error, and representativeness error.

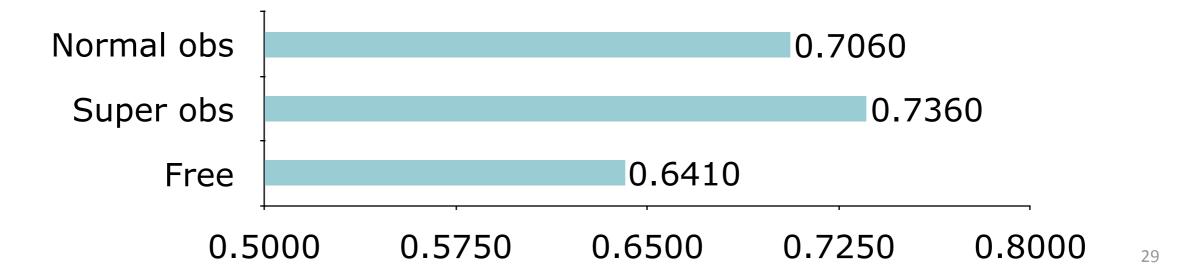
Super-observation approach



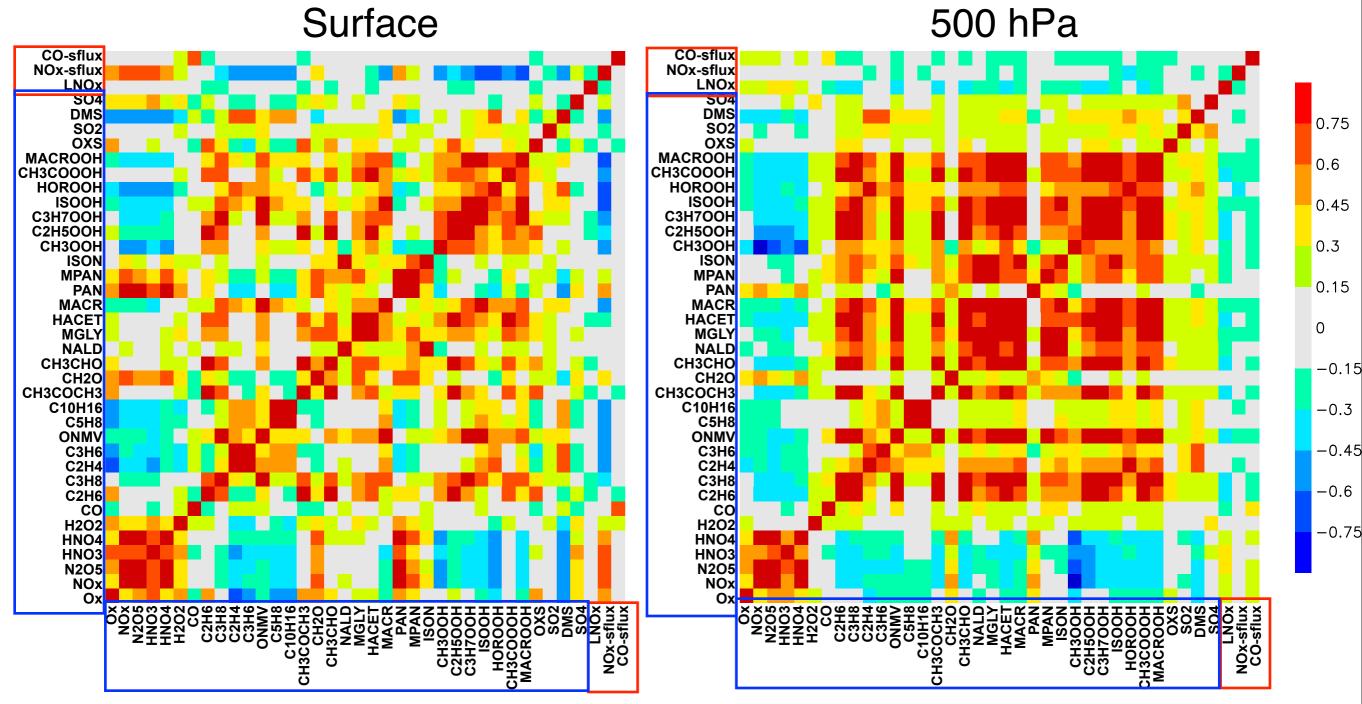
NOx emission increments: 11 January 2005



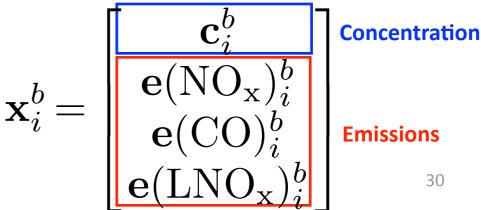
Spatial correlation



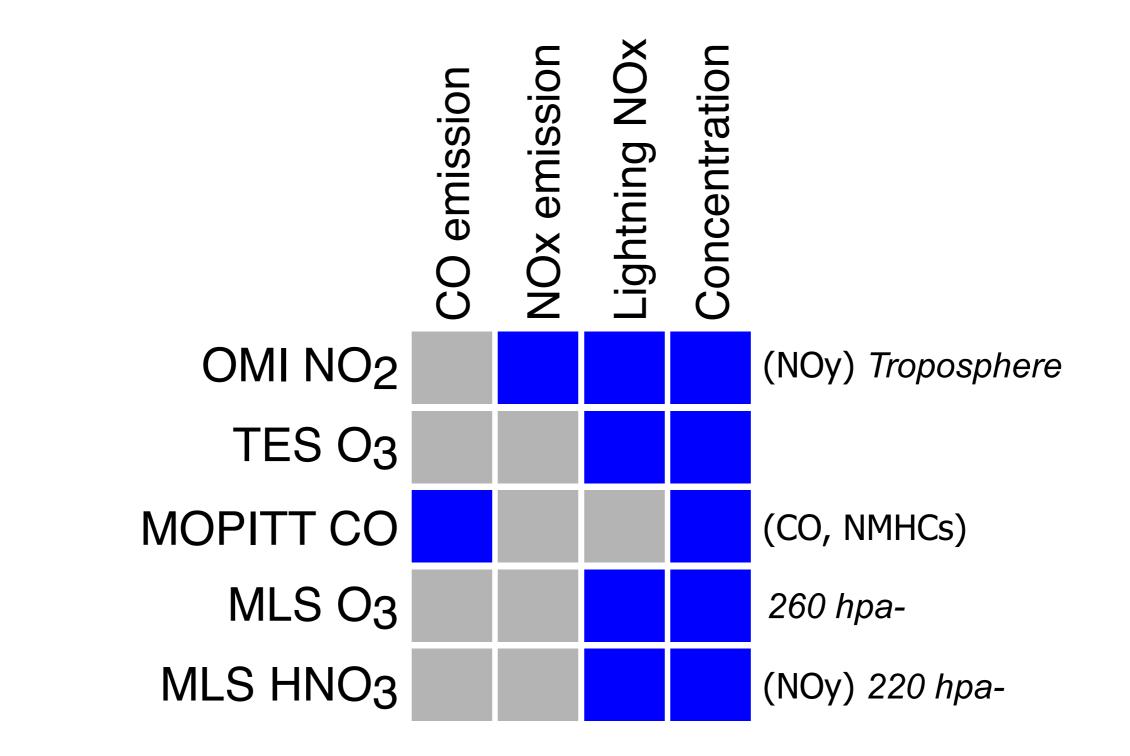
Background error covariance structure in CHASER-DAS



- Emission estimation based on state augmentation.
- Covariance among very weakly-related species is neglected (i.e., variable localization.

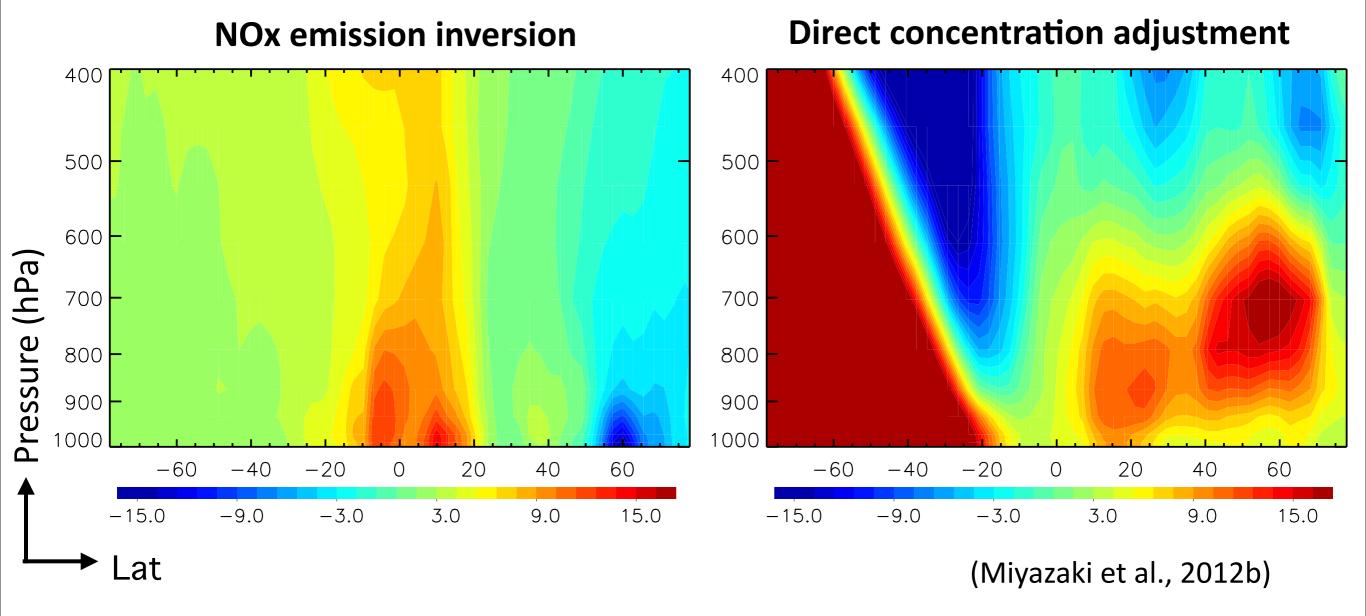


Background error covariance structure in CHASER-DAS



The variable localization (Kang et al., 2011)

The relative impact (in %) of the NOx emission inversion (left) and the direct concentration adjustment (right) through assimilation on the vertical O₃ profile



The simultaneous adjustment of the emissions and the concentrations is a powerful approach to optimize the whole tropospheric profiles

1. 大気組成データ同化とは

2. システムの開発

3. 解析結果の検証

4. 長期再解析の実施

5. 今後の課題

Self-consistency check: Chi-square test

An important test for the quality of data assimilation is whether the differences between the innovations are consistent with the covariance matrices for the model forecast and observations.

$$\mathbf{Y} = \frac{1}{\sqrt{m}} (\mathbf{H}\mathbf{P}^{b}\mathbf{H}^{T} + \mathbf{R})^{-1/2} (\mathbf{y}^{o} - H(\mathbf{x}^{b})). \qquad \chi^{2} = \operatorname{trace} \mathbf{Y}\mathbf{Y}^{T}$$

$$= \frac{1}{\sqrt{m}} (\mathbf{H}\mathbf{P}^{b}\mathbf{H}^{T} + \mathbf{R})^{-1/2} (\mathbf{y}^{o} - H(\mathbf{x}^{b})). \qquad \chi^{2} = \operatorname{trace} \mathbf{Y}\mathbf{Y}^{T}$$

$$= \frac{1}{\sqrt{m}} (\mathbf{H}\mathbf{P}^{b}\mathbf{H}^{T} + \mathbf{R})^{-1/2} (\mathbf{y}^{o} - H(\mathbf{x}^{b})). \qquad \chi^{2} = \operatorname{trace} \mathbf{Y}\mathbf{Y}^{T}$$

$$= \frac{1}{\sqrt{m}} (\mathbf{H}\mathbf{P}^{b}\mathbf{H}^{T} + \mathbf{R})^{-1/2} (\mathbf{y}^{o} - H(\mathbf{x}^{b})). \qquad \chi^{2} = \operatorname{trace} \mathbf{Y}\mathbf{Y}^{T}$$

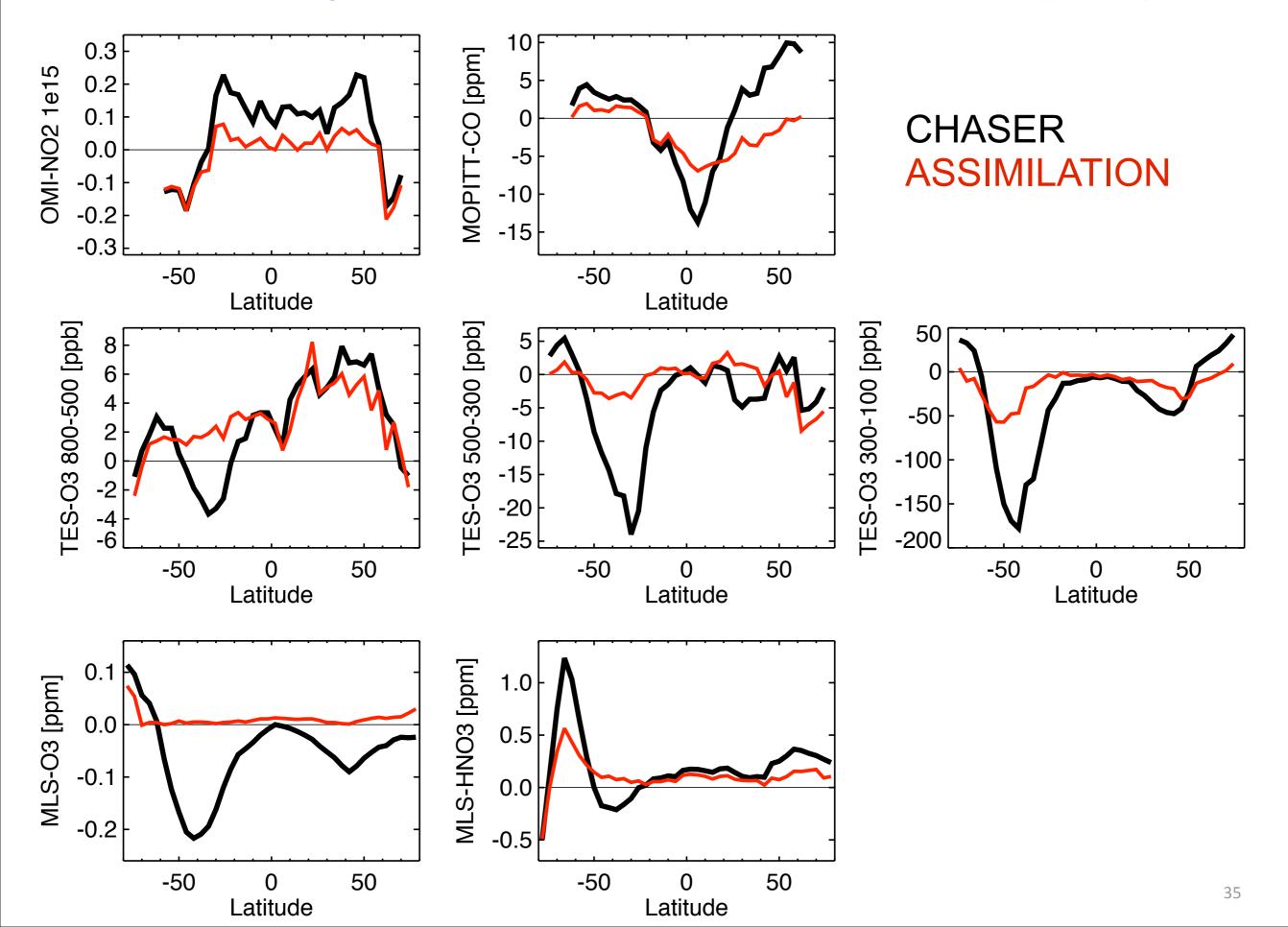
$$= \frac{1}{\sqrt{m}} (\mathbf{H}\mathbf{P}^{b}\mathbf{H}^{T} + \mathbf{R})^{-1/2} (\mathbf{y}^{o} - H(\mathbf{x}^{b})). \qquad \chi^{2} = \operatorname{trace} \mathbf{Y}\mathbf{Y}^{T}$$

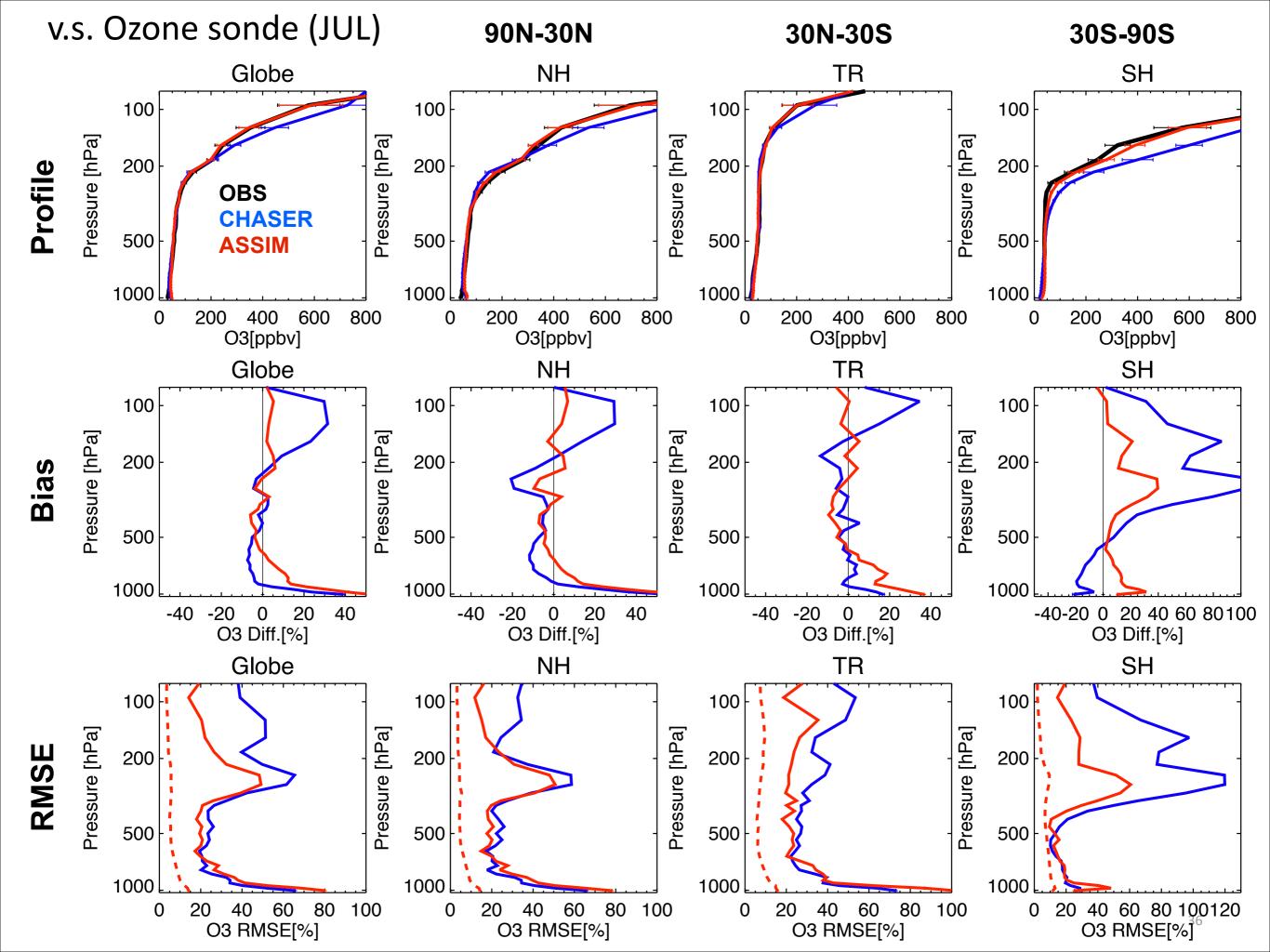
$$= \frac{1}{\sqrt{m}} (\mathbf{H}\mathbf{P}^{b}\mathbf{H}^{T} + \mathbf{R})^{-1/2} (\mathbf{y}^{o} - H(\mathbf{x}^{b})). \qquad \chi^{2} = \operatorname{trace} \mathbf{Y}\mathbf{Y}^{T}$$

$$= \frac{1}{\sqrt{m}} (\mathbf{H}\mathbf{P}^{b}\mathbf{H}^{T} + \mathbf{R})^{-1/2} (\mathbf{y}^{o} - H(\mathbf{x}^{b})). \qquad \chi^{2} = \operatorname{trace} \mathbf{Y}\mathbf{Y}^{T}$$

$$= \frac{1}{\sqrt{m}} (\mathbf{H}\mathbf{P}^{b}\mathbf{H}^{T} + \mathbf{R})^{-1/2} (\mathbf{y}^{o} - H(\mathbf{x}^{b})). \qquad \chi^{2}$$

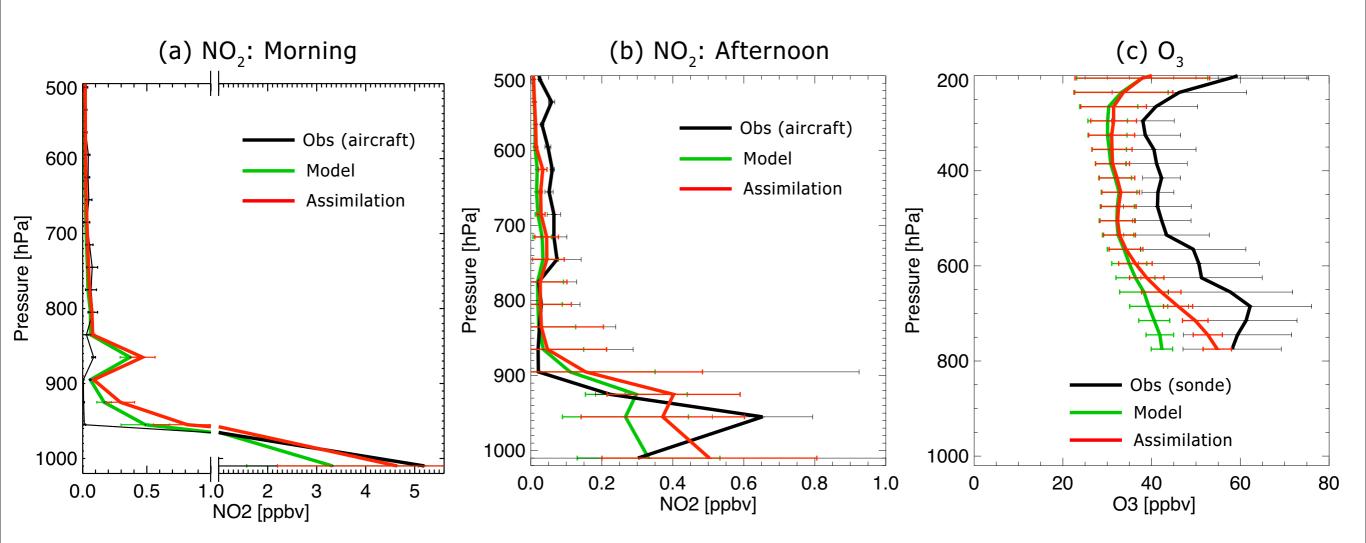
<u>Self-consistency check</u>: Observation-minus-Forecast (OmF) Mean



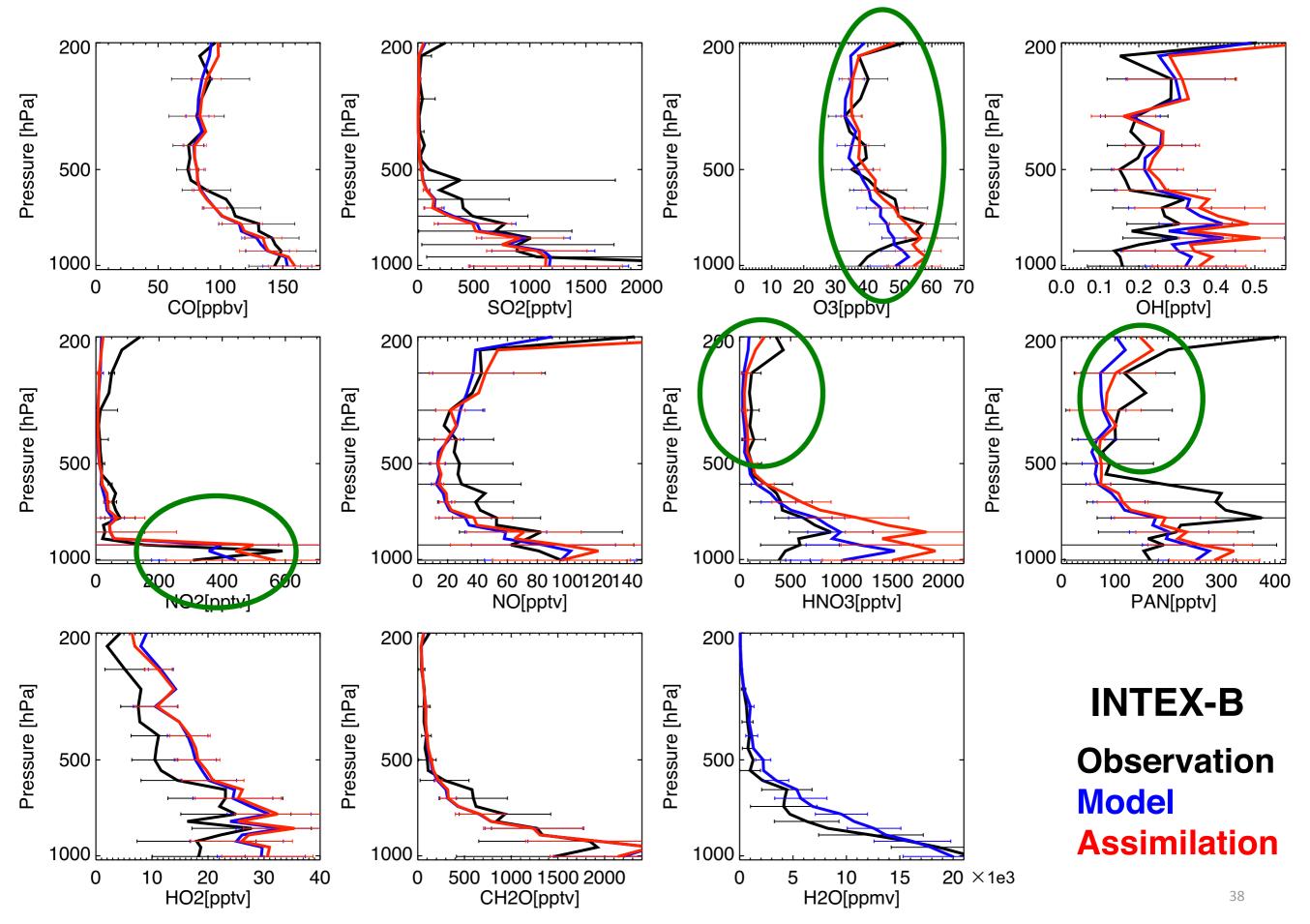




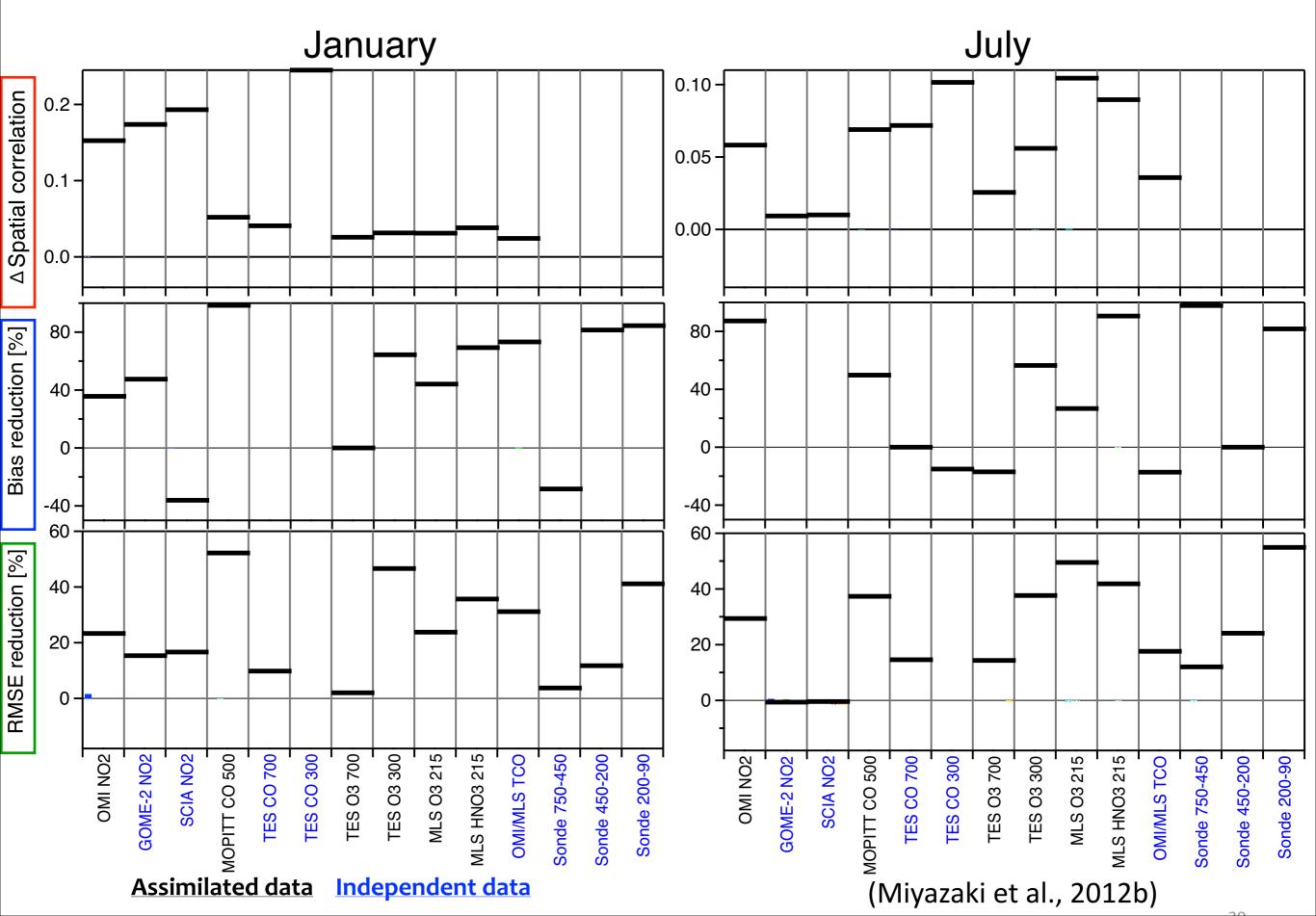
INTEX-B



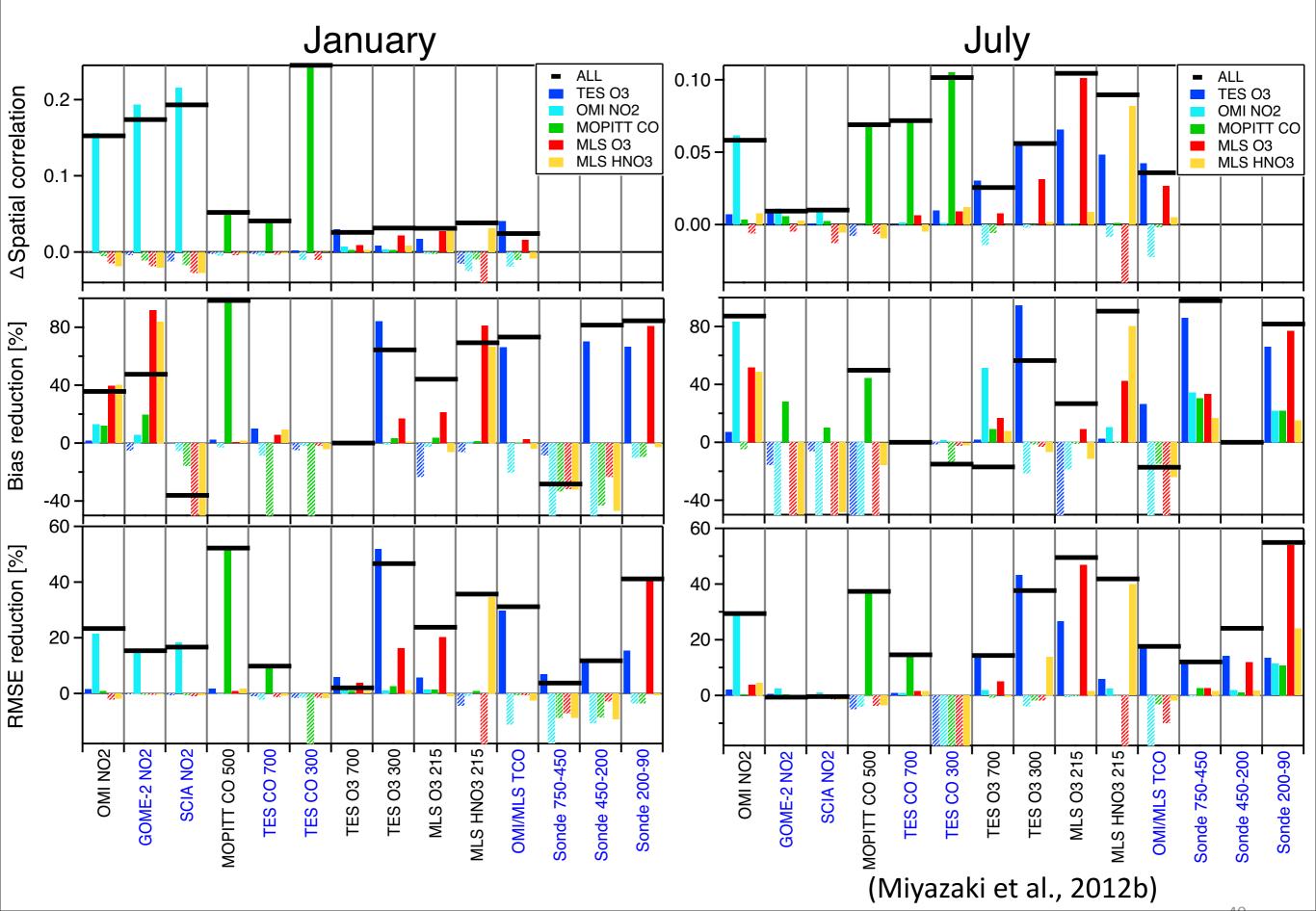
v.s. aircraft during INTEX-B



Spatial correlation increment BIAS reduction rate RMSE reduction rate



Observing System Experiments (OSEs)



Influences on the oxidation capacity

 Assimilation of each species data set has a strong influence on both assimilated/non-assimilated species.

•The inter-species influences are tightly associated with the changes in OH because of the chemical interactions in the CO-OH-Ox-NOx system.

20

10

0

-10

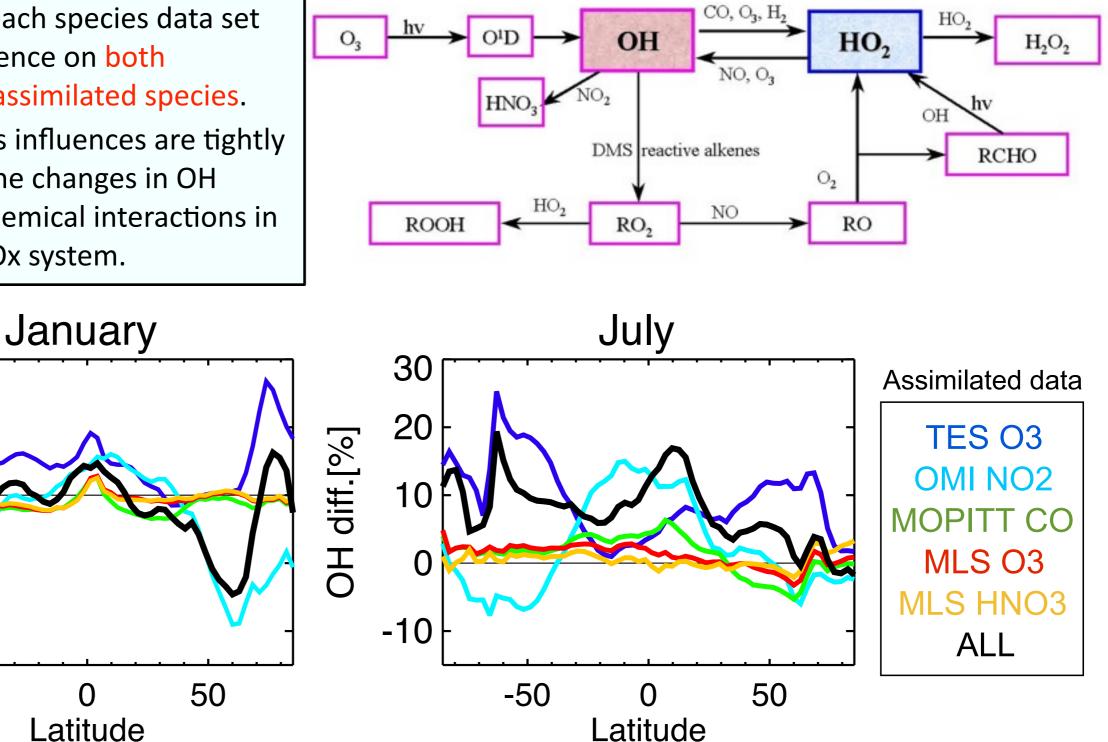
-20

-50

0

Latitude

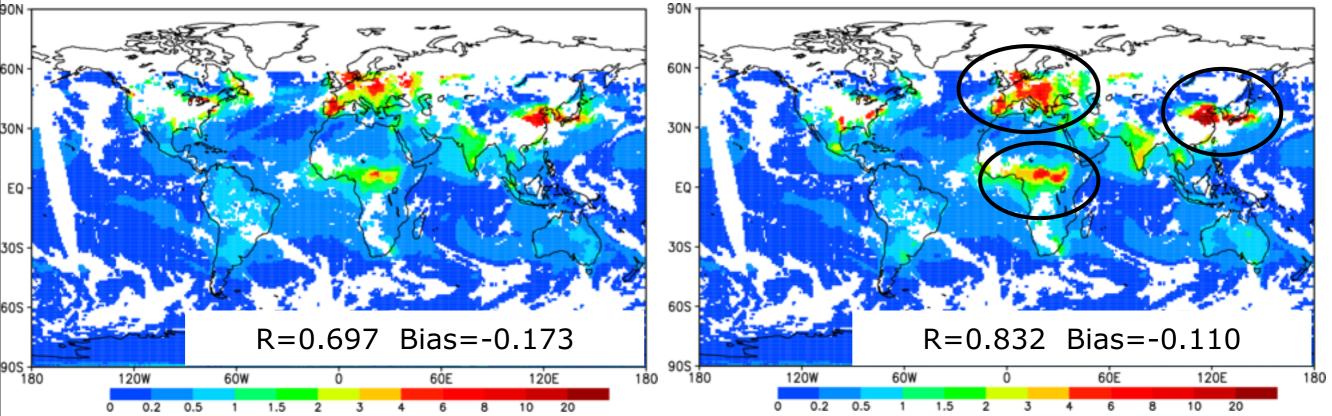
OH diff.[%]



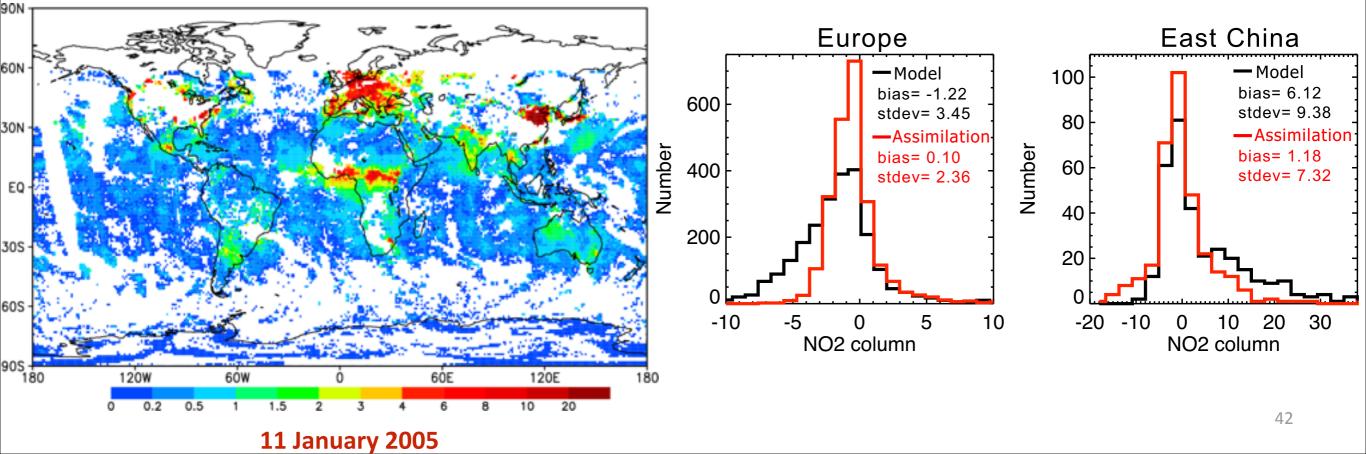
The obvious changes in the OH fields reveal the great potential of the multiple species assimilation to influence the NOx emission inversion etc.

NO₂ Simulation

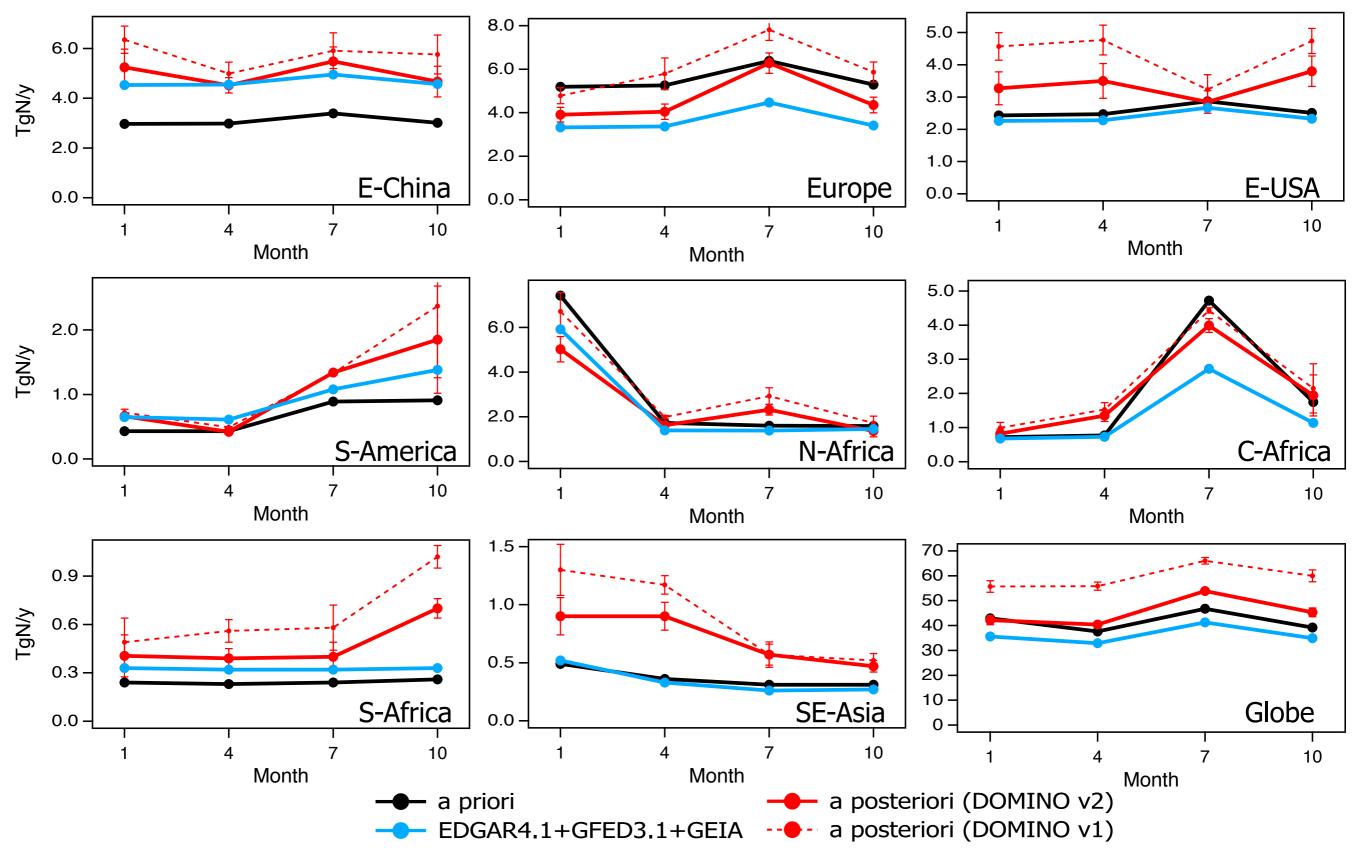
Assimilation

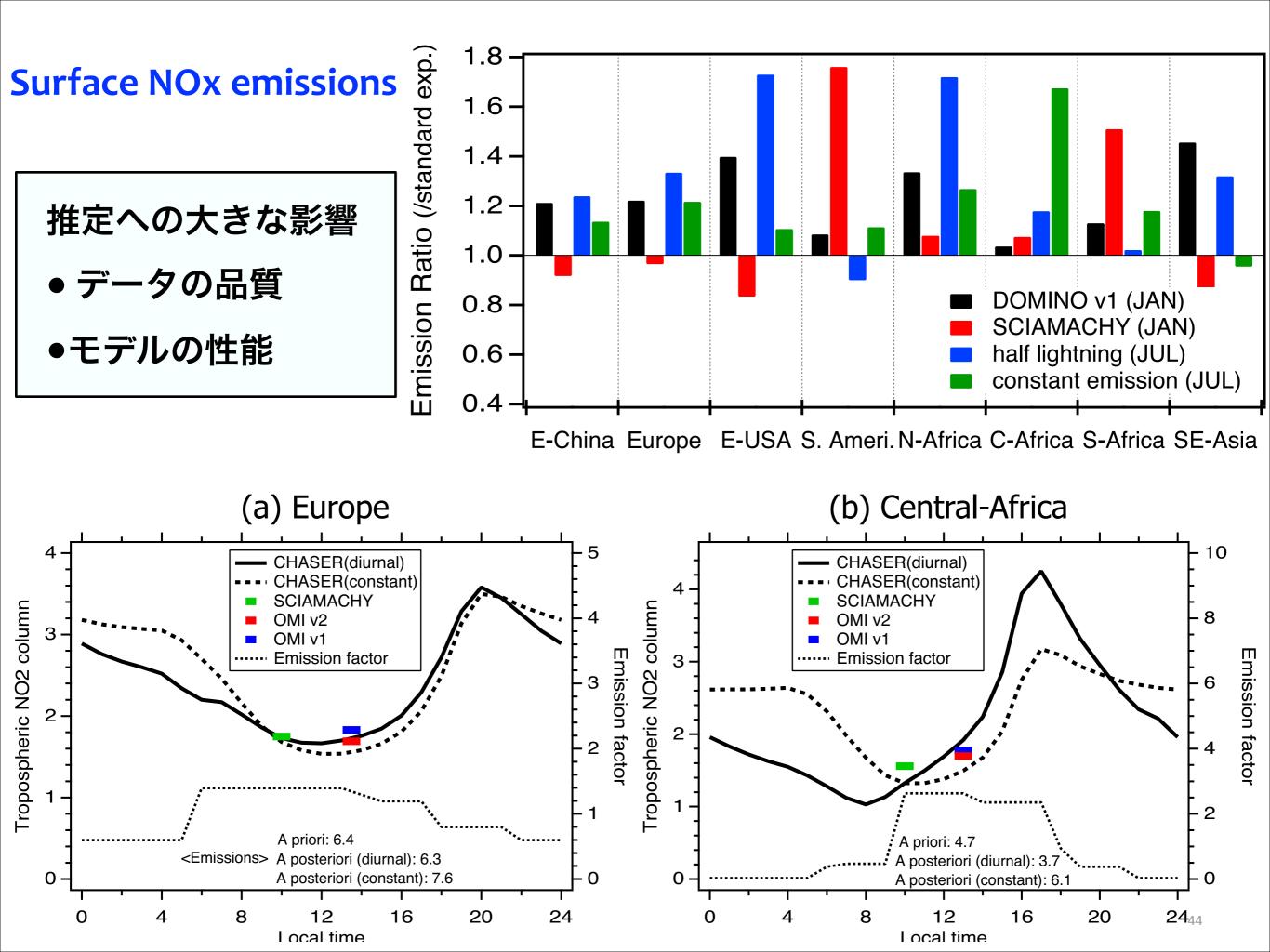


OMI

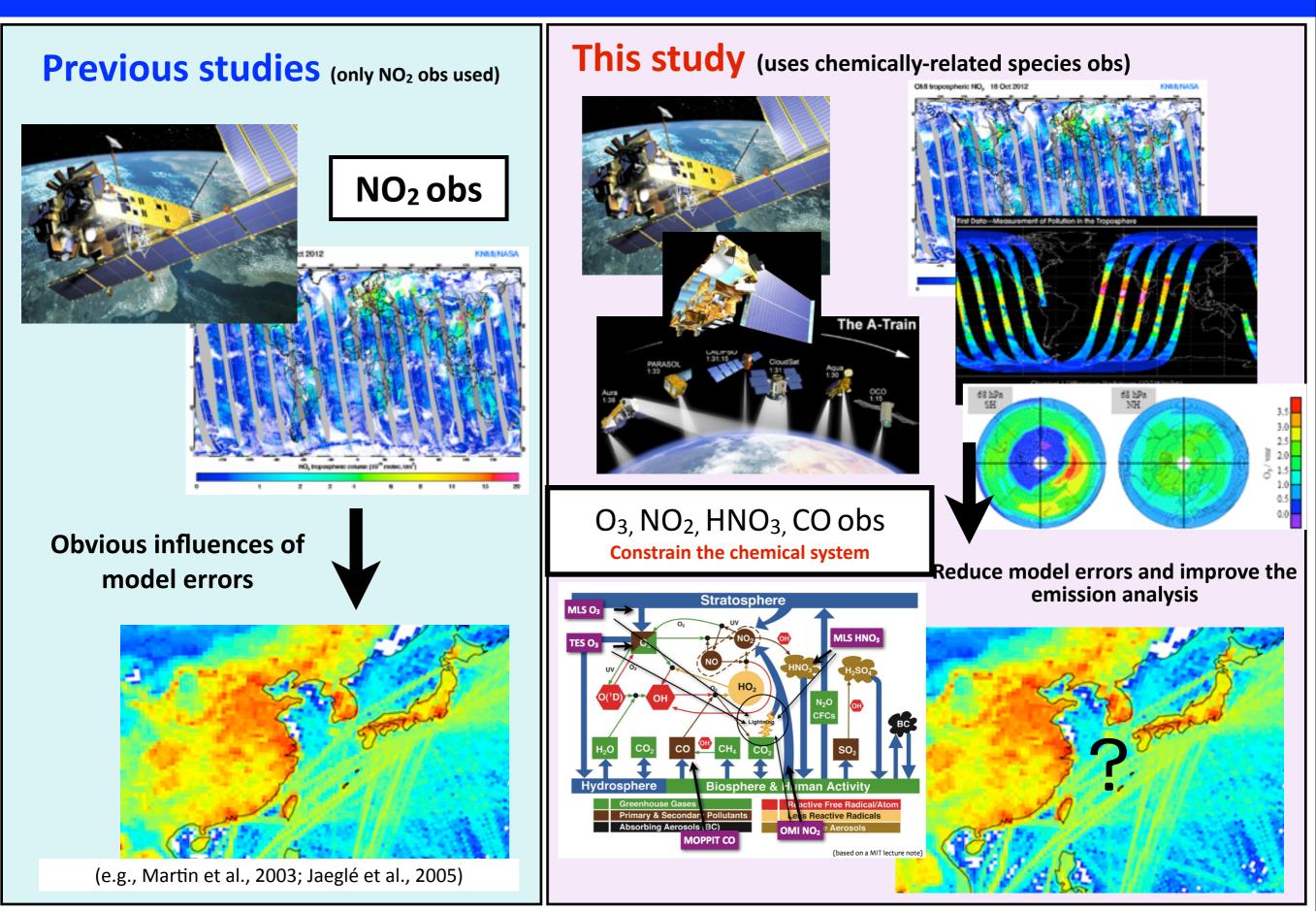


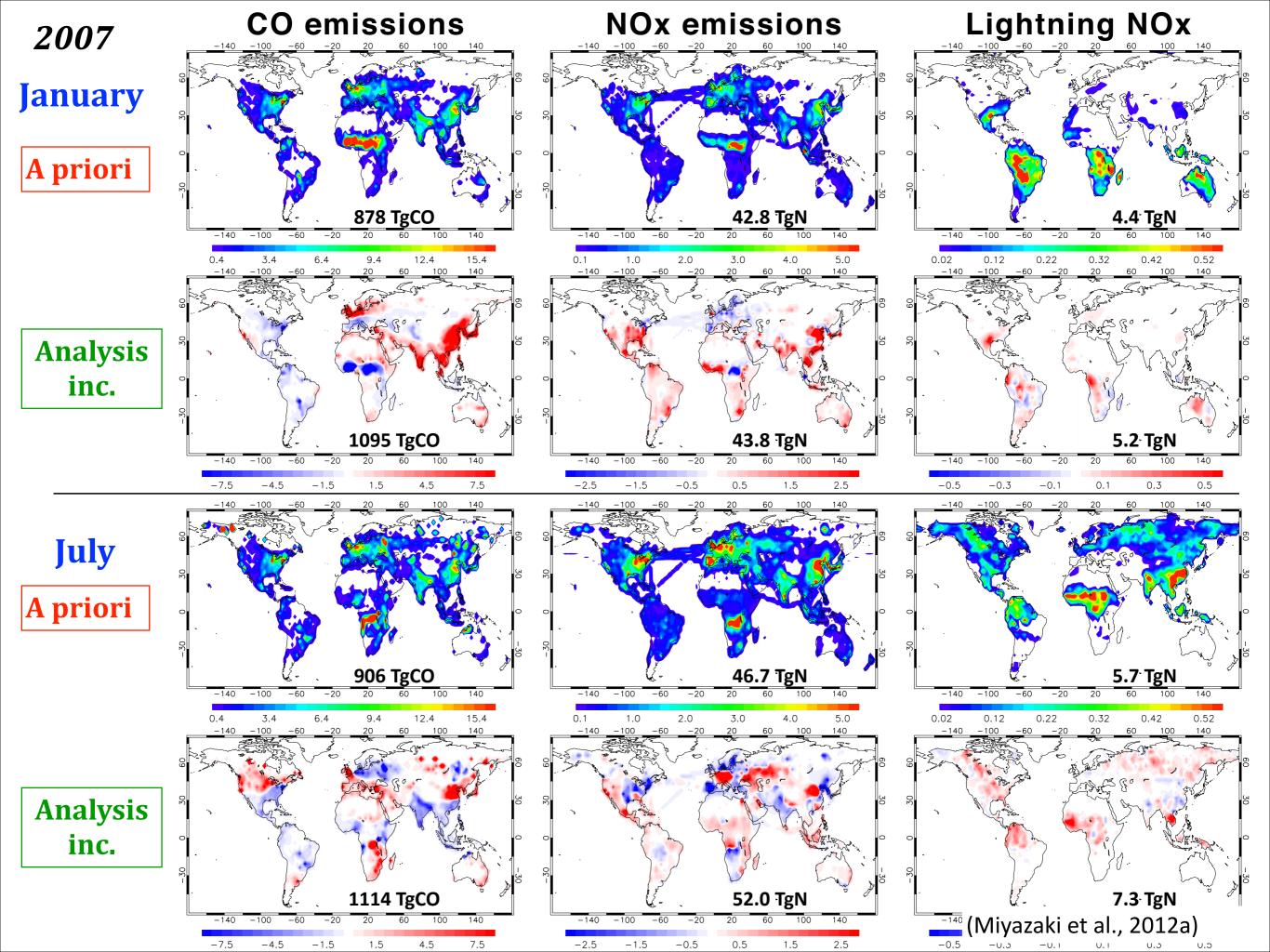
Surface NOx emissions





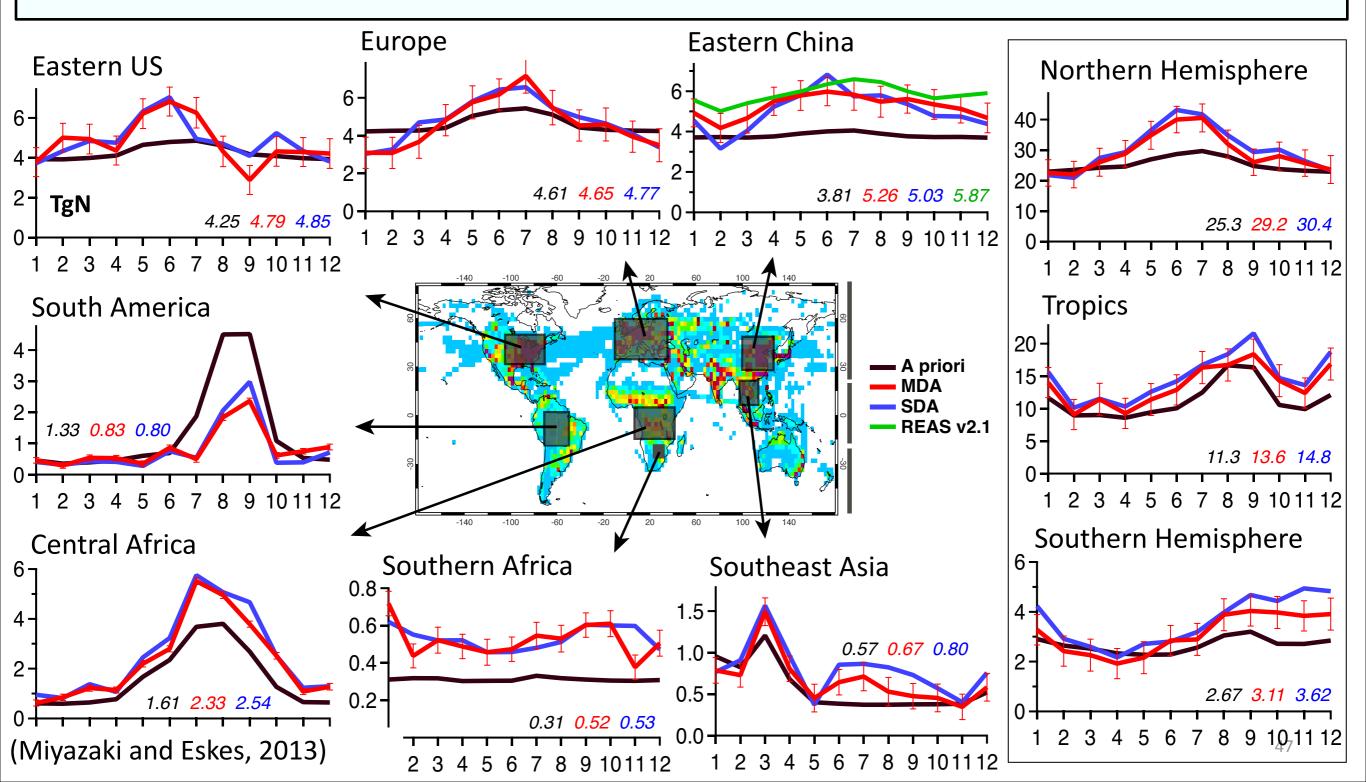
Top-down NOx emission estimates from satellite

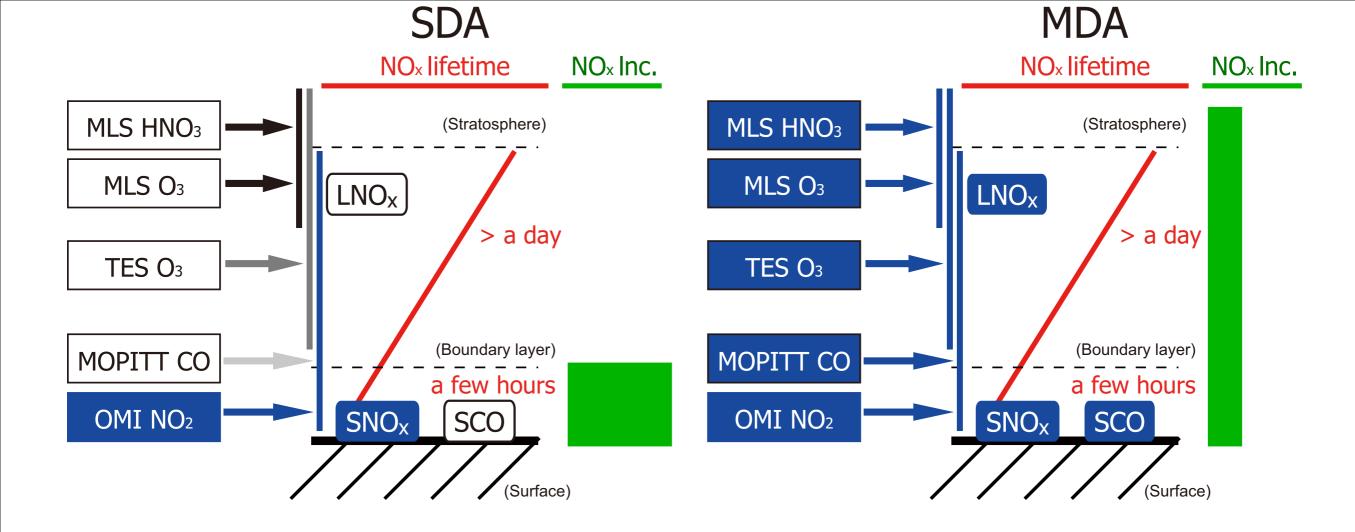




Multiple species constraints on surface NOx emissions

- The multiple datasets assimilation (MDA) provides additional constraints, as a consequence of the NO₂ profiles being modified by the non-NO₂ observations.
- The large influences of non-NO₂ data highlight the large uncertainty (by 58% on regional scale) in the NOx emissions inverted from NO₂ observations only (SDA: single dataset assimilation).

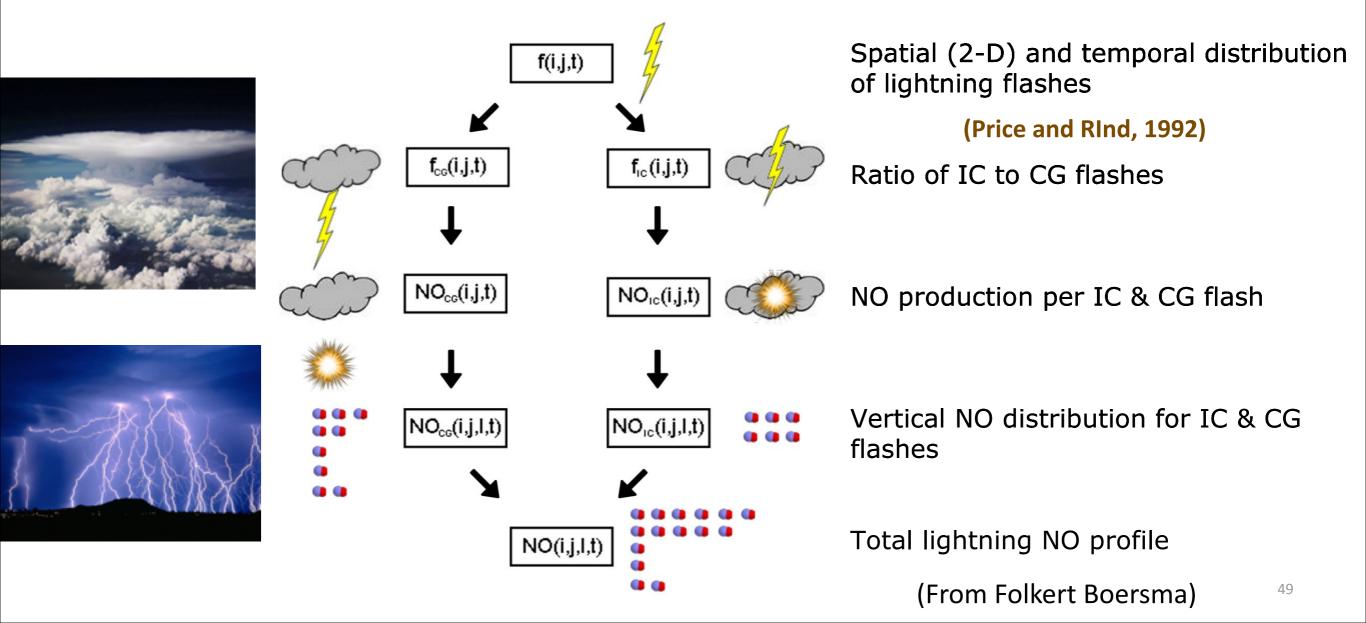




Accurate estimates of LNOx are important to understand variations in NOx, the oxidizing capacity, and several greenhouse gases (O₃, CH₄).

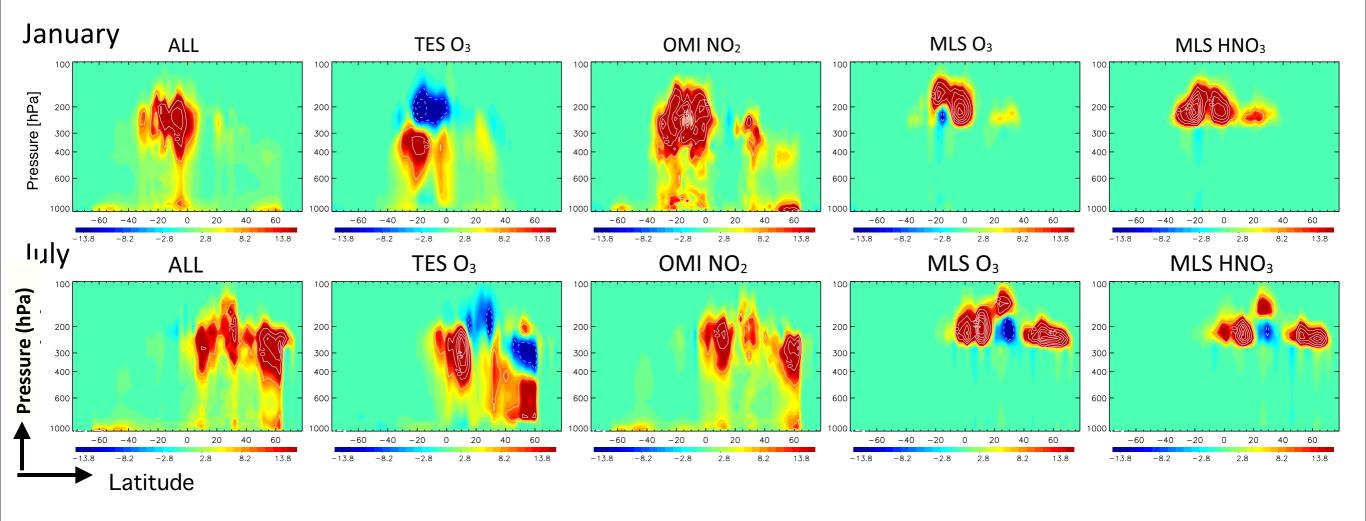
Larger uncertainly in the estimated total amount of NOx globally produced by lightning, i.e. ranging from 2 to 8 TgN/yr.

Bottom-up: The lightning and subsequent NOx formation are determined with the help of empirical parameterizations.



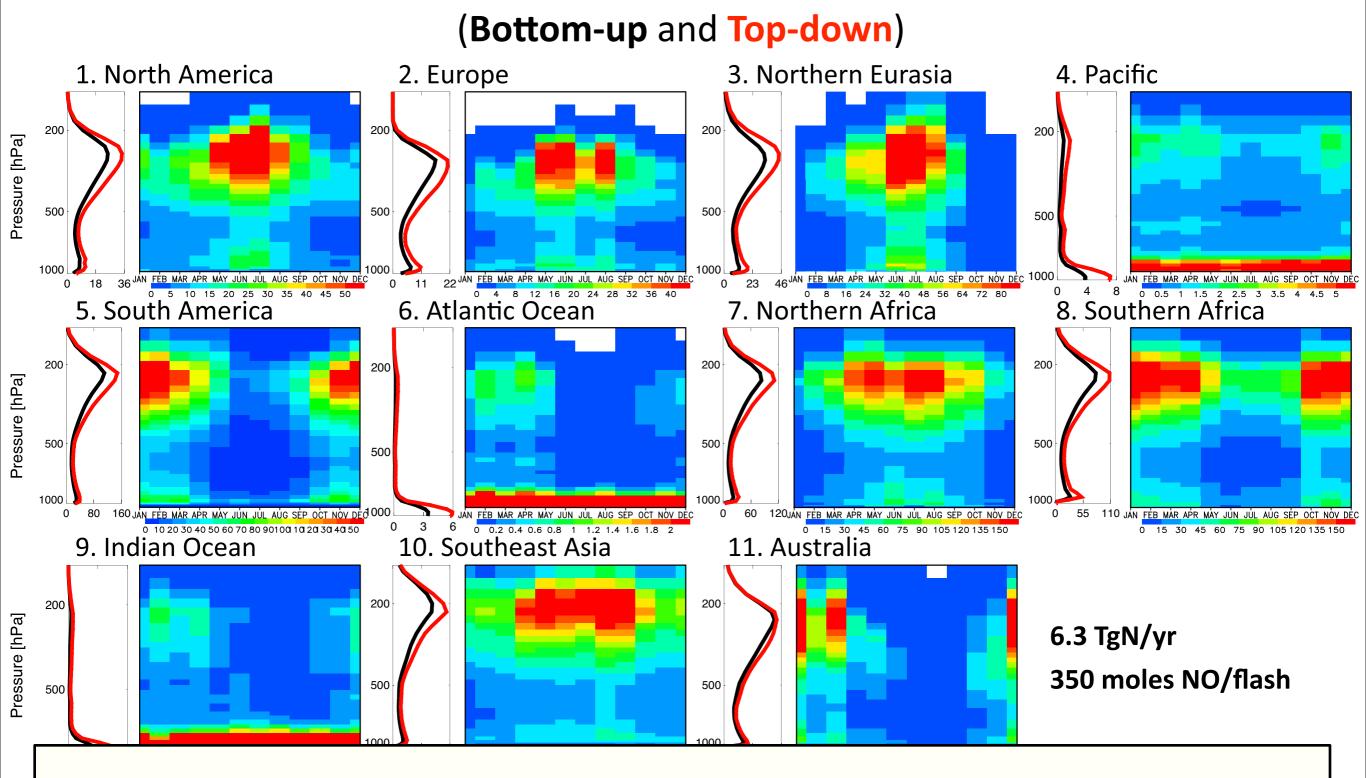
LNOx source increments from OSEs

90S-90N & 1000-100hPa cross-section



The combined use of the multiple datasets with different vertical sensitivities etc facilitates the estimation of the vertical LNOx profile and to distinguish between the surface NOx emissions and LNOx sources.

Seasonal variation of the LNOx sources



The widely used lightning parameterisation based on the C-shape assumption underestimates the source amounts in the upper troposphere and overestimates the peak source height in the upper troposphere by up to 1 km over land.

P

Error estimation

	January				July				
	NH	TR	SH	GL	NH	TR	SH	GL	
Control	0.78	3.99	1.39	6.15	4.69	2.99	0.50	8.18	
w/ OMI bias	0.87	3.97	1.46	6.31	4.61	3.08	0.50	8.18	
TES bias corr.	0.68	3.79	1.36	5.83	4.19	2.74	0.29	7.21	
w/o cloud OMI	0.76	4.04	1.31	6.09	4.13	2.89	0.29	7.33	
year 1997 SST	0.76	3.89	1.37	6.03	4.71	3.06	0.51	8.26	
+20% convection	0.80	3.76	1.37	5.89	4.27	2.99	0.50	8.09	
+20% LNOx err.	0.83	3.75	1.32	5.90	4.59	2.93	0.51	8.03	
+20% SNOx err.	0.81	3.77	1.27	5.85	4.58	2.83	0.50	7.90	
+15% LNOx prior	0.83	4.10	1.48	6.41	5.29	3.16	0.57	9.02	
Total bias	0.16	0.47	0.20	0.66	1.06	0.38	0.31	1.58	

(and more error sources in the chemical schemes etc (e.g., Stavrakou et al. 2013)

c.f. Schumann and Huntrieser (2007) have provided a best estimate of 5 ± 3 TgN

1. 大気組成データ同化とは

2. システムの開発

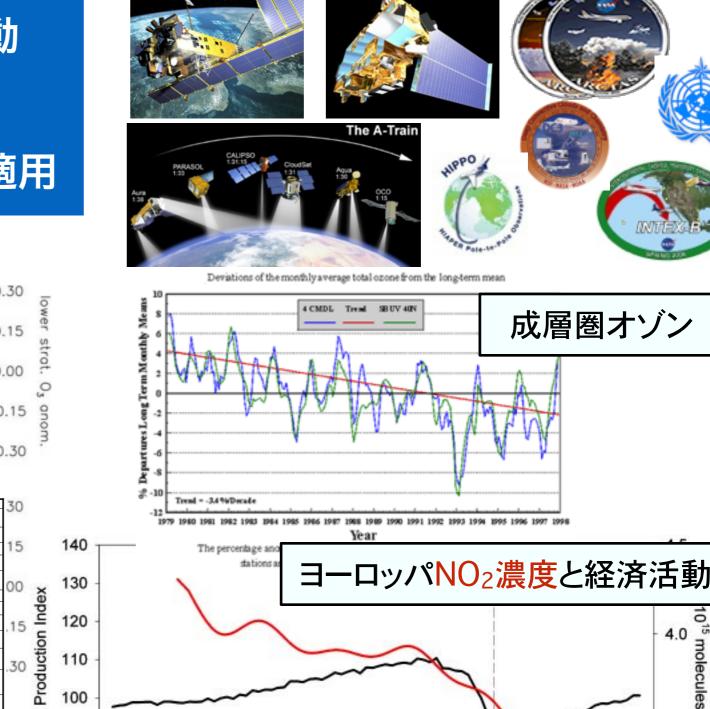
3. 解析結果の検証

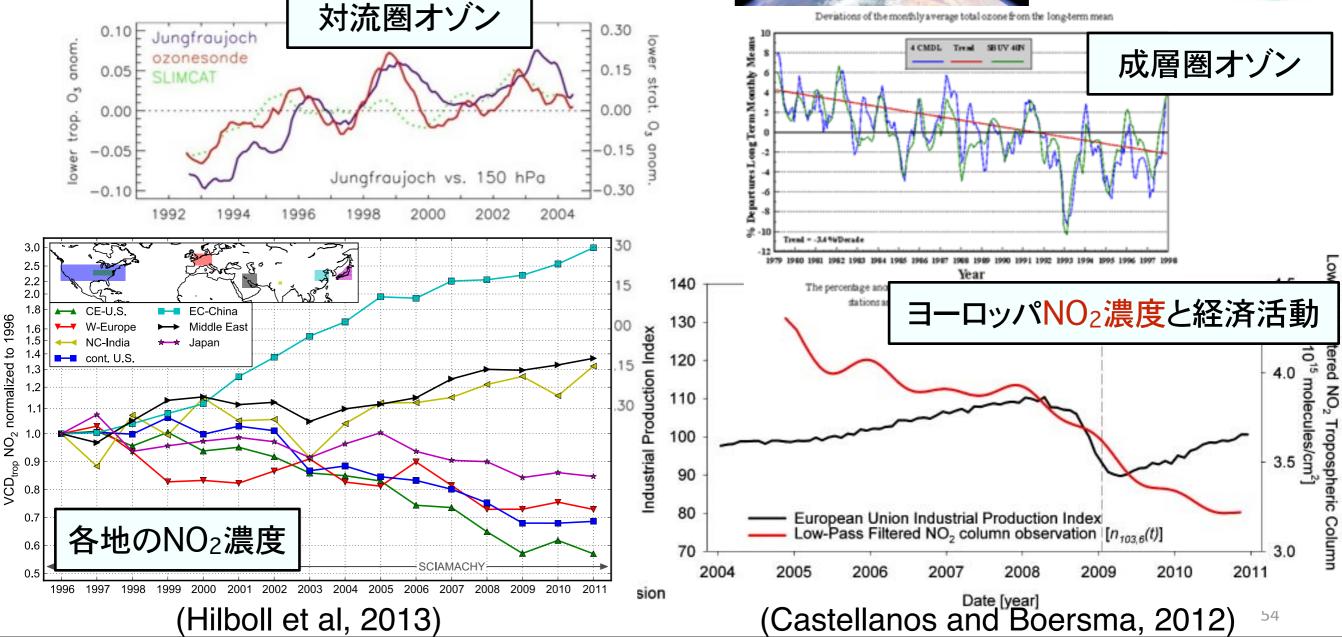
4. 長期再解析の実施

5. 今後の課題

大気組成の長期再解析

- ・大気汚染物質排出量の長期変動
- ・オゾン濃度変動要因の理解
- ・気候モデル・気象再解析への適用





1. 大気組成データ同化とは

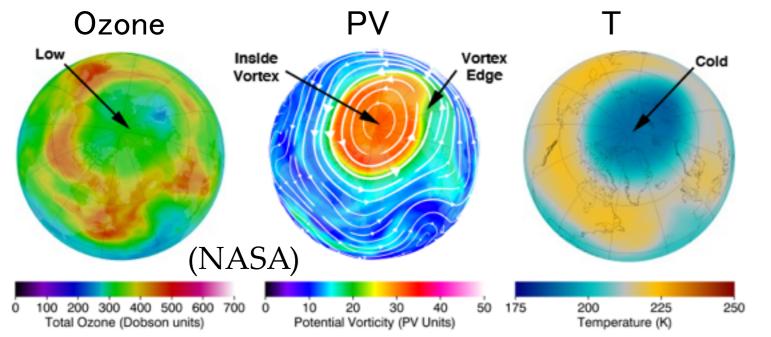
2. システムの開発

3. 解析結果の検証

4. 長期再解析の実施

5. 今後の課題

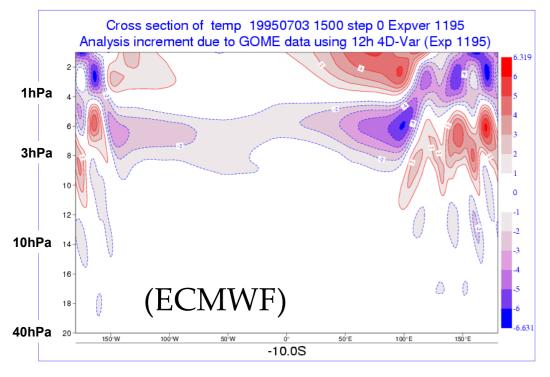
大気組成一気象統合解析

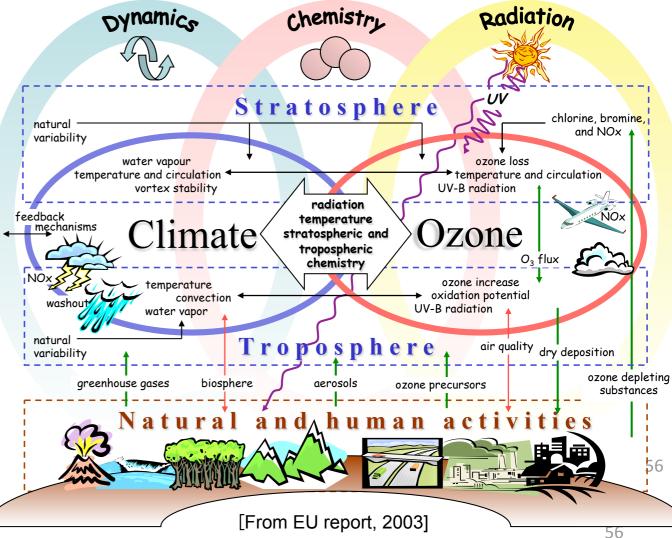


- 放射過程を介した結合
- 大気組成-PV(U)関係
- 気象場不確定性→背景誤差

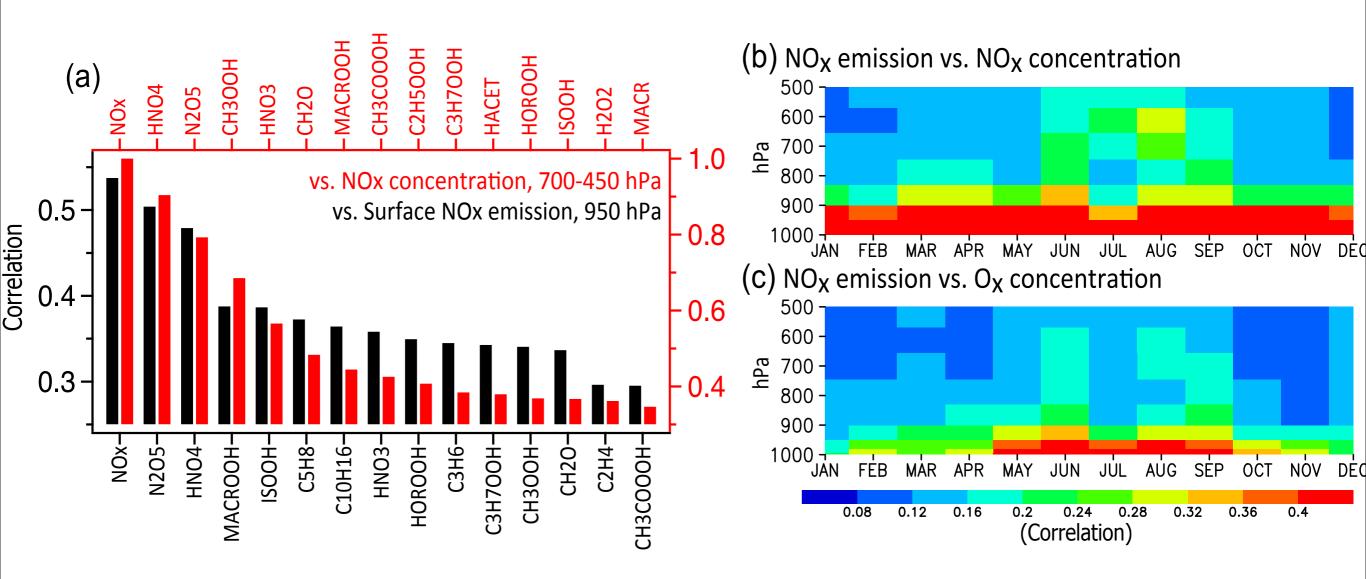
(気温→反応係数、風→輸送)



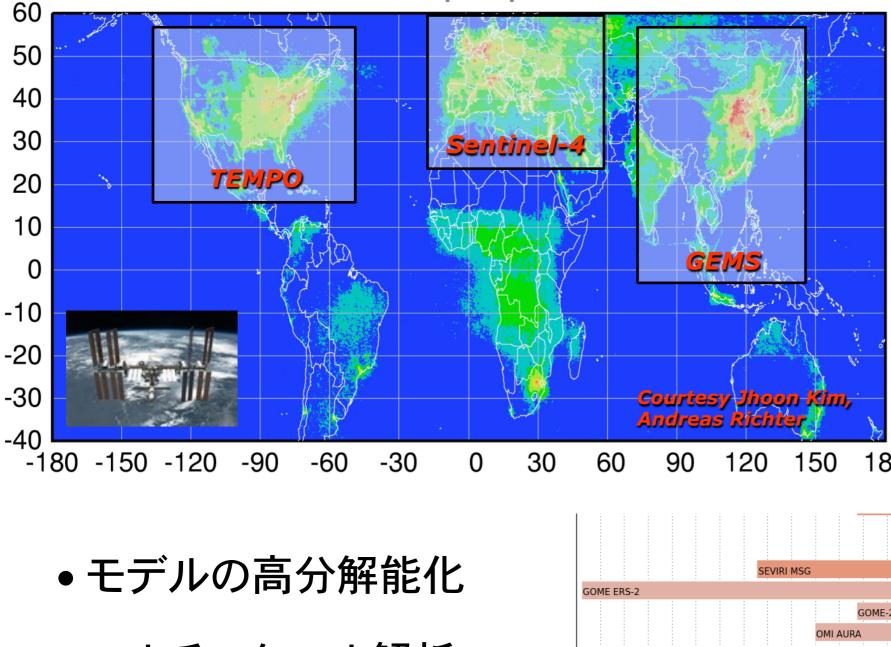




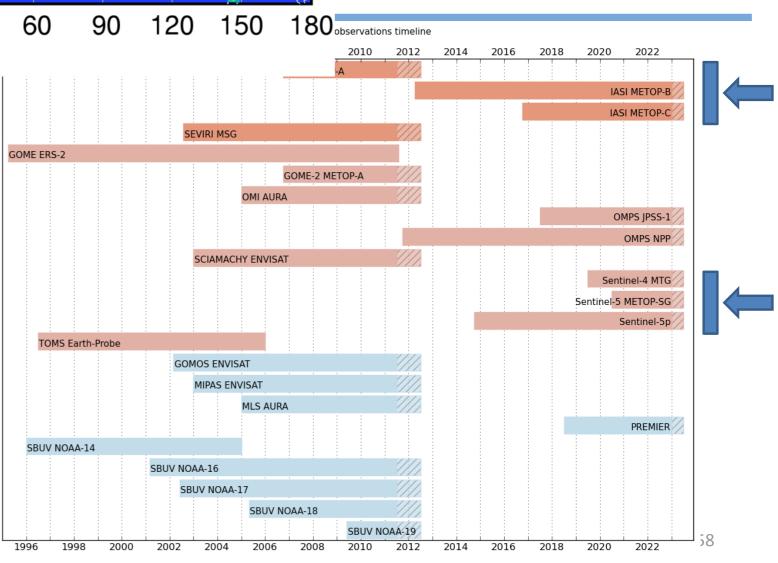
For further improvements in the emission estimates



OSSEs with a careful consideration of the complex chemical interactions and measurement characteristics for various species (incl. the seasonality) will support future instrumental design to improve the emission analysis.



- マルチスケール解析
- ●衛星・地上観測の統合
- インベントリーとの統合
- •環境政策へ活用



新たな観測データ

の利用に向けて

Past & future - O3

まとめと今後の課題

- •大気組成データ同化システム CHASER-DAS を開発
- 衛星観測データを統合した長期再解析を実施
- •大気汚染・大気組成変動・気候研究への提供を計画
- ・更なる観測データの利用、将来の観測計画への貢献
- •宇宙開発センターなどとの連携
- ・気象解析への貢献も重要