# Assimilation of Satellite Data for Atmospheric Composition

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with substantial contributions from

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**and many others**

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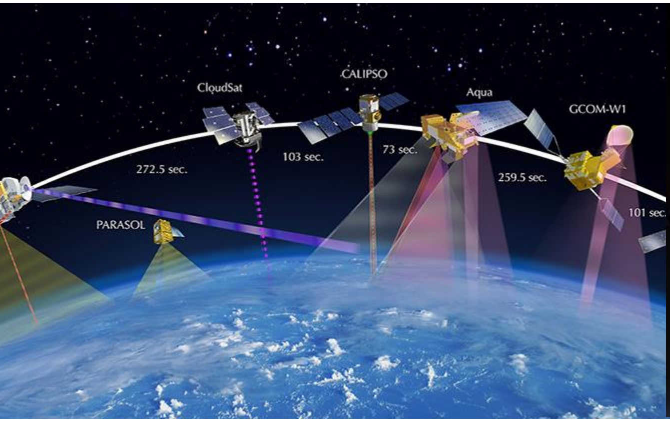


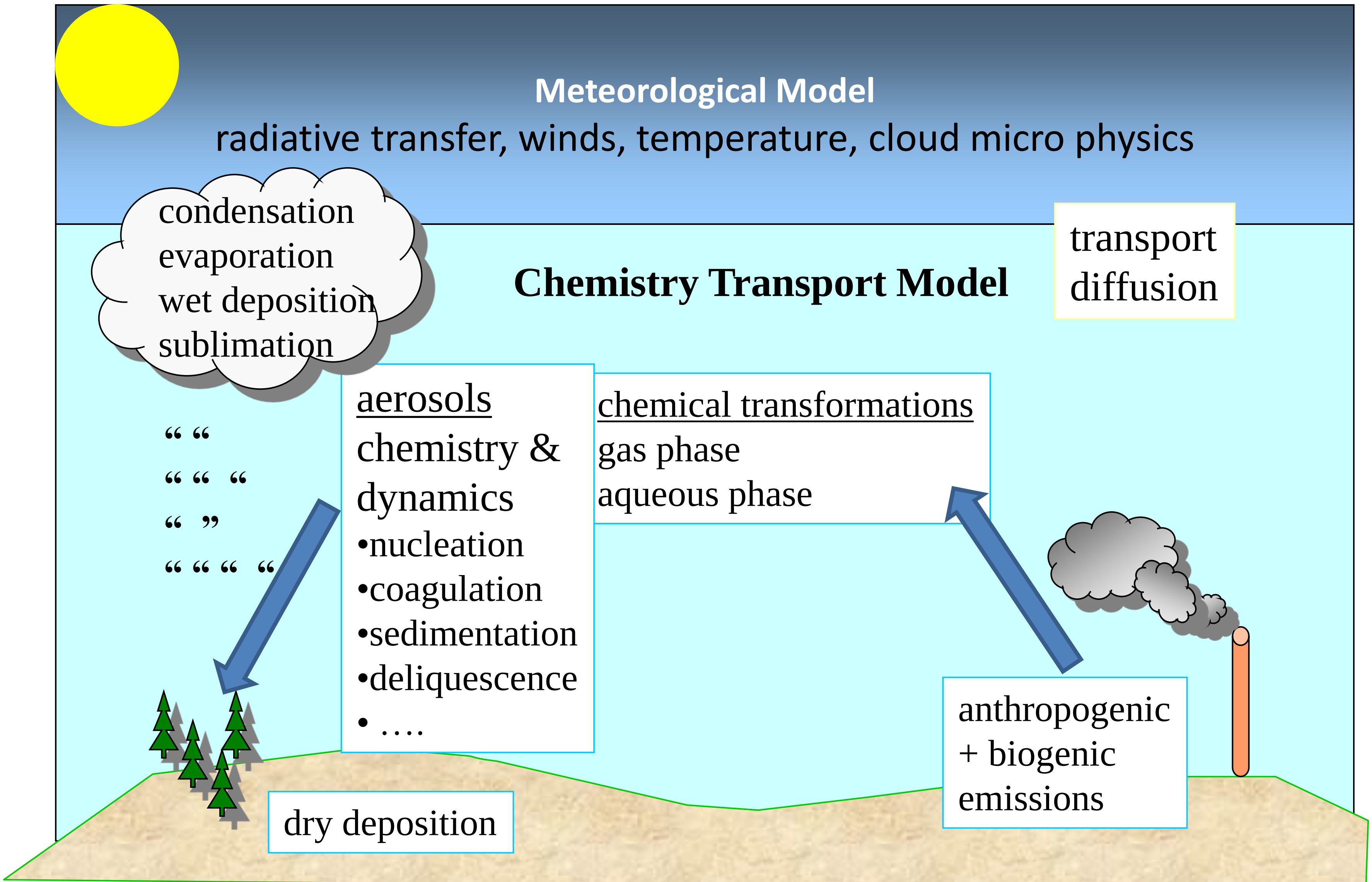


# 1. INTRODUCTION

# What do we expect from composition data assimilation?

- daily „**chemical weather“forecasts**=air quality prediction, the analog to NWP
  - exposure to polluted air and UV-B
- improve „classical“ NWP better calculation of the radiative transfer equation diabatic processes (aerosols, O3,…)
- budget calculations of various constituents
- optimal chemical state analyses (=**monitoring**) or reanalyses:
  - earlier detection/attribution of climate change signals
  - (re-)assessment of radiative forcing

# Processes in a complex chemistry-transport model dim ~ $O(10^7)$



# Characteristics of chemistry data assimilation (1)
# <u>physical viewpoint</u>

## Main sources of uncertainty:

- direct parameters
  - Initial values,
  - emission rates (in tropospheric data assimilation),
  - deposition and sedimentation velocities
  - reaction rates, J-values

- indirect parameters (in trop. data assimilation),
  - boundary layer height
  - vertical exchange mechanisms: convection

## Characteristics of tropospheric chemistry data assimilation (2), 
## mathematical viewpoints

- highly underdetermined system - on 2 levels
  - variables/gridpoint: ~ 60 -200
  - satellite data: scalar column value → profile vector

- regionally/locally highly nonlinear chemical dynamics (photo chemistry)

- constraints by physical laws/models are insufficient, however central manifolds variable ("initialisation" problem, chemical balance not guaranteed)

- assimilation or inversion problem to be solved?

# Transport-diffusion-reaction equation and its adjoint

**Tendency Equations**

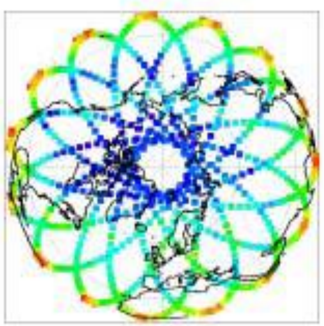
direct chemistry transport equation

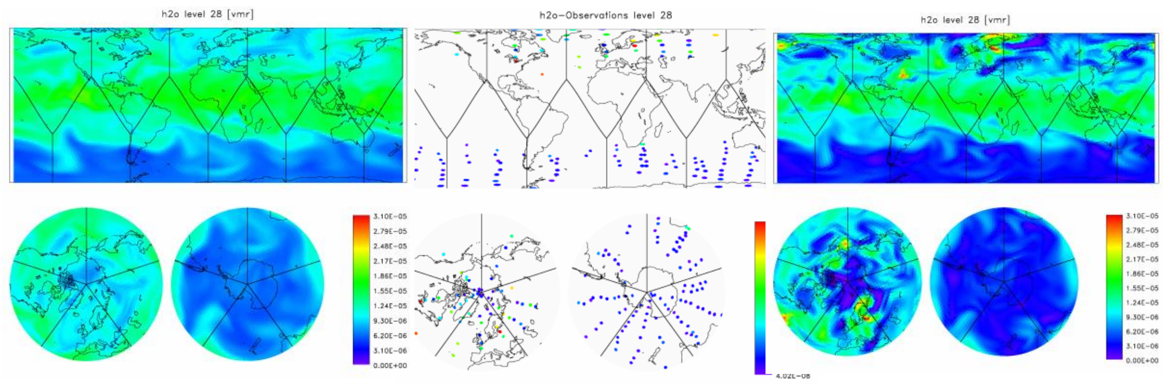
$$\frac{\partial c_i}{\partial t} + \nabla \cdot (\mathbf{v} c_i) - \nabla \cdot (\rho \mathbf{K} \nabla \frac{c_i}{\rho}) - \Sigma_{r=1}^{R} \left( k(r) \left( s_i(r_+) - s_i(r_-) \right) \Pi_{j=1}^{U} c_j^{s_j(r_-)} \right) = E_i + D_i$$

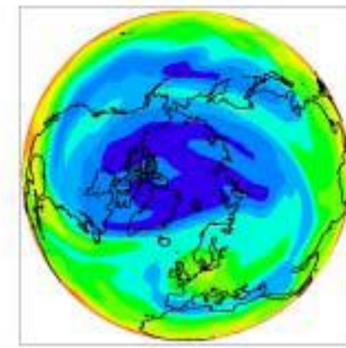
| | | | |
|---|---|---|---|
| $c_i$ | concentration of species $i$ | $c_i^*$ | adjoint of concentration of species $i$ |
| $\mathbf{v}$ | wind velocity | $s$ | stoichiometric coefficient |
| $k(r)$ | reaction rate of reaction $r$ | $\mathbf{K}$ | diffusion coefficient |
| $U$ | number of species in the mechanism | $R$ | number of reactions in the mechanism |
| $E_i$ | emission rate of species $i$ (source) | $D_i$ | deposition rate of species $i$ (sink) |

adjoint chemistry transport equation

$$-\frac{\partial \delta c_i^*}{\partial t} - \mathbf{v} \nabla \delta c_i^* - \frac{1}{\rho} \nabla \cdot (\rho \mathbf{K} \nabla \delta c_i^*) + \Sigma_{r=1}^{R} \left( k(r) \frac{s_i(r_-)}{c_i} \Pi_{j=1}^{U} \bar{c_j}^{s_j(r_-)} \Sigma_{n=1}^{U} \left( s_n(r_+) - s_n(r_-) \right) \delta c_n^* \right) = 0$$





# 2. STRATOSPHERIC CHEMISTRY DATA ASSIMILATION

# stratospheric chemistry example

167 gas phase reactions +

10 heterogeneous reactions on polar strat. clouds

**Table 1.** Photolysis reactions included in the SA(

represents constituents that are not con

| Reaction | |
|---|---|
| (R1) | $O_2 + h\nu \rightarrow O(^3P) + O(^3P)$ |
| (R2) | $O_3 + h\nu \rightarrow O(^3P) + O_2$ |
| (R3) | $O_3 + h\nu \rightarrow O(^1D) + O_2$ |
| (R4) | $H_2O + h\nu \rightarrow H + OH$ |
| (R5) | $H_2O_2 + h\nu \rightarrow OH + OH$ |
| (R6) | $NO_2 + h\nu \rightarrow O(^3P) + NO$ |
| (R7) | $NO_3 +$ |
| (R8) | $NO_3 +$ |
| (R9) | $N_2O +$ |
| (R10) | $N_2O_5 +$ |
| (R11) | $HNO_3$ |
| (R12) | $HNO_4$ |
| (R13) | $Cl_2O_2 +$ |
| (R14) | $Cl_2 + h$ |
| (R15) | $OClO +$ |
| (R16) | $HCl +$ |
| (R17) | $HOCl +$ |
| (R18) | $ClONO$ |
| (R19) | $CH_3Cl$ |
| (R20) | $CCl_4 +$ |
| (R21) | $CFCl_3$ |
| (R22) | $CF_2Cl_2$ |
| (R23) | $CHF_2C$ |
| (R24) | $CF_2ClC$ |
| (R25) | $CH_3CC$ |
| (R26) | $BrO +$ |
| (R27) | $BrCl +$ |
| (R28) | $HOBr +$ |
| (R29) | $BrONC$ |
| (R30) | $CH_3Br$ |
| (R31) | $CF_2ClE$ |
| (R32) | $CF_3Br$ |
| (R33) | $HNO_4$ |
| (R34) | $ClONO$ |
| (R35) | $N_2O_5 +$ |
| (R36) | $CH_2O + h\nu \rightarrow H + HCO$ |
| (R37) | $CH_2O + h\nu \rightarrow H_2 + CO$ |

**Table 2.** Gas phase reactions that are included in

"products" represents constituents which are not consi

| Reaction | |
|---|---|
| (R38) | $O(^3P)+O_3 \rightarrow O_2+O_2$ |
| (R39) | $O(^1D)+O_2 \rightarrow O(^3P)+O_2$ |
| (R40) | $O(^1D)+O_3 \rightarrow O_2$ |
| (R41) | $O(^1D)+O_3 \rightarrow O($ |
| (R71) | $OH+HO_2 \rightarrow H_2($ |
| (R72) | $OH+H_2O_2 \rightarrow H_2$ |
| (R73) | $HO_2+O_3 \rightarrow OH+$ |
| (R74) | $HO_2+HO_2 \rightarrow H_2$ |

**Table 2.** (continued)

| Reaction | |
|---|---|
| (R105) | $ClO+OH \rightarrow Cl+HO_2$ |
| (R106) | $ClO+OH \rightarrow HCl+O_2$ |
| (R107) | $OClO+OH \rightarrow HOCl+O_2$ |
| (R108) | $HCl+OH \rightarrow Cl+H_2O$ |
| (R141) | $Br+HO_2 \rightarrow HBr+O_2$ |
| (R142) | $BrO+HO_2 \rightarrow HOBr+O_2$ |
| (R143) | $Br+O_3 \rightarrow BrO+O_2$ |
| (R144) | $CH_2O+Br \rightarrow HBr+HCO$ |

**Table 3.** Heterogeneous reactions included in the SACADA reaction scheme. The notation "(c)" indicates a species in the condensed (liquid or solid) phase. The term "products" represents constituents which are not considered in the reaction scheme.

| Reaction | | Uptake coefficient | | |
|---|---|---|---|---|
| | | liquid/STS | NAT | ice |
| (R168) | $BrONO_2 + H_2O(c) \rightarrow HOBr + HNO_3$ | $f(t, p_{H_2O})^a$ | - | 0.26 |
| (R169) | $N_2O_5 + H_2O(c) \rightarrow HNO_3 + HNO_3$ | $f(t, p_{H_2O})^a$ | 0.0004 | 0.02 |
| (R170) | $ClONO_2 + H_2O(c) \rightarrow HNO_3 + HOCl$ | $f(t, p_{H_2O}, p_{HCl})^b$ | 0.004 | 0.3 |
| (R171) | $ClONO_2 + HCl(c) \rightarrow Cl_2 + HNO_3$ | $f(t, p_{H_2O}, p_{HCl})^b$ | 0.2 | 0.3 |
| (R172) | $HOCl + HCl(c) \rightarrow Cl_2 + H_2O$ | $f(t, p_{H_2O}, p_{HCl})^b$ | 0.1 | 0.2 |
| (R173) | $N_2O_5 + HCl(c) \rightarrow HNO_3 +$ products | - | 0.003 | 0.03 |
| (R174) | $HOBr + HCl(c) \rightarrow BrCl + H_2O$ | 0.01 | - | 0.3 |
| (R175) | $ClONO_2 + HBr(c) \rightarrow BrCl + HNO_3$ | - | 0.3 | 0.3 |
| (R176) | $HOCl + HBr(c) \rightarrow BrCl + H_2O$ | - | - | 0.05 |
| (R177) | $BrONO_2 + HCl(c) \rightarrow BrCl + HNO_3$ | 0.3 | - | 0.3 |

*a*: as recommended by *Sander et al.* [2006]

*b*: *Shi et al.* [2001], as recommended by *Sander et al.* [2006]

# The early challenge: Polar zone depletion motivated data assimilation with Chemistry-Transport Models

- CTMs driven by off-line winds and temperatures, e.g.:
  - Khattatov *et al.* 1999;
  - Errera and Fonteyn 2001;
  - Stajner *et al.* 2001;
  - Eskes *et al.* 2003,
  - Marchand *et al.* 2004
- assimilation of ozone (profiles and total columns) now operational at a number of institutions making use of CTMs:
  - KNMI http://www.temis.nl/ **TM5**
  - BIRA-IASB http://www.bascoe.oma.be/ **BASCOE**
  - DLR-DFD http://taurus.caf.dlr.de **SACADA**
  - NASA http://gmao.gsfc.nasa.gov/operations/ **GEO**S

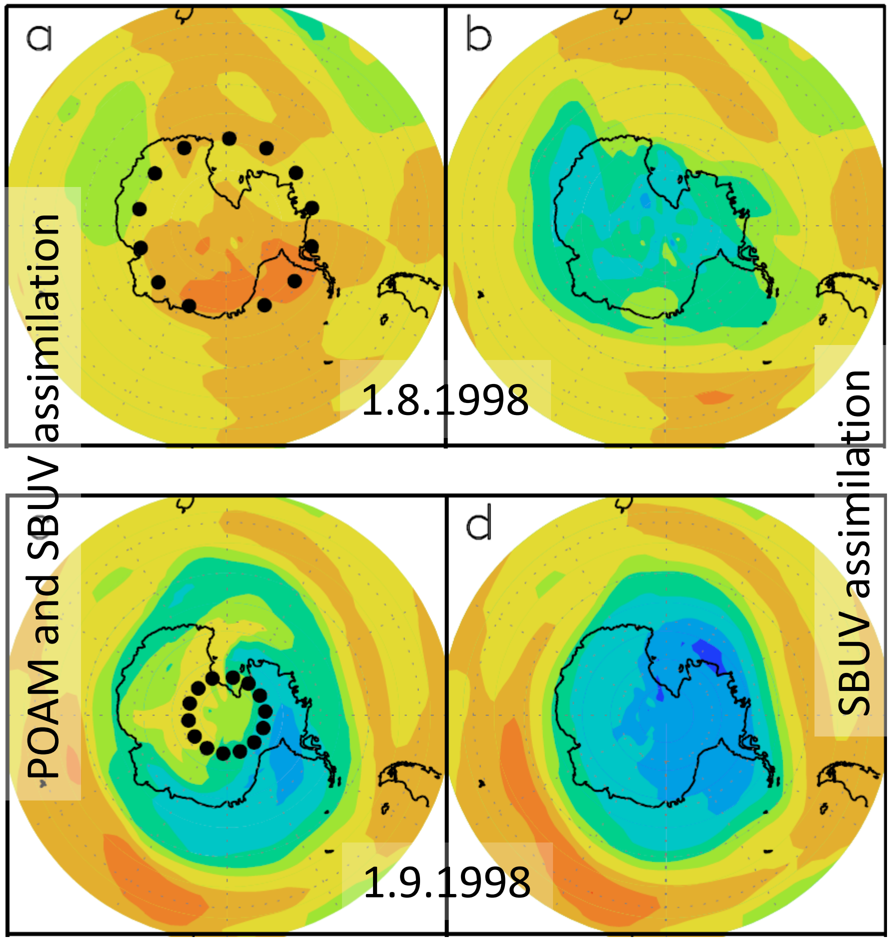
# Early operational ozone analyses (Štajner *et al.,* 2001).

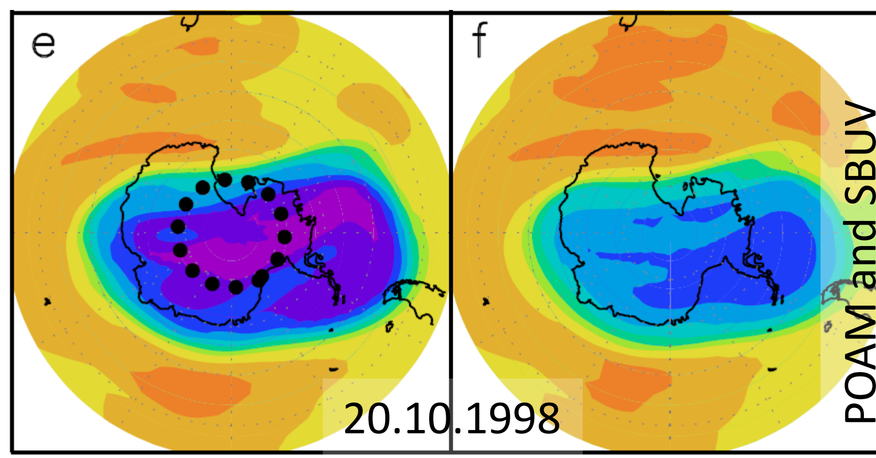
- Goddard Earth Observation System (GEOS) ozone data assimilation system 3-D CTM with parametrized ozone chemistry,
- $\chi 2$ diagnostics to estimate the system parameters,
- operational in 1999,
- stratospheric ozone analyses
- SBUV/2 and TOMS

# Example ozone hole focus: SBUV/2 and POAM-III (Štajner and Wargan 2004), combined **occultation**

**Ozone mixing ratio (in ppmv) at 70 hPa**

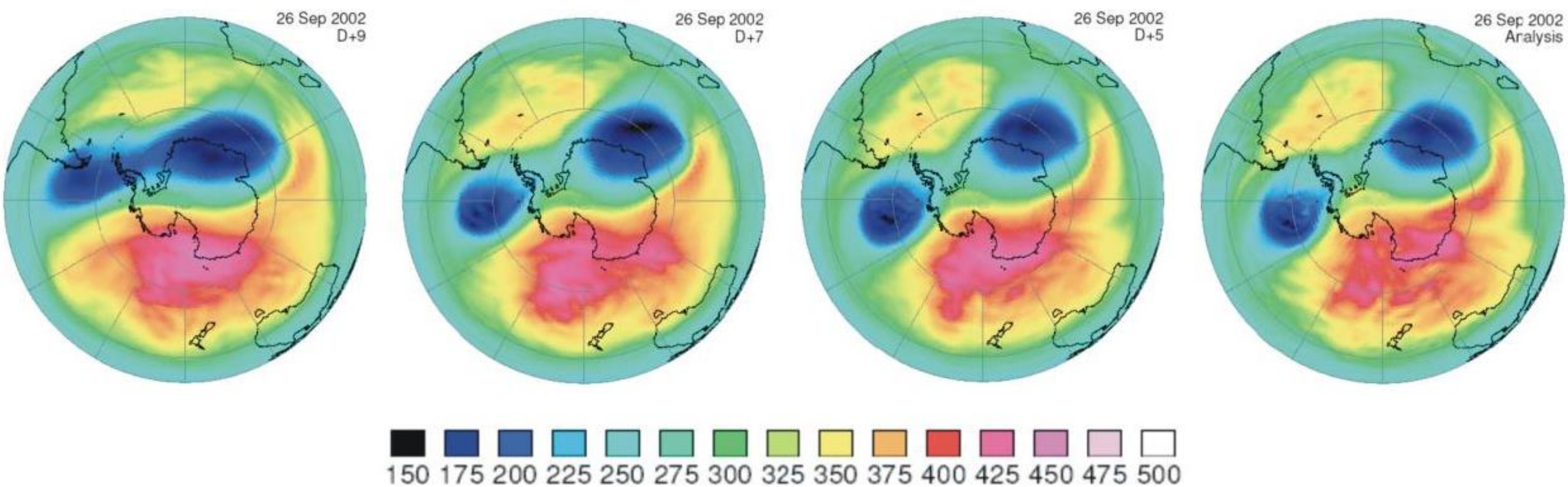
POAM III ozone data solar occultation austral winter and spring in 1998.
sun-synchronous satellite orbit,
14–15 sunsets and sunrises per day,
25.4 longitude apart,
two latitude circles 54N to 71N, 63S to 88S
vertical resolution of v3 ozone 1.1 km
random errors < 5% for z > 15 km




● **POAM III occultation positions**

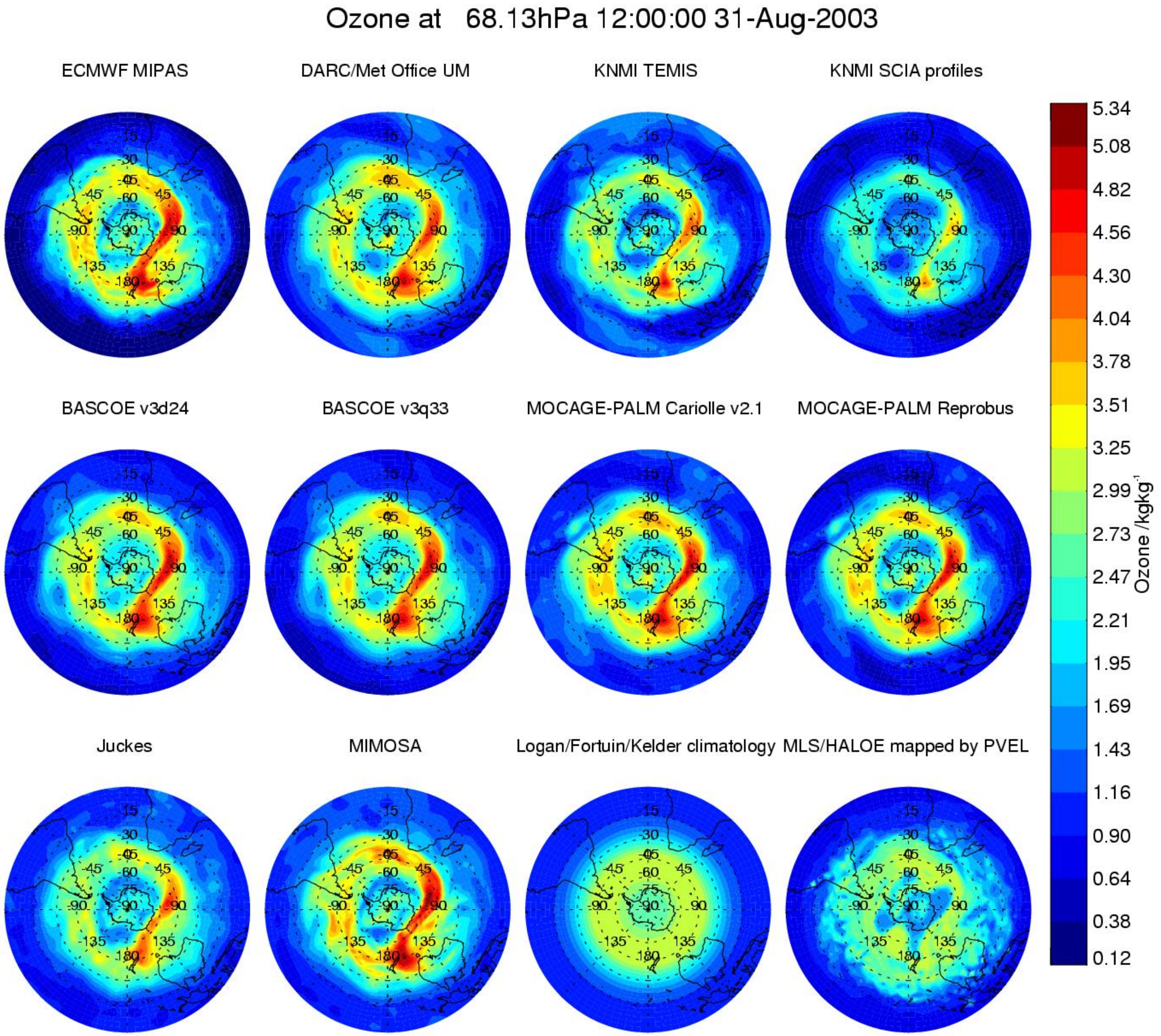
# O3 **total column data assimilation** (GOME) Forecasts and analysis of the first southern vortex split event




**Ozone total column on 26 September 2002, KNMI operational ozone assimilation system. From left to right: 9-, 7-, 5-day forecasts, and the corresponding analysis.**

**From Eskes *et al.* (2005), KNMI.**

# ASSET data assimilation analysis comparison:

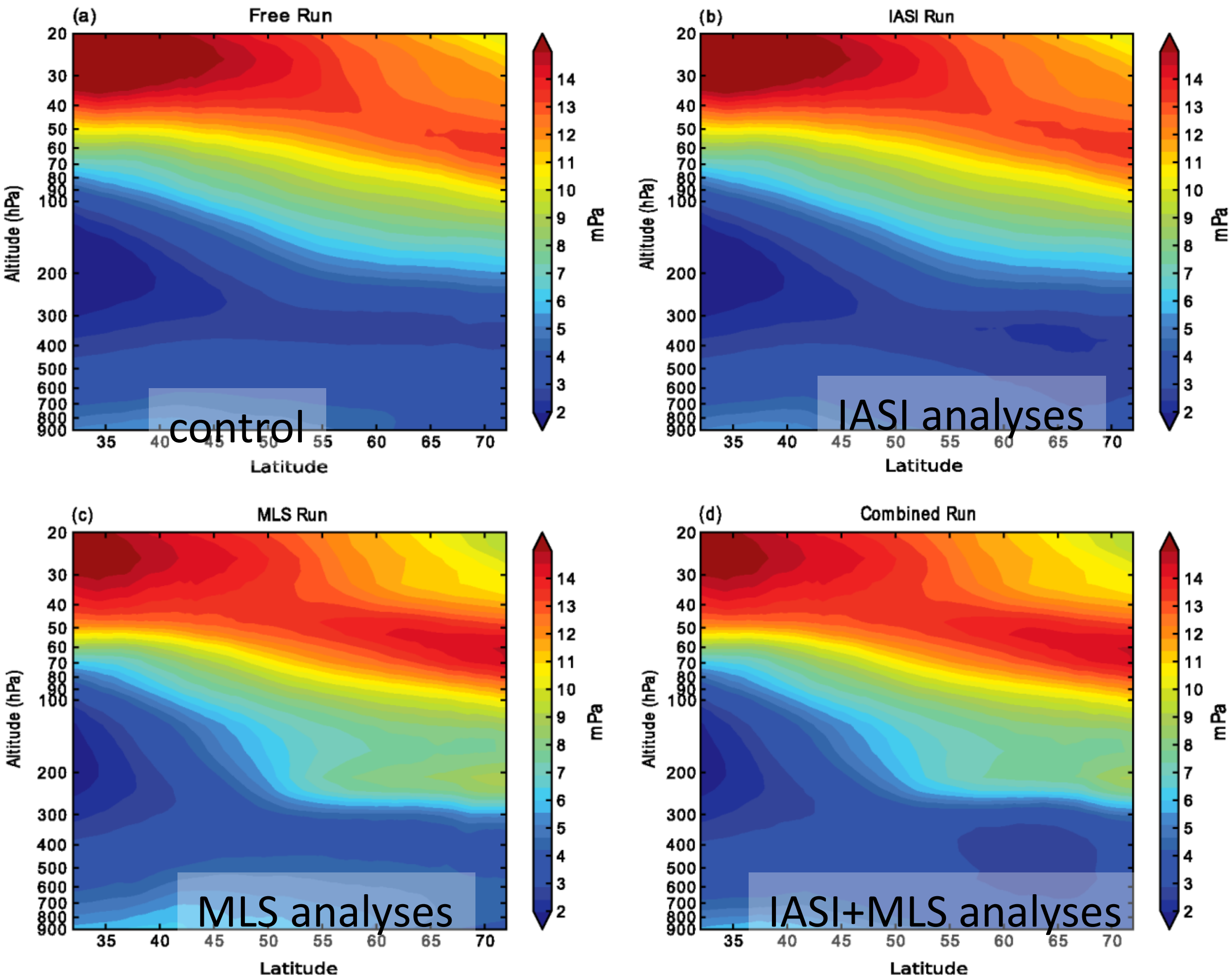


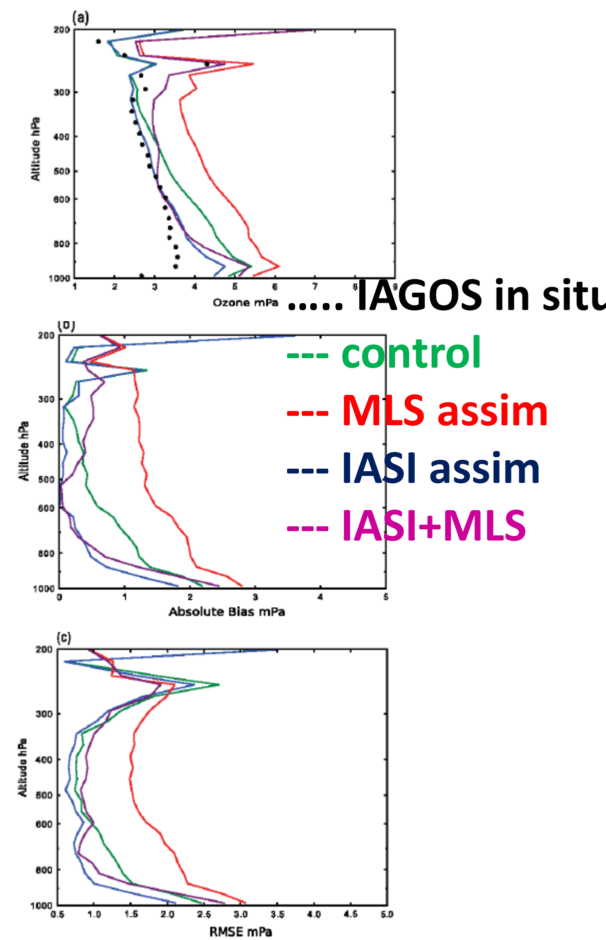

Ozone (ppm) at 68 hPa in the southern hemisphere on 31st August 2003.

**from Lahoz et al, 2010**

# Combined assimilation of **IASI** ozone tropospheric columns and stratospheric **MLS** profiles

by Barre, J Peuch, VH Lahoz, WA Attie, JL Josse, B Piacentini, Eremenko, M Dufour, Nedelec, P; von Clarmann, T El Amraoui, (2014)




**zonal mean of O3 field July 2009 over Europe 15W-35**E

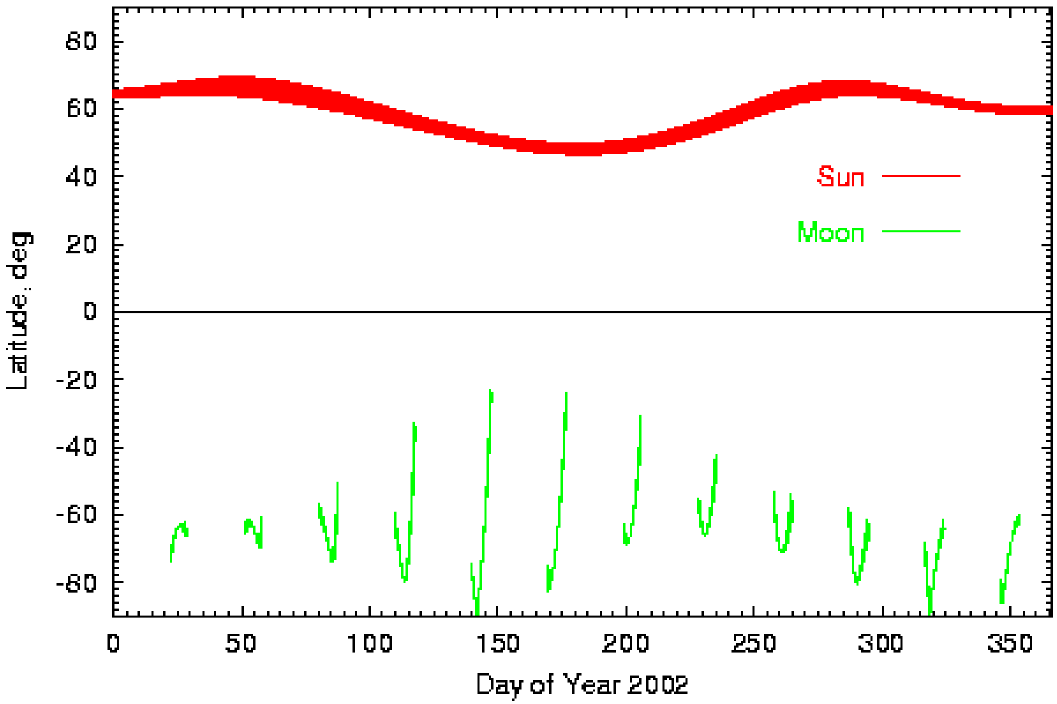
# ENVISAT MIPAS and SCIAMACHY by SACADA 4D-var-assimilation system

## Data Availability 21. Oct. – 14. Nov. 2003

| | MIPAS-IMK | | SCIA-Limb | | SCIA-Occ | |
|---|---|---|---|---|---|---|
| | Available | Assimilated | Available | Assimilated | Available | Assimilated |
| O3 | X | X | X | | X | |
| NO2 | X | X | X | | X | |
| N2O | X | X | | | | |
| HNO3 | X | X | | | | |
| HNO4 | X | | | | | |
| NO | X | | | | | |
| N2O5 | X | X | | | | |
| H2O | X | X | | | | |
| CH4 | X | X | | | | |
| CFC-11 | X | X | | | | |
| CFC-12 | X | X | | | | |
| ClO | X | | | | | |
| ClONO2 | X | X | | | | |
| BrO | | | X | | | |

MIPAS : von Clarman, Stiller et al., KIT Karlsruhe
SCIAMACHY: Bovensmann and coworkers, Uni Bremen

# SCIAMACHY Solar Occultation Data Analysis for SACADA




$O_3$ and $NO_2$

J. Meyer, A. Bracher, L. Amekudzi, S. Noel, A. Rozanov, B. Hoffmann, H. Bovensmann, J. P. Burrows

Institute for Environmental Physics, University of Bremen, Germany

# Scatter plots for Nov. 13, 2003

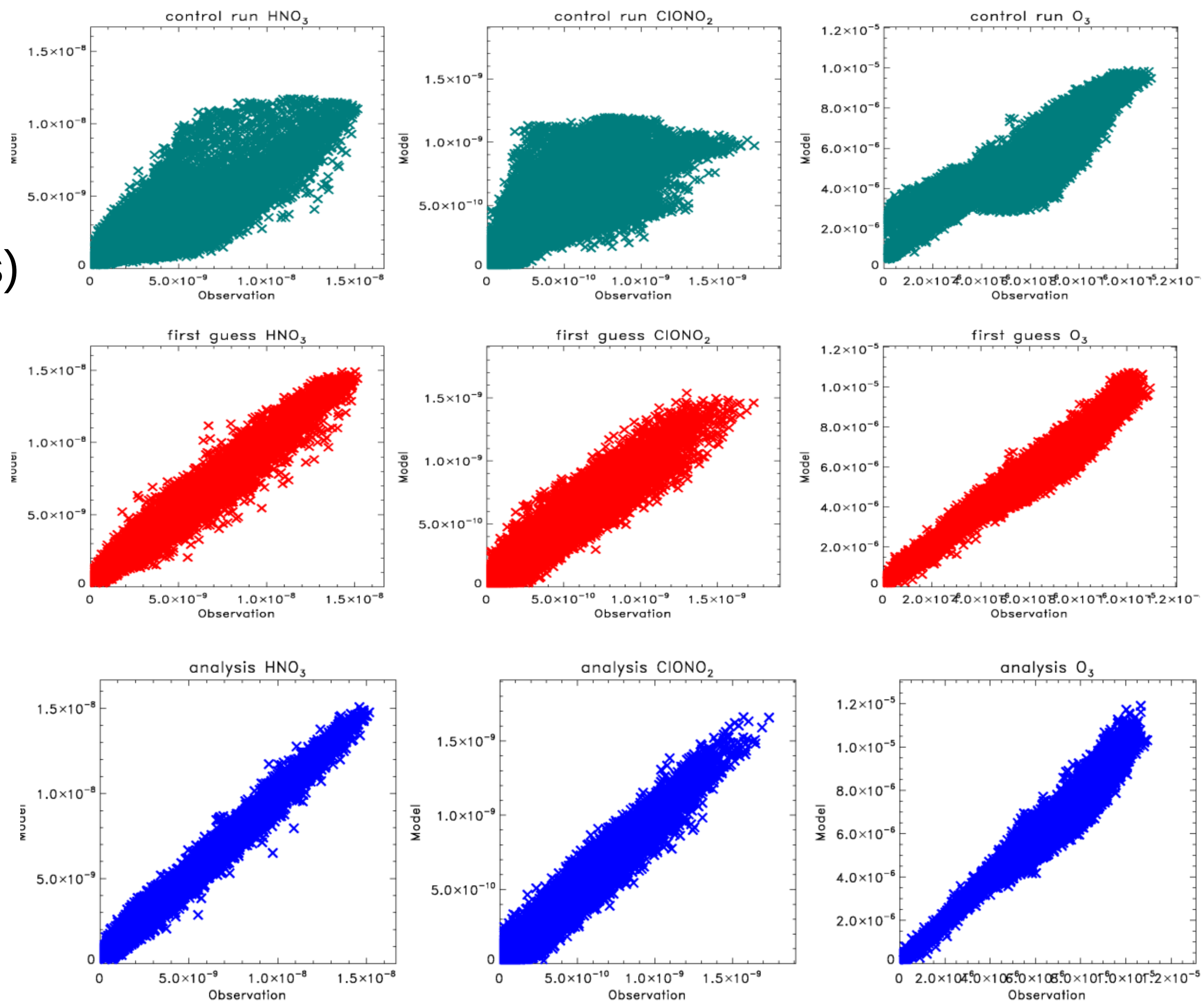
**$HNO_3$** **$ClONO_2$** **$O_3$**

Control Run
(after 23 days of free integration with SOKRATES (2D) initial values)

23 days consecutive 4D-var:

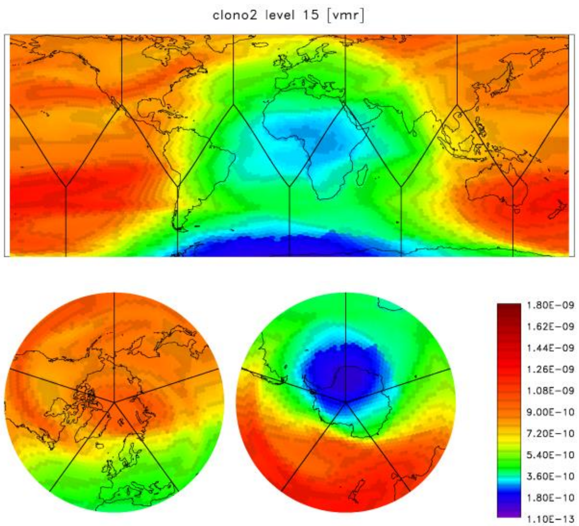
Background

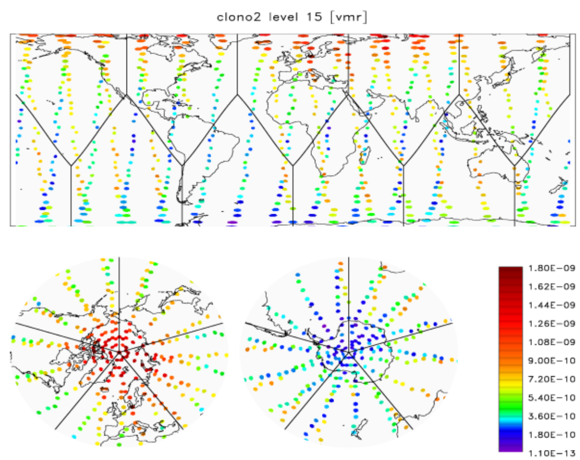
Analysis

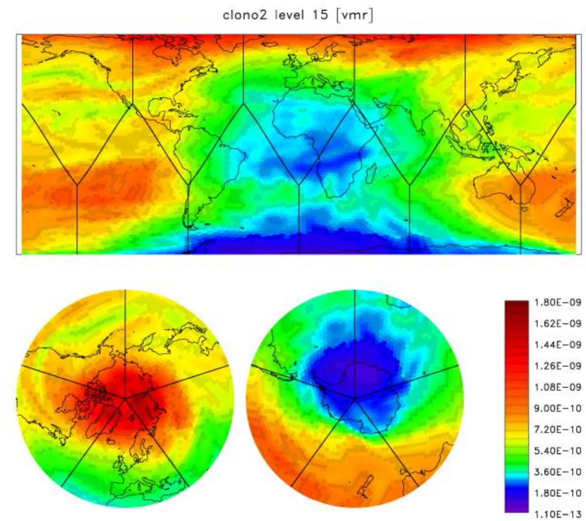


# SACADA 4D-var, 24 h assimilation window

# Results for $ClONO_2$ at 7.6 hPa (~33 km), Nov. 13, 2003 12:00 UTC




**Control Run**

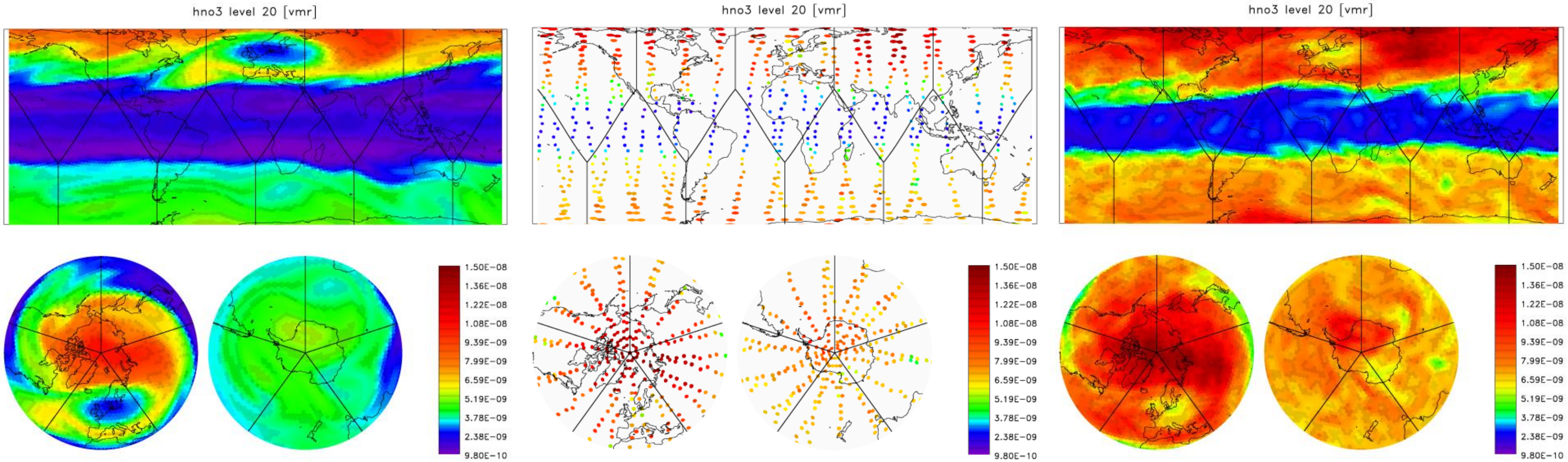
**(no assimilation)**

**MIPAS Observations**

**Analysis**

# SACADA 4D-var, 24 h assimilation window

## $HNO_3$ at 28 hPa (~24 km), Nov. 4, 2003 12:00 UTC

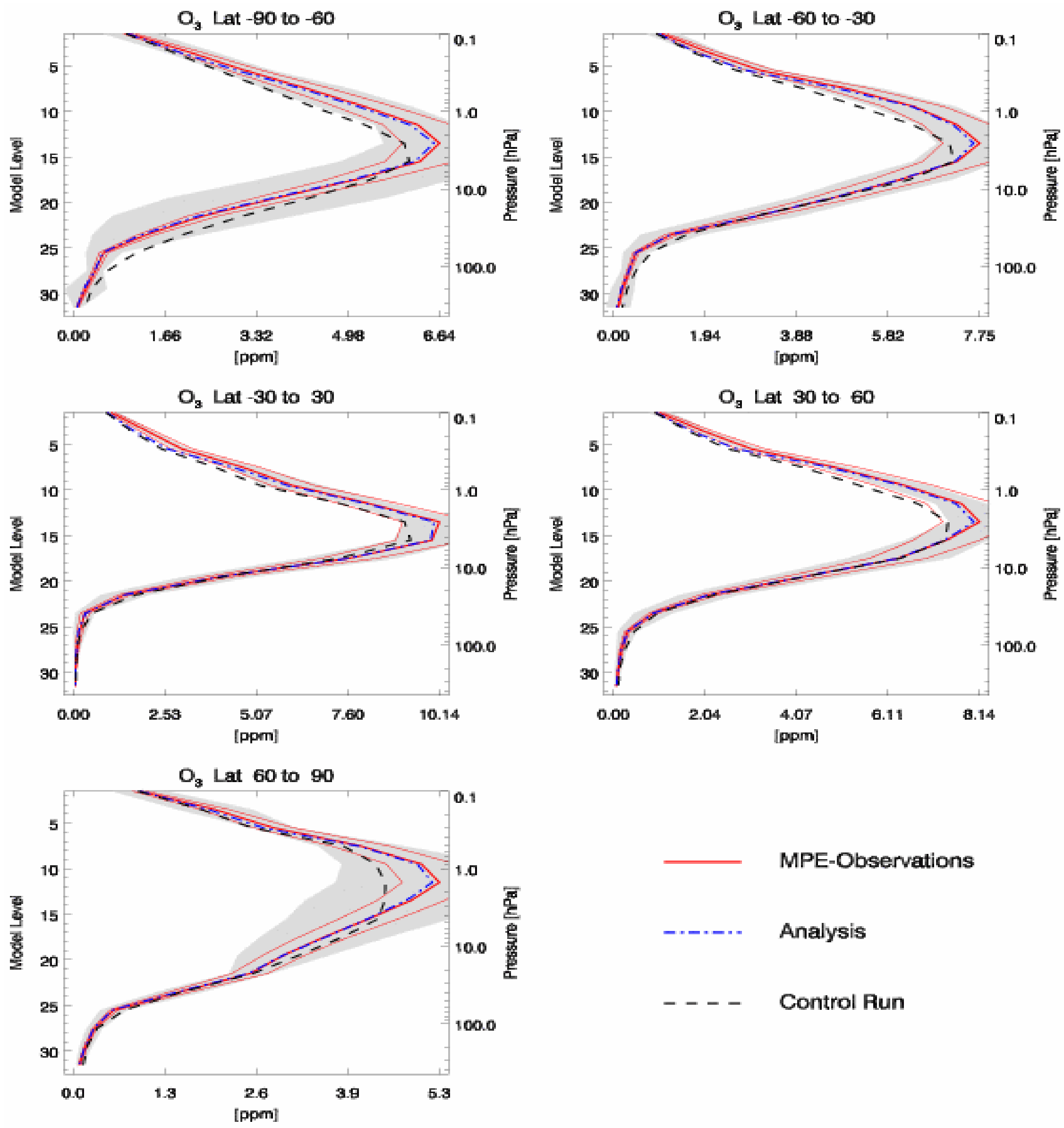



Control Run
(no assimilation)

MIPAS Observations

Analysis

Ozone profiles averaged over the latitude belts indicated and the time span 8.9.-15.10.2002



# Full global atmosphere: Data used in MACC NRT system

| Instrument | Satellite | Satellite operator | Data provider | Species | Status |
|---|---|---|---|---|---|
| **MODIS** | Terra | NASA | NASA/NOAA | Aerosol, fires | **Active** |
| **MODIS** | Aqua | NASA | NASA/NOAA | Aerosol, fires | **Active** |
| **SEVIRI** | Meteosat-9 | EUMETSAT | IM | Fires | **Active** |
| **Imager** | GOES-11, 12 | NOAA | NOAA | Fires | **Passive** |
| **Imager** | MTSAT-2 | JMA | JMA | Fires | Planned |
| **MLS** | Aura | NASA | NASA | $O_3$ | **Active** |
| **OMI** | Aura | NASA | NASA | $O_3$ | **Active** |
| **SBUV-2** | NOAA-16,19 | NOAA | NOAA | $O_3$ | **Active** |
| **SCIAMACHY** | Envisat | ESA | KNMI | $O_3$ | **Died** |
| **GOME-2** | Metop-A | EUMETSAT | DLR | $O_3$ | **Active** |
| **GOME-2** | Metop-B | EUMETSAT | DLR | $O_3$ | **Passive** |
| **IASI** | Metop-A | EUMETSAT | LATMOS/ULB | CO | **Active** |
| **IASI** | Metop-B | EUMETSAT | LATMOS/ULB | CO | **Passive** |
| **MOPITT** | Terra | NASA | NCAR | CO | **Active** |
| **GOME-2** | Metop-A | EUMETSAT | DLR | $NO_2$ | **Passive/Tests** |
| **GOME-2** | Metop-B | EUMETSAT | DLR | $NO_2$ | **Passive/Tests** |
| **OMI** | Aura | NASA | KNMI | $NO_2$ | **Active** |
| **OMI** | Aura | NASA | NASA | $SO_2$ | **Active** |
| **GOME-2** | Metop-A | EUMETSAT | DLR | $SO_2$ | **Passive/Tests** |
| **GOME-2** | Metop-A | EUMETSAT | DLR | $SO_2$ | **Passive/Tests** |
| **GOME-2** | Metop-B | EUMETSAT | DLR | HCHO | **Passive** |
| **Offline tests:** | | | | | |
| **IASI** | Metop-A | EUMETSAT | LATMOS/ULB | O3 | **Tests** |

**Courtesy: A. Benedetti, R. Engelen, J. Flemming, A. Inness, S. Massart, ECMWF, MACC**

# Setup for the reactive gases assimilation

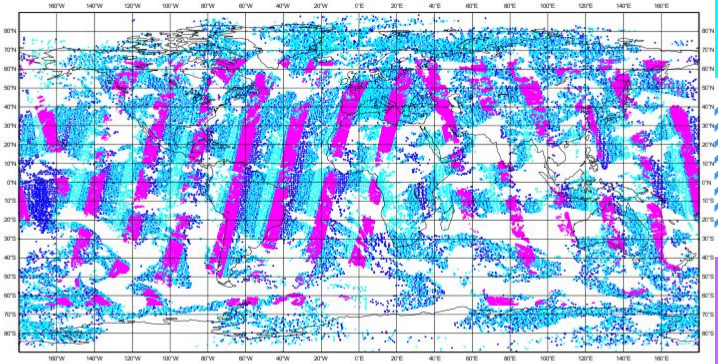
- IFS species: $O_3$, CO, $NO_2$, $SO_2$, HCHO
- More species available from CTM output (and in C-IFS)
- Coupled system or C-IFS
- Background errors calculated with:
  - NMC method (CO, NOx, HCHO)
  - Analysis ensemble method ($O_3$)
  - Prescribed profile ($SO_2$)
- Difficulties assimilating species with short lifetimes (e.g. $NO_2$): NOx as control variable and $NO_2$-NOx interconversion operator
- Variational bias correction used for reactive gases
- Chemistry included in outer loop (ifstraj) not in minimisation; adjoint of transport only



Courtesy: A. Benedetti, R. Engelen, J. Flemming, A. Inness, S. Massart, ECMWF, MACC

# Reactive gases data usage in MACC NRT system: 20130801, 12z

## CO

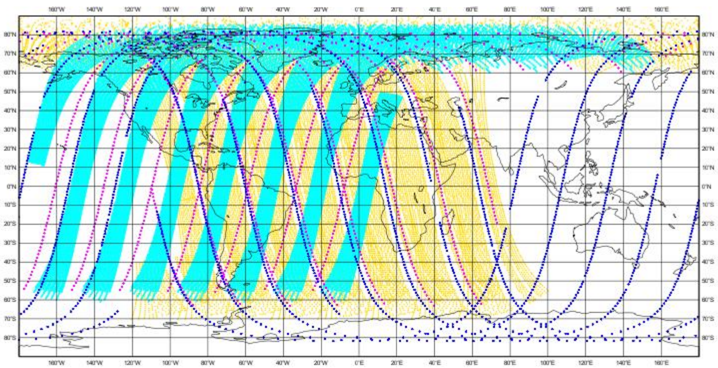


IASI Metop-A

IASI Metop-B

MOPITT TERRA

## O3



GOME-2 Metop-A

OMI AURA

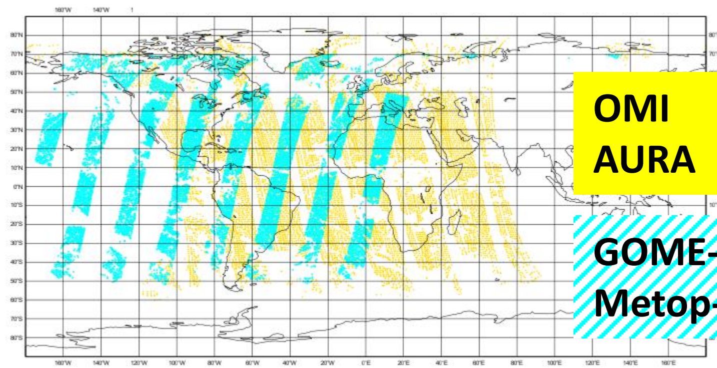
MLS AURA

SBUV/2 NOAA-16 NOAA-19

assimilated

monitored

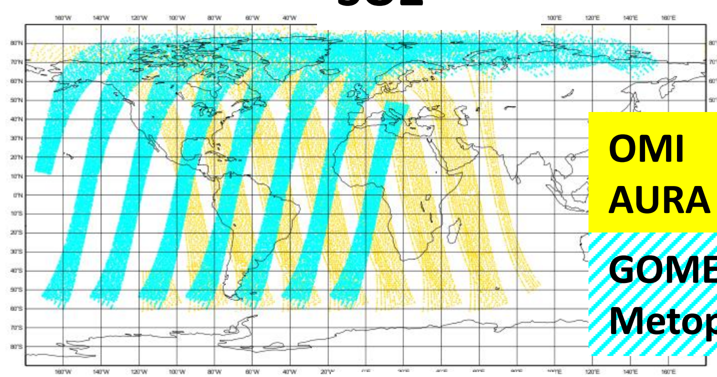
## Tropospheric NO2



OMI AURA

GOME-2 Metop-A

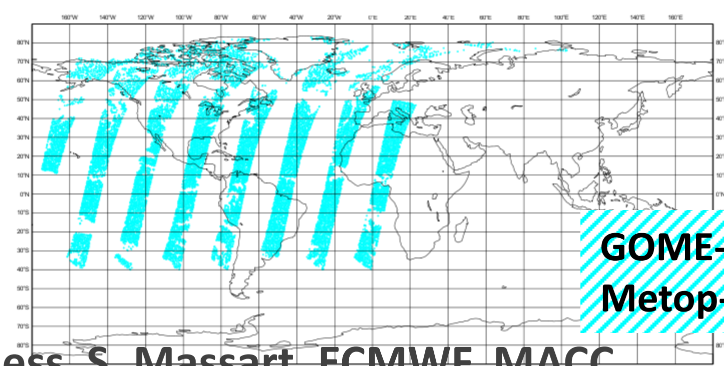
## SO2



OMI AURA

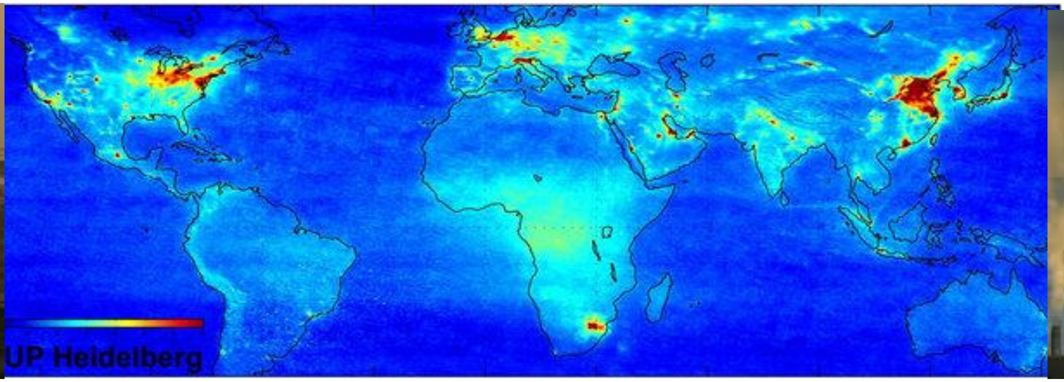
GOME-2 Metop-A

## HCHO



GOME-2 Metop-A

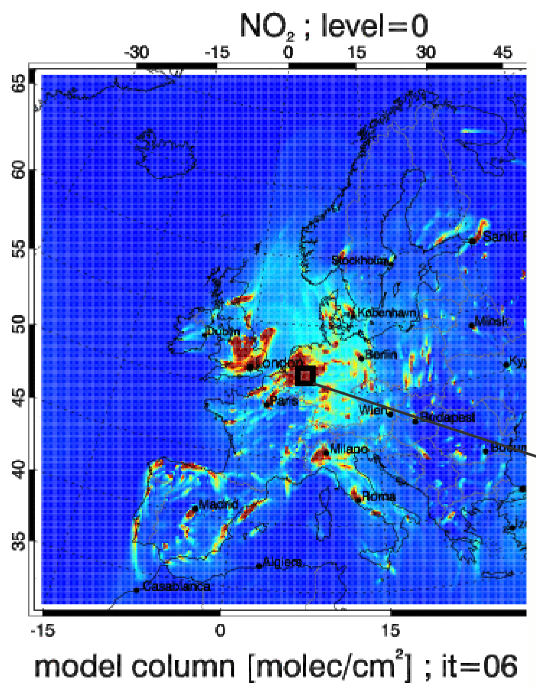
Courtesy: A. Benedetti, R. Engelen, J. Flemming, A. Inness, S. Massart, ECMWF, MACC

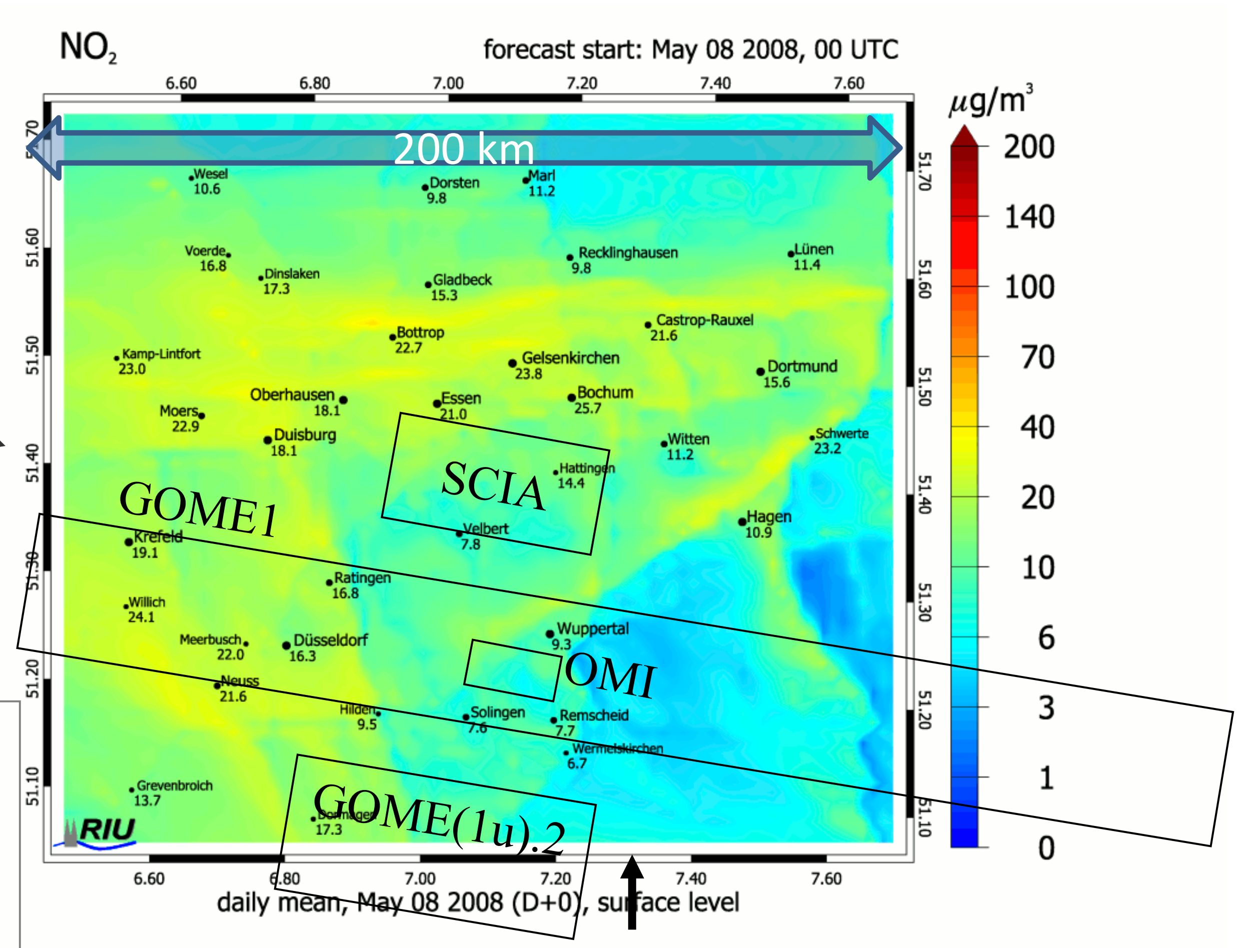



# 3. SATELLITE DATA ASSIMILATION FOR TROPOSPHERE AND AIR QUALITY

# NO2 tropospheric column satellite information:

ESA UV-VIS satellite footprints  Ruhr area comparison



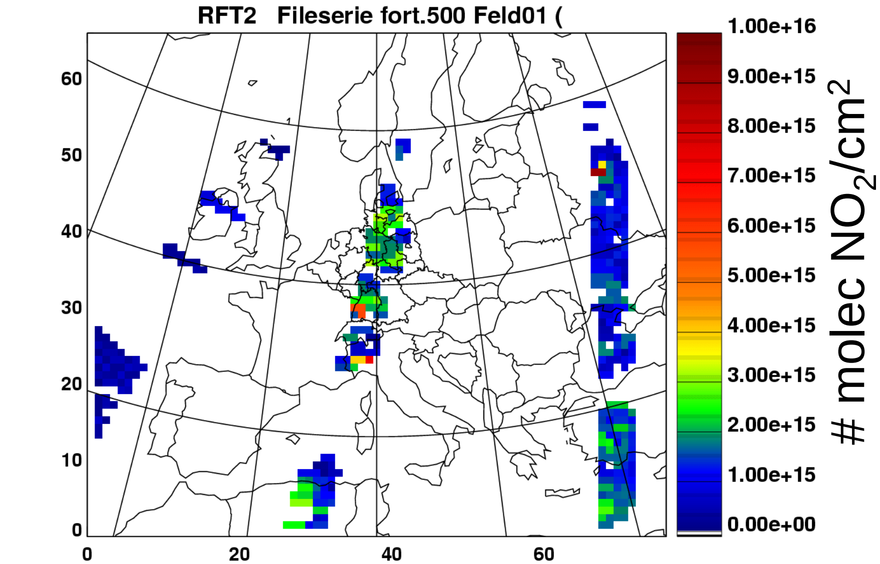




| nadir areas: | |
|---|---|
| GOME 1 | 320 x 40 $km^2$ |
| (special mode) | 80 x 40 “ |
| SCIAMACHY | 60 x 30 “ |
| GOME 2 | 80 x 40 “ |
| OMI | 24 x 13 “ |

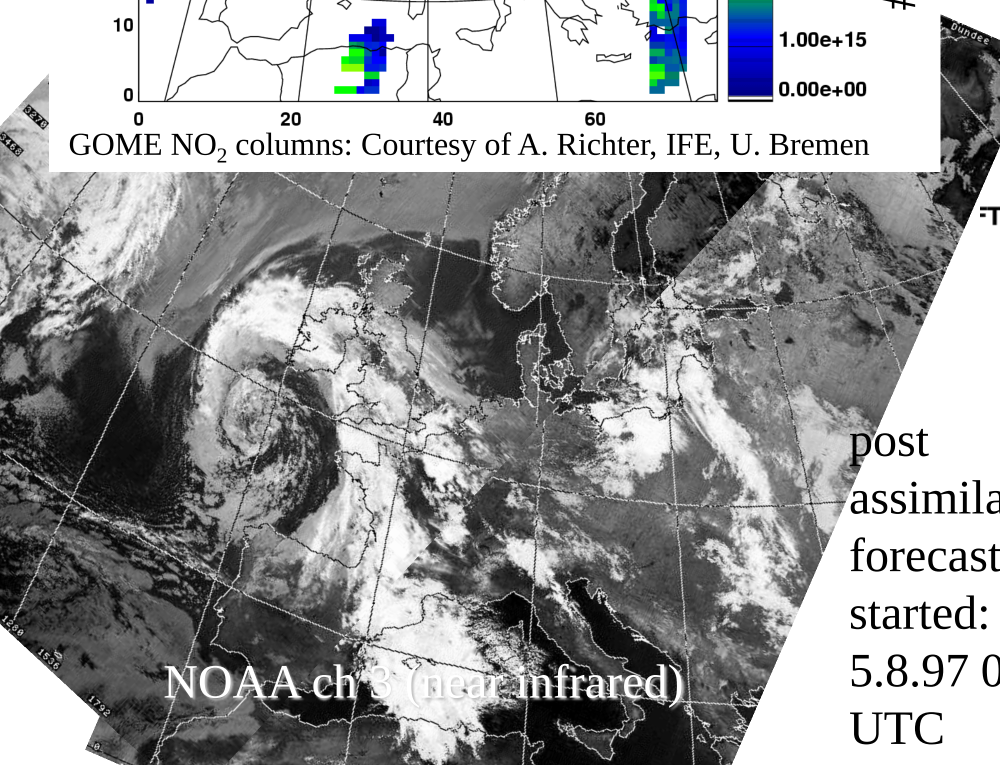
Ruhr area domain

(~12 000 000 inhabitants)

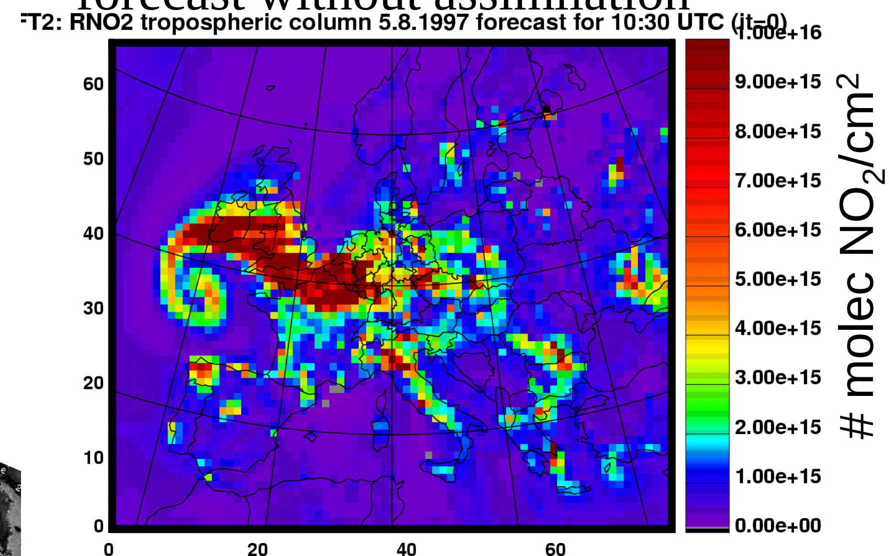
# Assimilation of GOME $NO_2$ tropospheric columns, 4Dvar with EURAD-IM



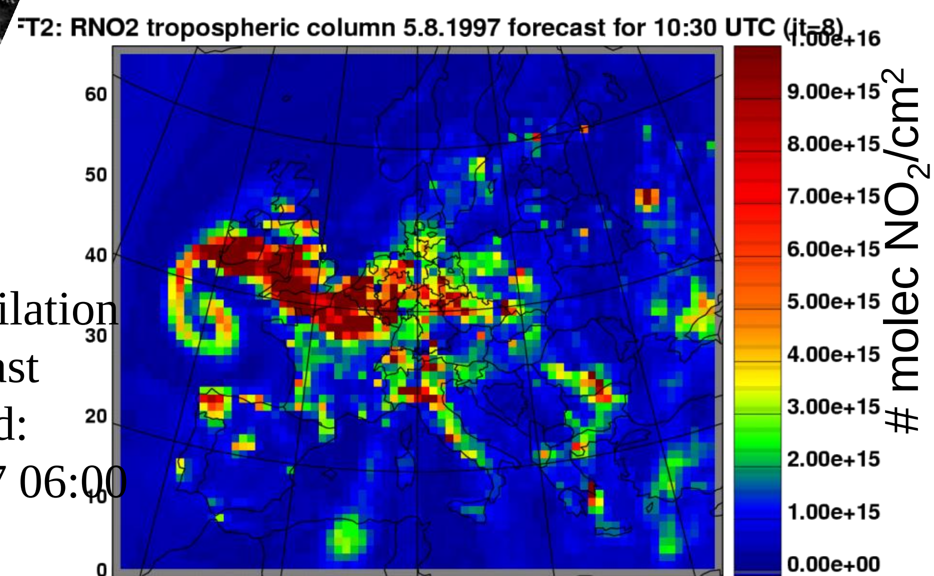

GOME $NO_2$ columns: Courtesy of A. Richter, IFE, U. Bremen




forecast without assimilation



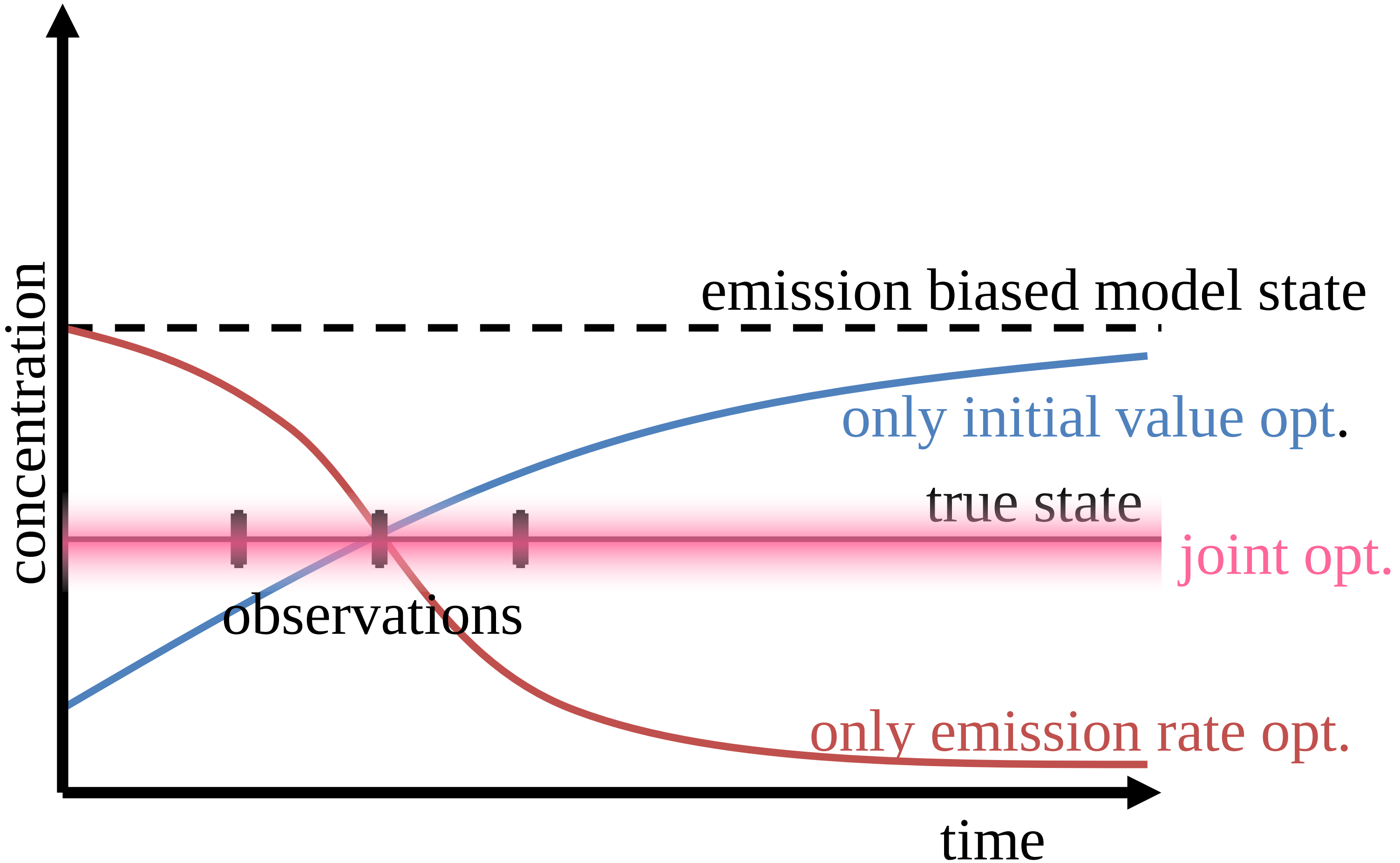

post assimilation forecast started: 5.8.97 06:00 UTC



## Question: Which parameter to be optimized?

Hypothesis:

initial state and emission rates are least known



# In the troposphere, for **emission rates,** the product (*paucity of knowledge*importance*) is high

Emission Rate Optimization

minimize cost function

$$J(\mathbf{x}(t_0),\mathbf{e}) = \frac{1}{2}(\mathbf{x}^b(t_0)-\mathbf{x}(t_0))^T\mathbf{B}_0^{-1}(\mathbf{x}^b(t_0)-\mathbf{x}(t_0)) +$$

deviations from background initial state

$$\frac{1}{2}\int_{t_0}^{t_N}(\mathbf{e}_b(t)-\mathbf{e}(t))^T\mathbf{K}^{-1}(\mathbf{e}_b(t)-\mathbf{e}(t))dt +$$

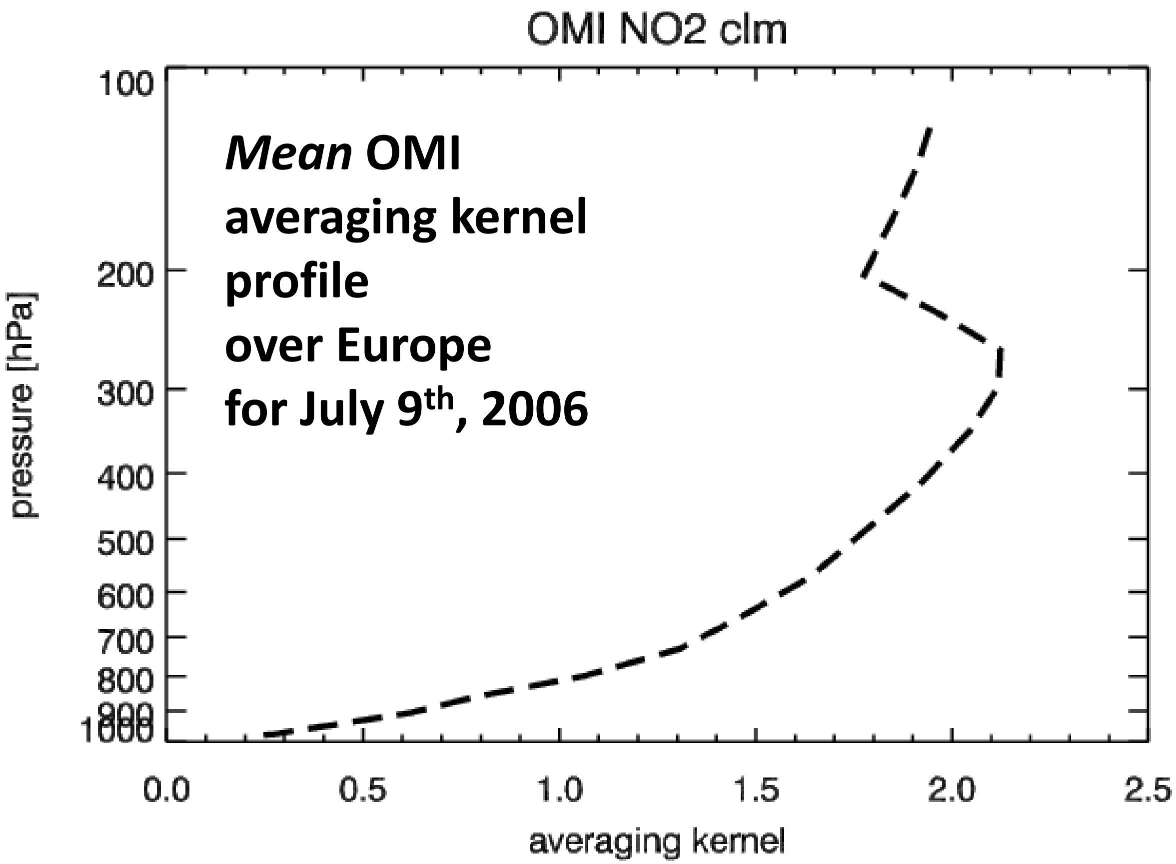
deviations from a priori emission rates

$$\frac{1}{2}\int_{t_0}^{t_N}\left(\mathbf{y}^0(t)-H[\mathbf{x}(t)]\right)^T\mathbf{R}^{-1}(\mathbf{y}^0(t)-H[\mathbf{x}(t)])dt$$

model deviations from observations

| | |
|---|---|
| $\mathbf{x}^b(t_0)$ | background state at $t=0$ |
| $\mathbf{x}(t)$ | model state at time t |
| $\mathbf{e}_b(t_0)$ | background emission rate at $t=0$ |
| $\mathbf{e}(t)$ | emission rate field at time t |
| $\mathbf{K}$ | emission rate error covariance matrix |
| $H[\ \ ]$ | forward interpolator |
| $\mathbf{y}^0(t)$ | observation at time t |
| $\mathbf{B}_0$ | background error covariance matrix |

# *UV-VIS retrievals:*
# *Assimilation by averaging kernels*




max. sensitivity of model domain mean averaging kernel **above boundary layer!**

**How can we still make best use of it?**

## How to proceed to obtain benefit from trop. column integral information?

(A typical problem of Inverse Modelling by Integral Equations)

Two more specific questions:

- When is it justified to project averaging kernel information to the surface?
- Can this be done without heuristics, destroying the BLUE property of the assimilation algorithm?

# Observation operator **H**

Formally an integral equation to be solved for vertical $NO_2$ molecule density function $x$ ($\sigma$ vertical coordinate)

$$y = \int_1^0 w(\sigma)x(\sigma)d\sigma$$

$$y = \sum^K h_k x_k$$

At the minimum $\mathbf{x} =: \mathbf{x}_a$

$$d\mathbf{x}_a := \mathbf{x}_a - \mathbf{x}_b = (\mathbf{B}_0^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}\mathbf{H}^T\mathbf{R}^{-1}\left\{\mathbf{y}^0 - H[\mathbf{x}_b]\right\}$$

$$= \mathbf{B}\mathbf{H}^T(\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^T)^{-1}\left\{\mathbf{y}^0 - H[\mathbf{x}_b]\right\}$$

For scalar column retrieval:

$$d\mathbf{x}_a^c = \underbrace{\mathbf{B}\mathbf{h}^T(r+b)^{-1}}\left\{y^0 - H[\mathbf{x}_b]\right\}$$

adjoint representer

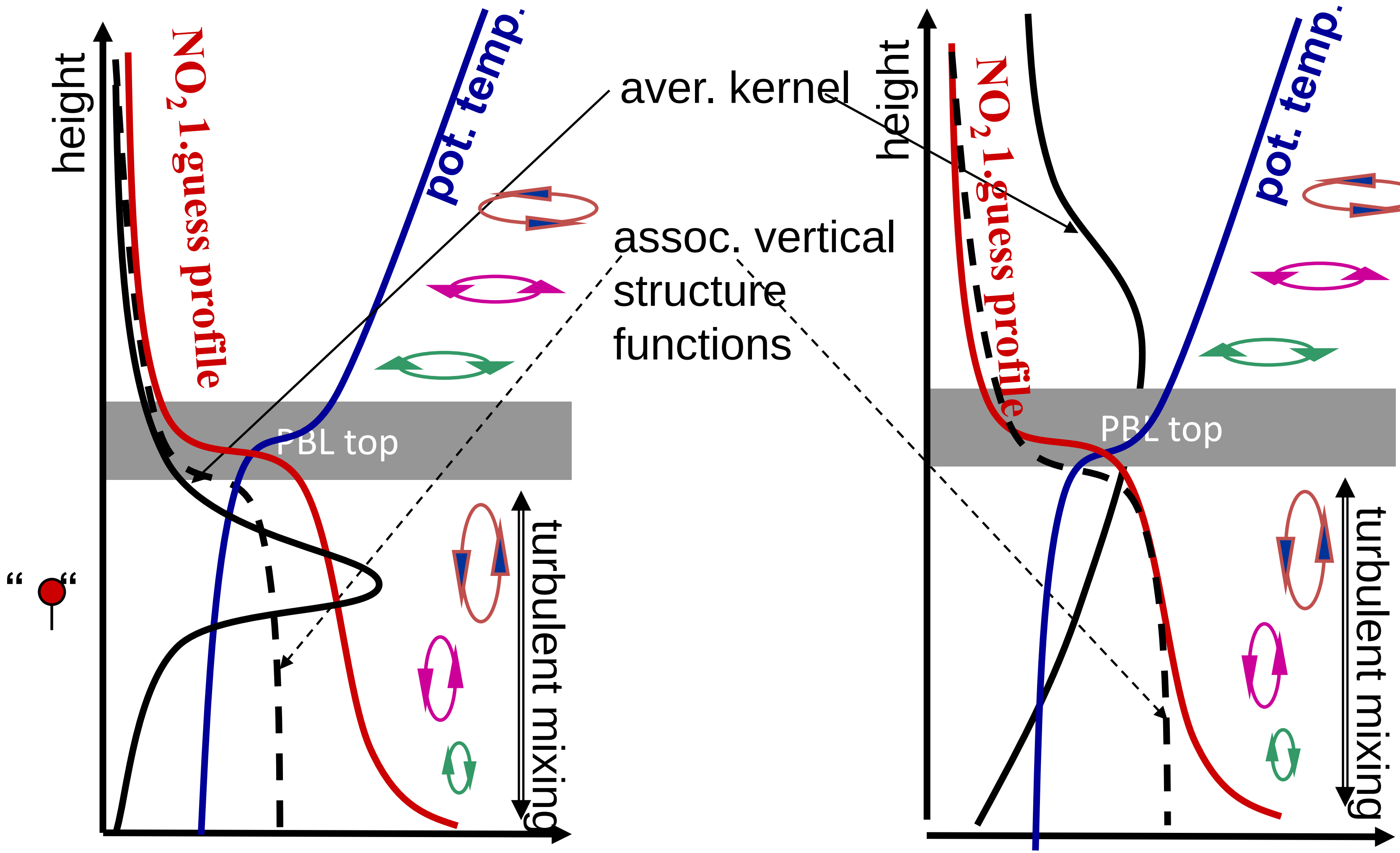
→ vertical structure function in B essential!

# 4. Focus: joint emission rate initial value optimisation

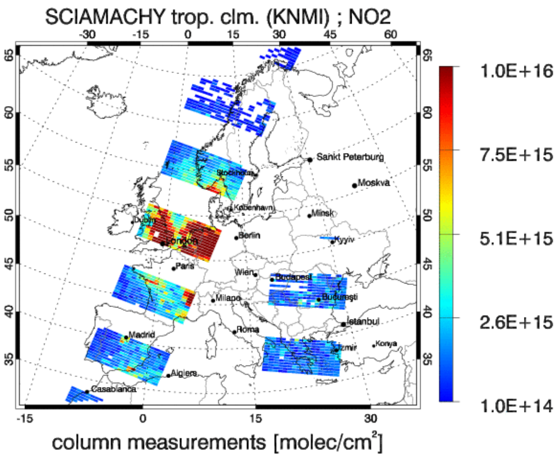
Vertical structure function:

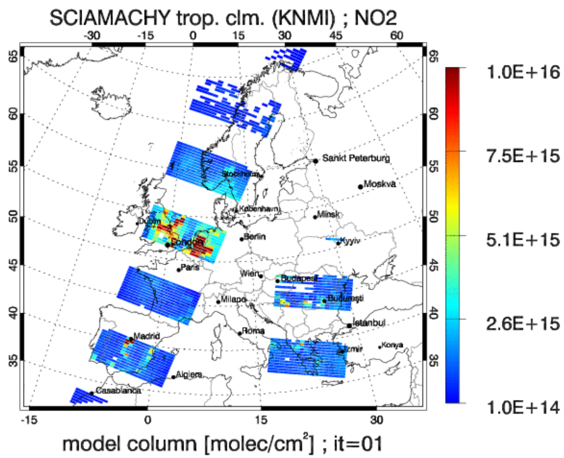
Extending the information from observation location by vertical exchange of polutants and information

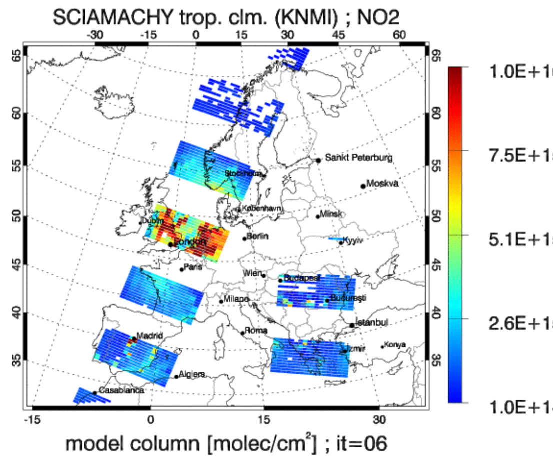
***ideal case real***



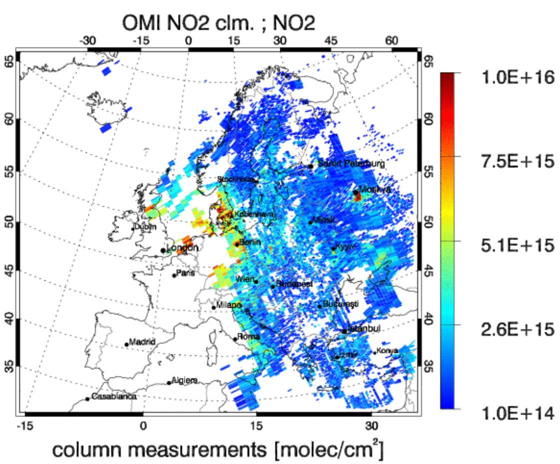
# Comparison of NO2 tropospheric columns in molecules/cm2 for July 6th, 2006, 09-12 UTC.

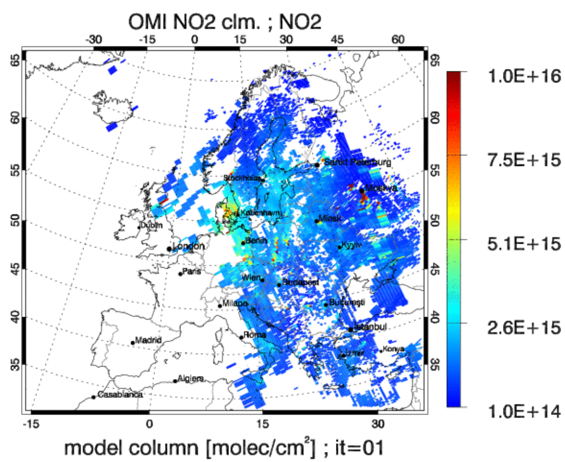


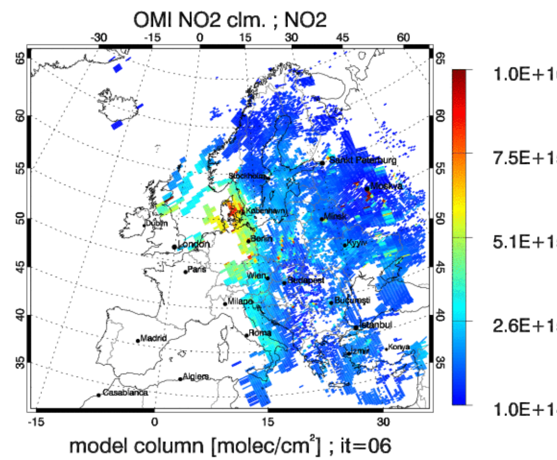



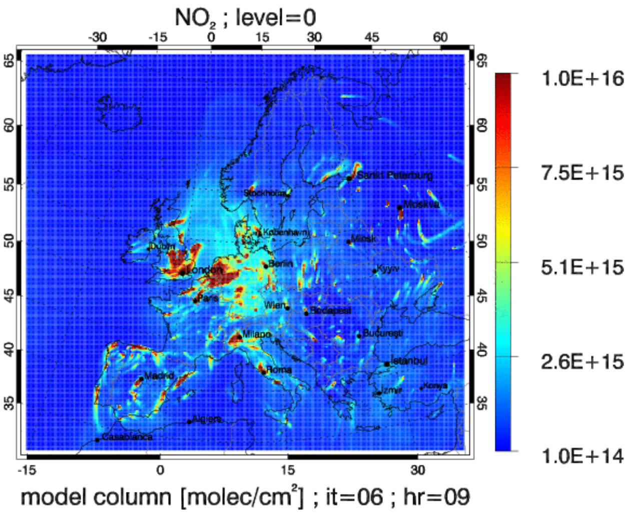

rerievals (**y**); :EURAD forecasted ($\mathbf{Hx}_b$); column analyses ($\mathbf{Hx}_a$).

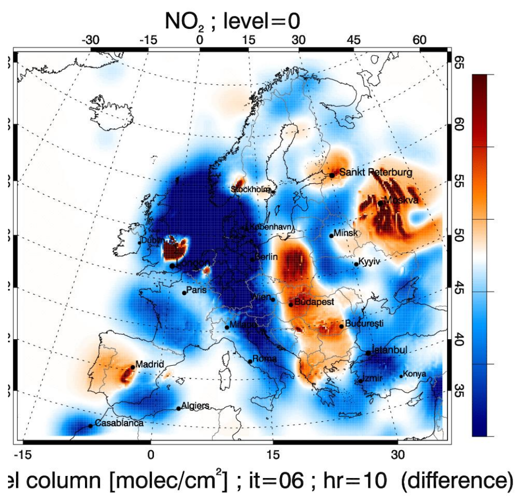


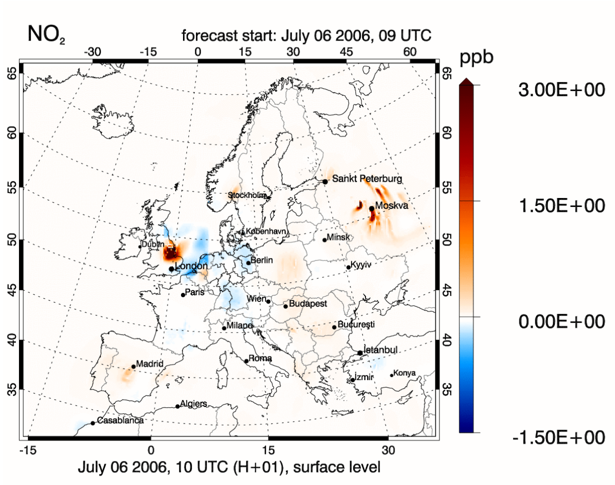



Data assimilation result in terms of tropospheric columns for July 6th, 2006. NO2 model columns based on OMI and SCIAMACHY assimilation within interval, 09-12 UTC.

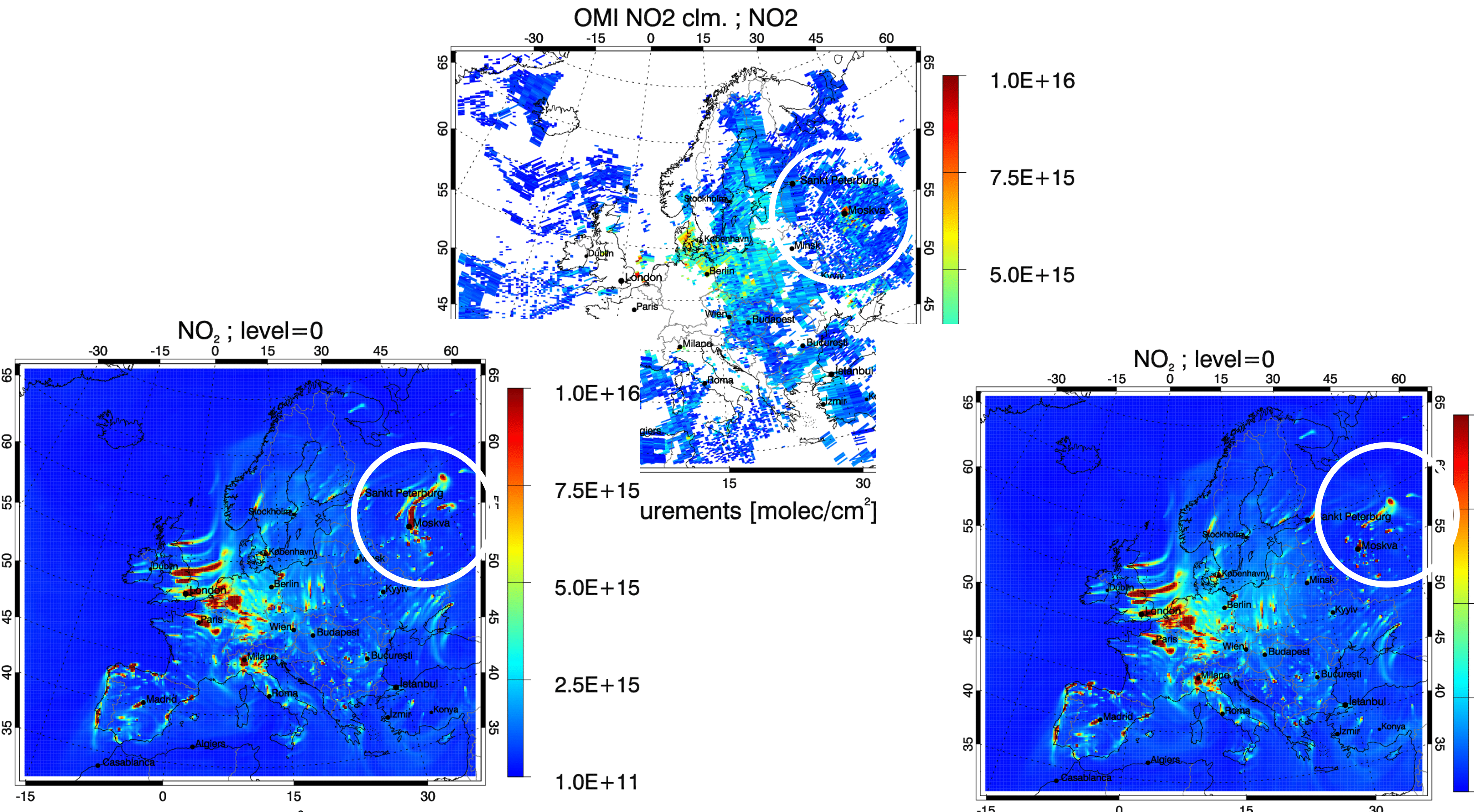


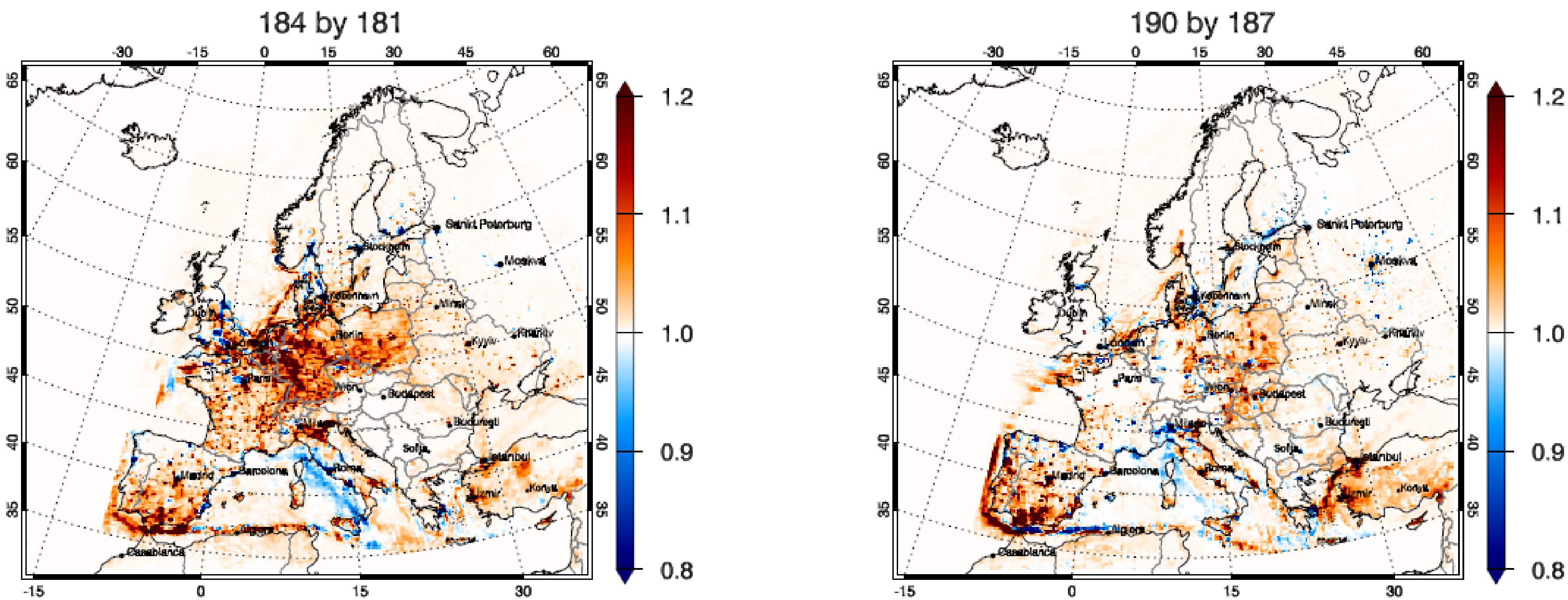

Difference field giving implied changes for tropospheric columns by assimilation (middle), and induced surface concentration changes by NO2 ppb (right)

Data assimilation result in terms of tropospheric columns for **July 7th**, 2006. NO2 model columns based on OMI  and SCIAMACHY assimilation within the assimilation interval, 09-12 UTC.



# Emission rate optimisation factors for NO2 after assimilation of

## OMI retrieved NO2 tropospheric columns



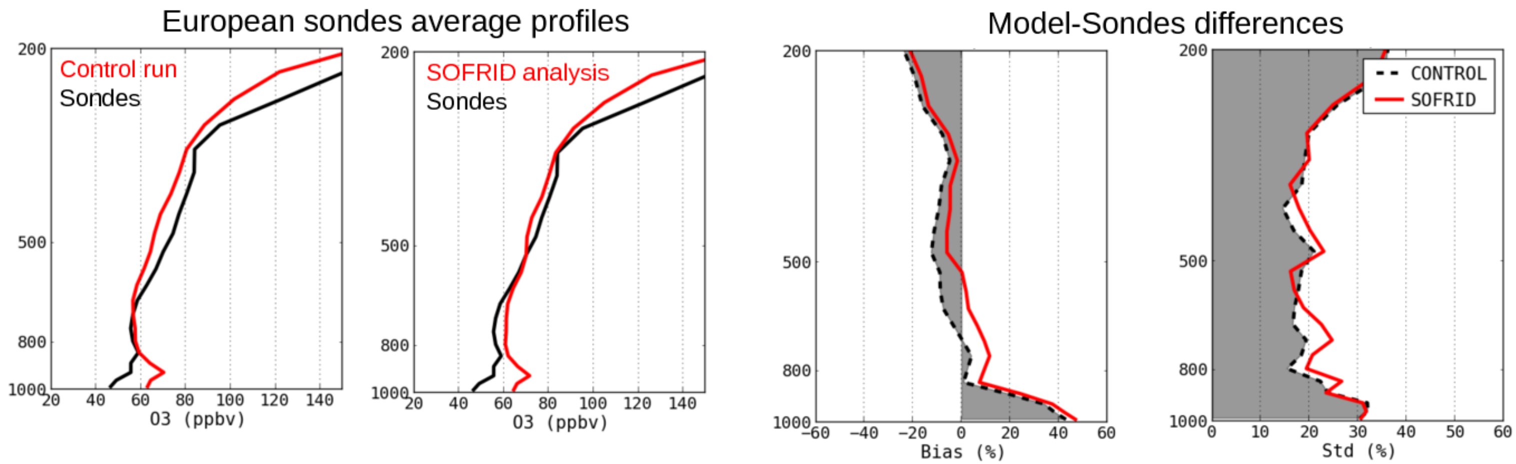

2 x 4 days assimilation sequence. Left panel shows results after assimilation procedures from July 1.-4. 2006, right panel for July 7.-11., 2006. OMI data from KNMI

# IASI SOFRID $O_3$ re-analysis (CERFACS)

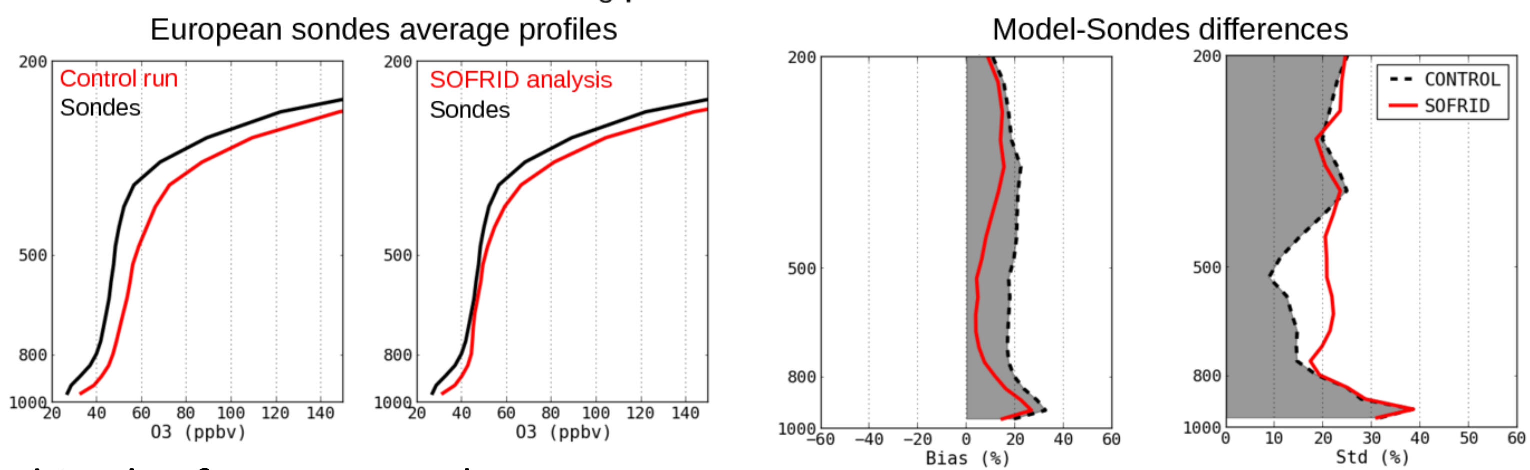
Validation of IASI analysis with ozonesonde data:

BIAS = model minus observations

$O_3$ profiles in July 2010:



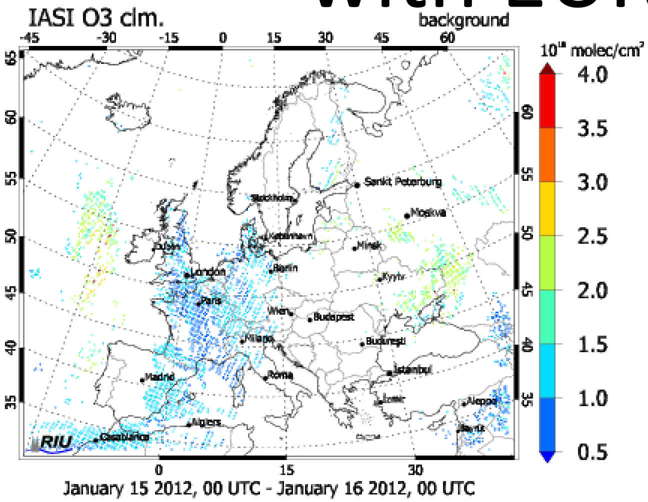

$O_3$ profiles in Jan 2012:

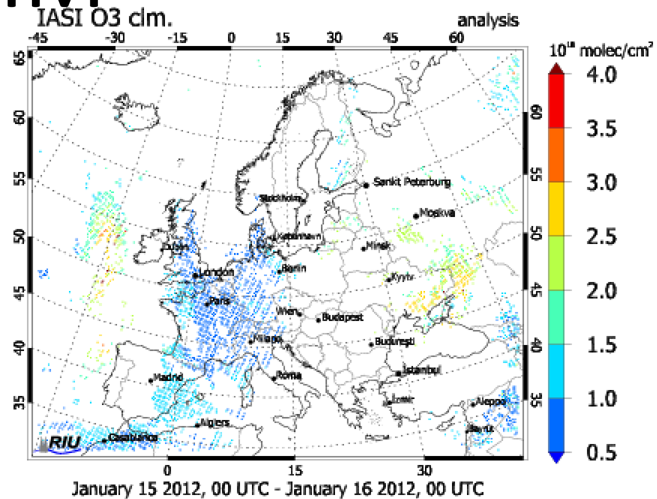


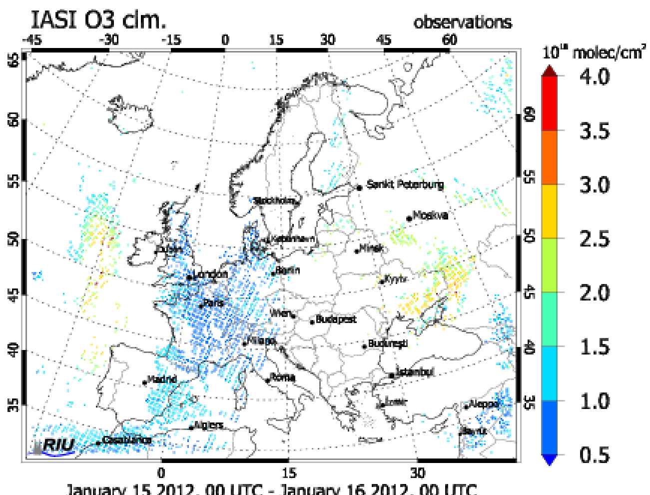

- Bias reduced in the free troposphere
- Surface ozone impact is minor
- MOZAIC-IAGOS as additional validation? (only 2012 available)

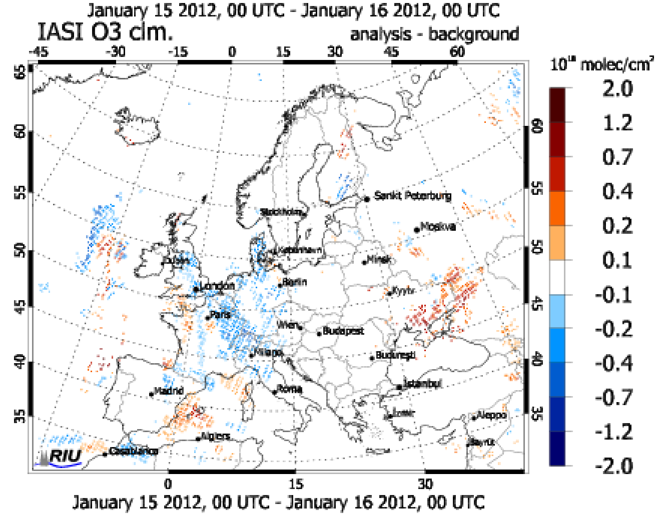
Courtesy: E. Emili, CERFACS

# IASI partial Ozone column assimilation with EURAD-IM

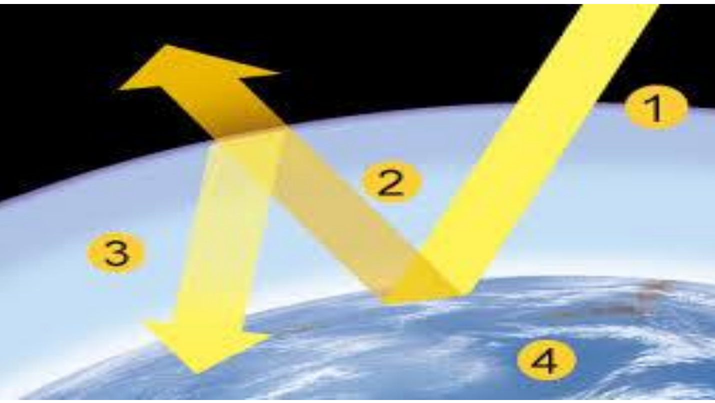



*IASI partial Ozone columns above 800 mb for January 15, 2012 interpolated on the EURAD-IM grid with 15 km resolution.*





# GREENHOUSE GAS INVERSION

# $CO_2$ satellite inversion

- small signals relative to large background values enforce accuracy requirements at the limits of today‘s space borne spectroscopy
- preferred assimilation method is 4D-var for source/sink inversion

# Satellite data types and status resumé

- thermal infra-red spectral domain, with a peak sensitivity in the middle troposphere
  - **AIRS, IASI, TES, GOSAT-TANSO**
- solar infra-red domain  with a more uniform sensitivity to GHGs throughout the atmospheric column, including the boundary layer.
  - **SCIAMACHY, GOSAT-TANSO, OCO-2**
- of both measurement types in the 12-hour 4D-Var useful,
- but: systematic errors caused by **uncertainties in the spectroscopy** or by **aliasing with other atmospheric signa**ls like aerosols
- **the inversion of CO2 surface fluxes from satellite retrievals up to now hampered**.

(from F. Chevallier, MACC report 2014)

# GOSAT observations
# Characteristics and error estimates

(example from Chevallier et al., 2010)

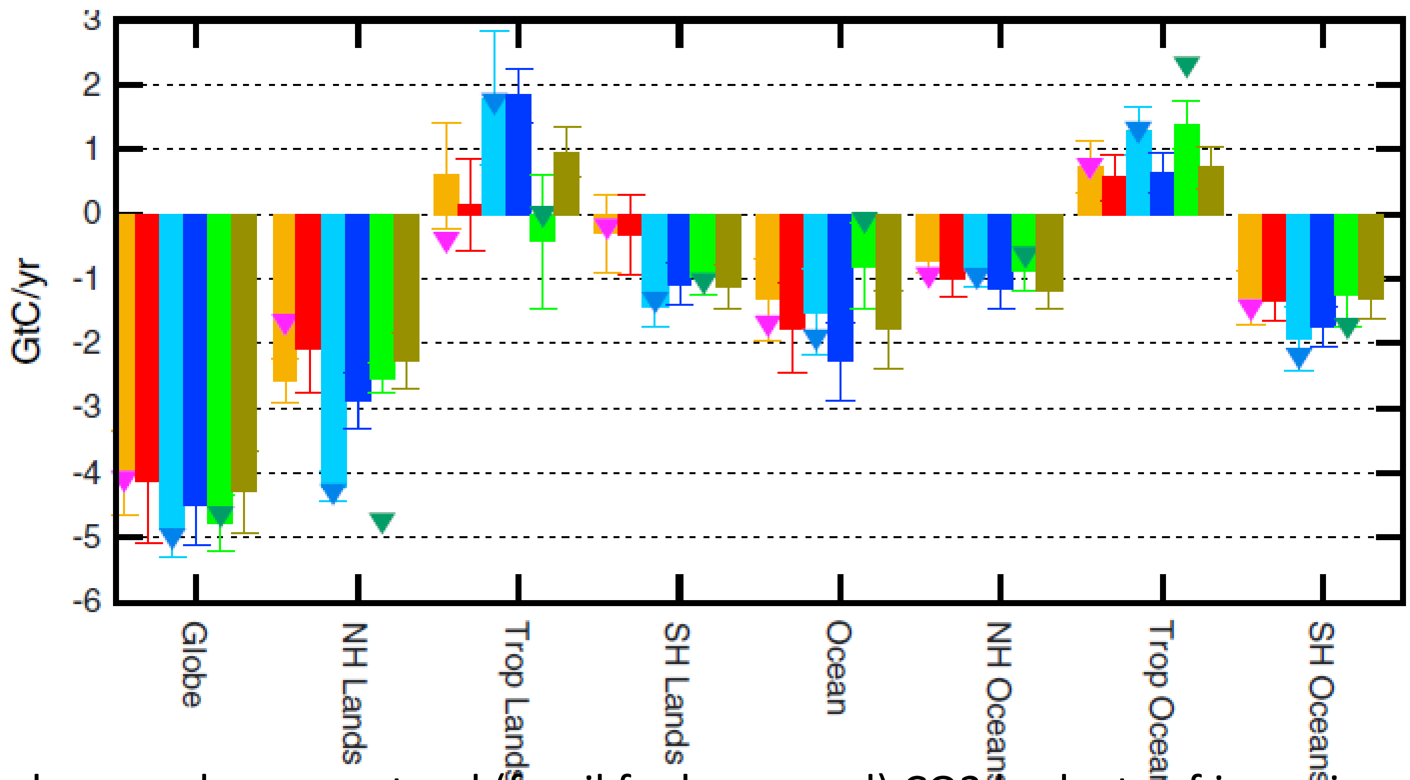
**Features**

- sun-synchronous GOSAT radiation data in the near infrared
- 12-level averaging kernels for XCO2 retrieval
- simultaneous fit to 2 CO2 bands (1.61, 2.06 mm) and O2-A Band (0.765 mm)
- quality check results in ~300,000 soundings/a (~1/20 of total)

**error budget**

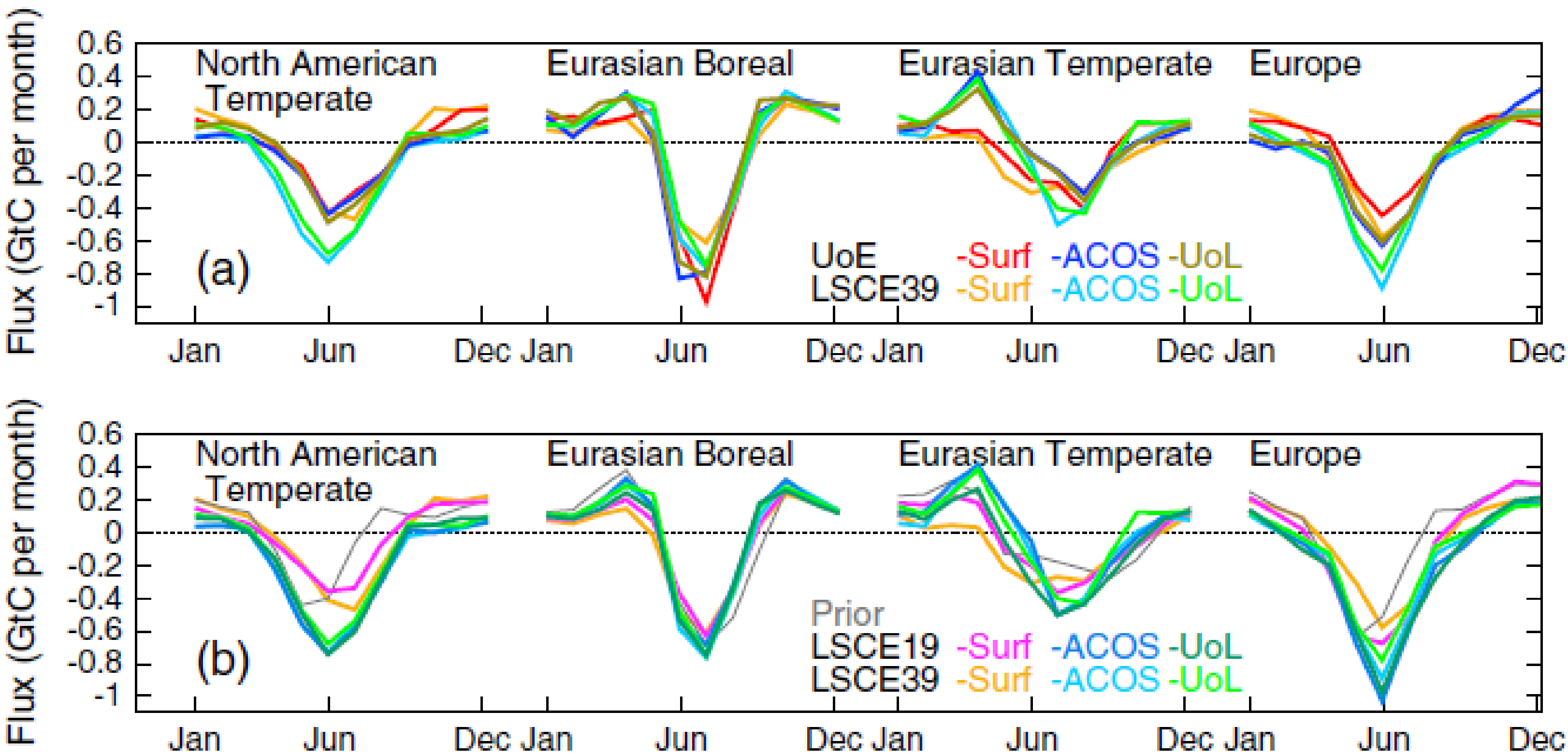
- retrieval error scene-specific
- 1 ppm to errors associated with the radiation model, representativity, and transport model →
- **1.8 - 7.2 ppm total error,** needed are < 0.5 ppm

# Fluxes derived from GOSAT XCO2 backscattered sunlight at short-wave IR for 2010




Large-scale annual mean natural (fossil fuel removed) CO2 budgets of inversions
Comparison of the UoE (Kalman F. University of Edinburgh )
LSCE-39 (variational ,Laboratoire des Sciences du Climat et de l'Environnement )
ACOS (Bayesian; NASA), UoL (Bayesian; Univ. of Leicester) results.

# Differences

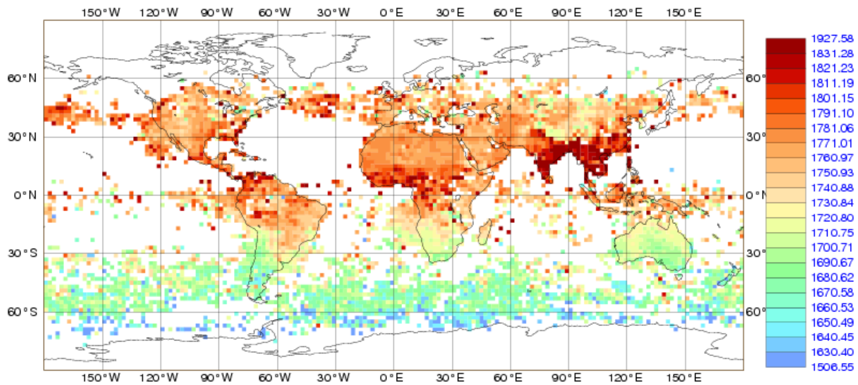



**Chevallier et al, 2014**

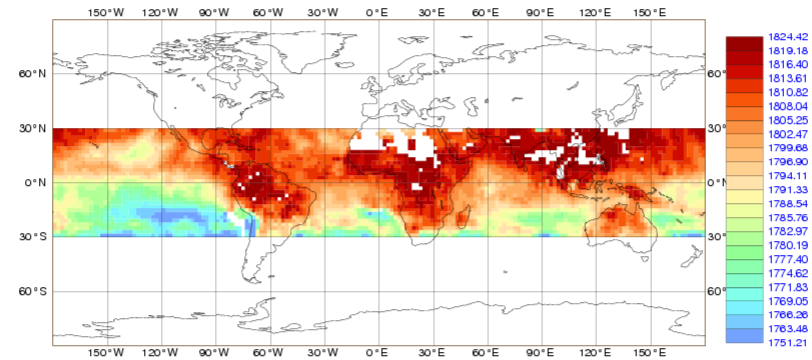
Regional seasonal CO2 flux estimates 2010
Comparison of the UoE (Kalman F. University of Edinburgh )
LSCE-39 (variational ,Laboratoire des Sciences du Climat et de l'Environnement )
ACOS (Bayesian; NASA), UoL (Bayesian; Univ. of Leicester) results.
(b) Comparison of the LSCE-19 results, the LSCE-39 results, and the LSCE prior fluxes.

# ECMWF-MACC: Assimilated GHG satellite data

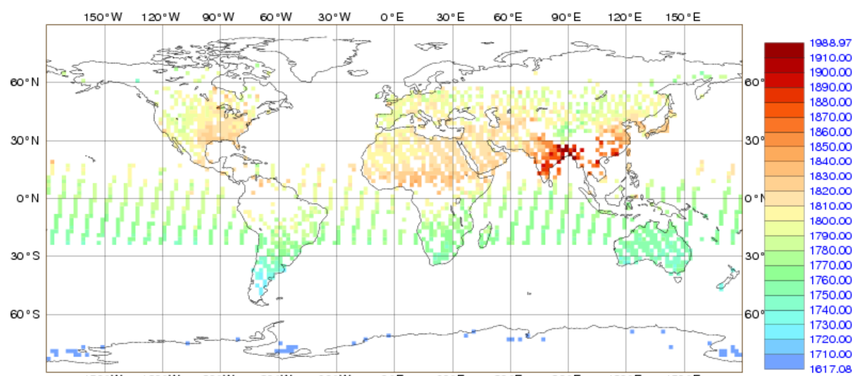
ENVISAT/SCIAMACHY
CH4 and CO2 – Lower tropo.




METOP-A/IASI
CH4 and CO2 – Middle tropo.




GOSAT/TANSO
CH4 and CO2 – Lower tropo.




*Monthly averages of the observed XCH4 for October 2011*

Column-averaged dry-air mole fractions of CO2 and CH4 provided by:

SRON Netherlands Institute for Space Research

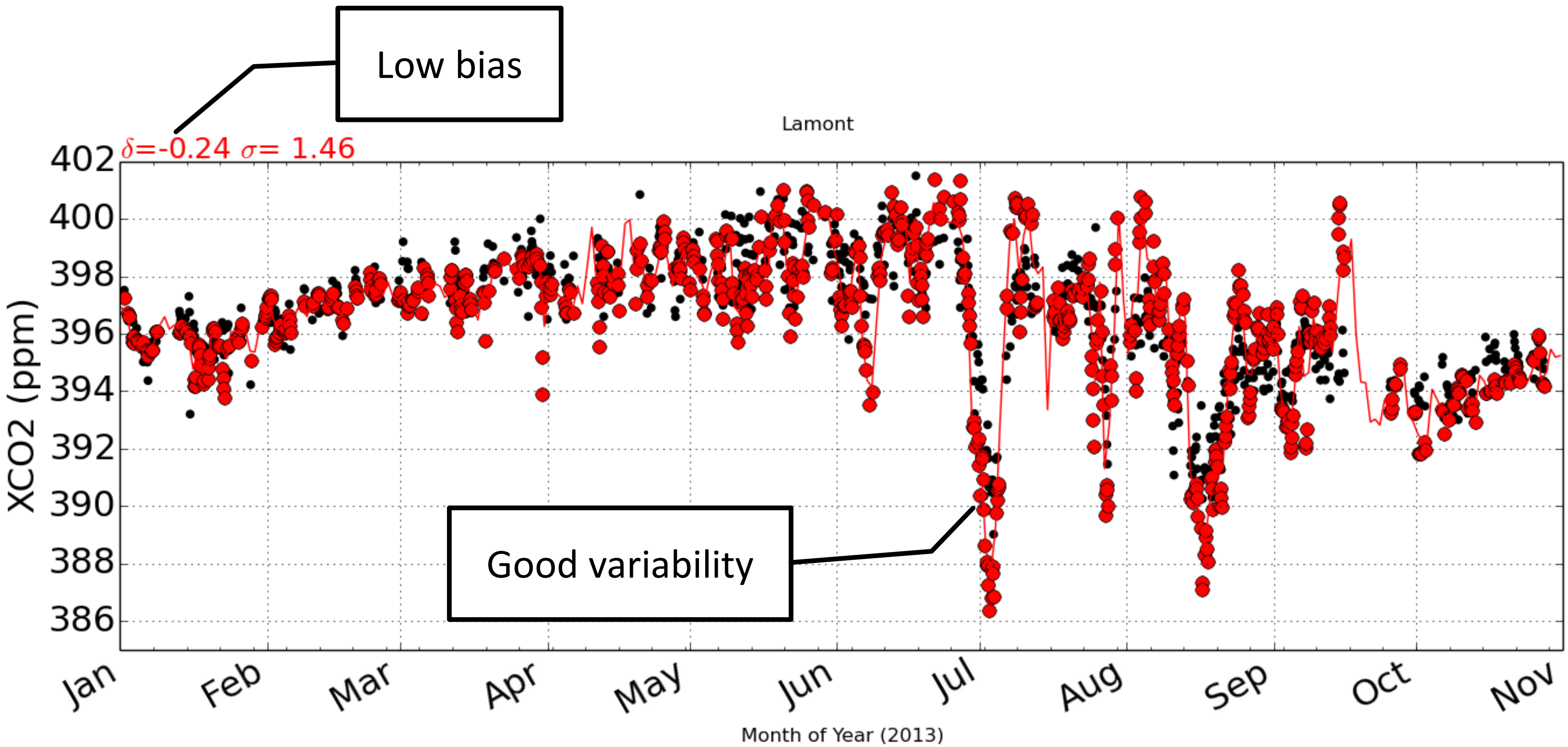
LMD

Universität Bremen

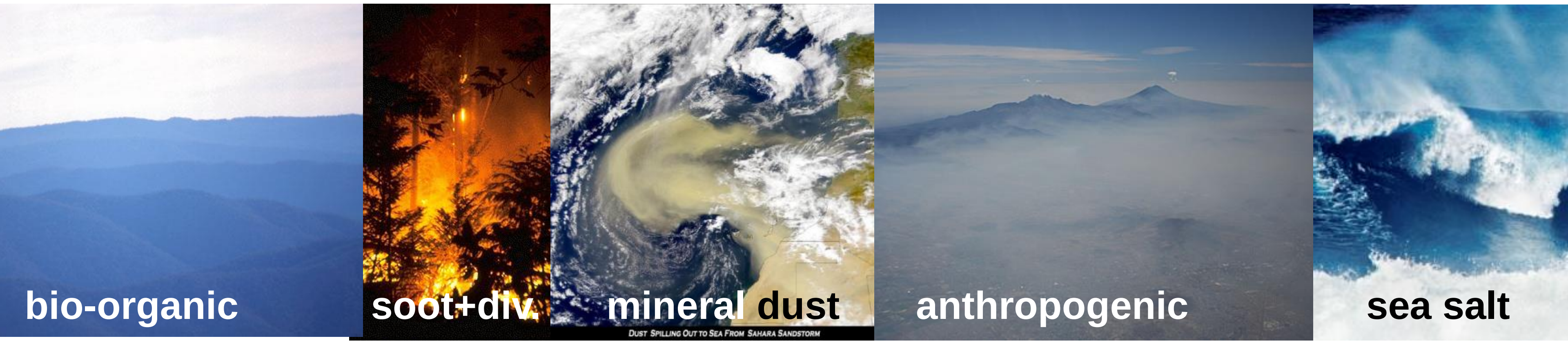
Tests with AIRS and IASI radiances for CO2

**Courtesy S. Massart@ECMWF**

# Zoom over 2013



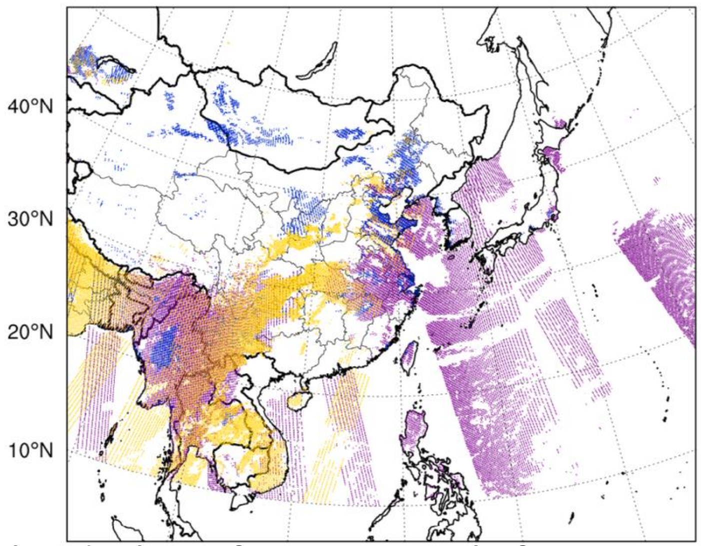

**Courtesy S. Massart@ECMWF**




# SATELLITE AEROSOL DATA ASSIMILATION

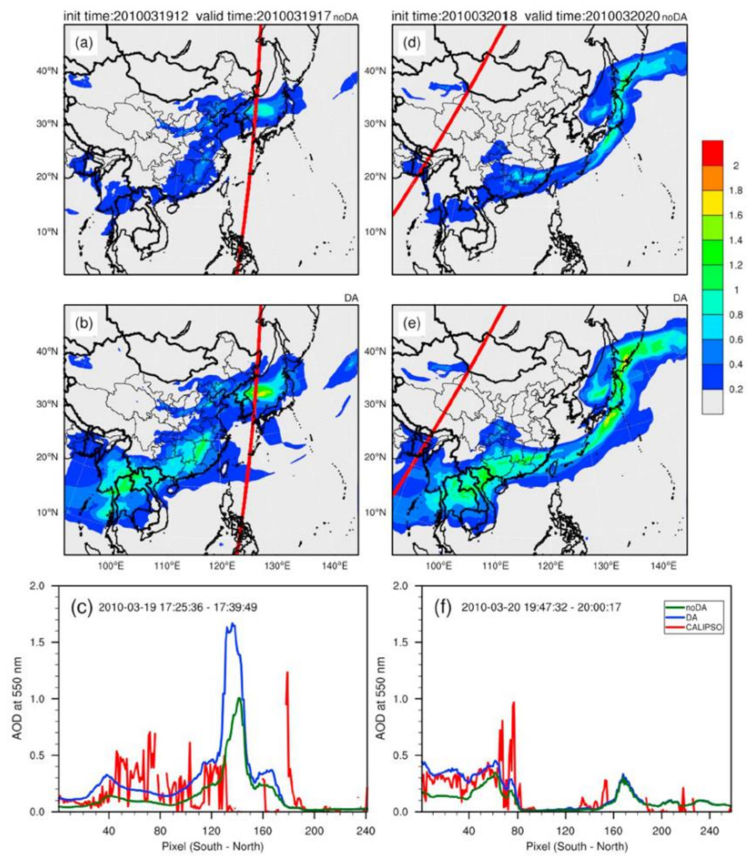
# Three-dimensional variational Assimilation of MODIS aerosol optical depth:

(MODIS) AOD coverage from
the Aqua and Terra
at 06:00 UTC 21 March 2010.




Purple: dark surface retrievals from Aqua;
gold: dark surface Terra;
blue: deep blue produced from Aqua.

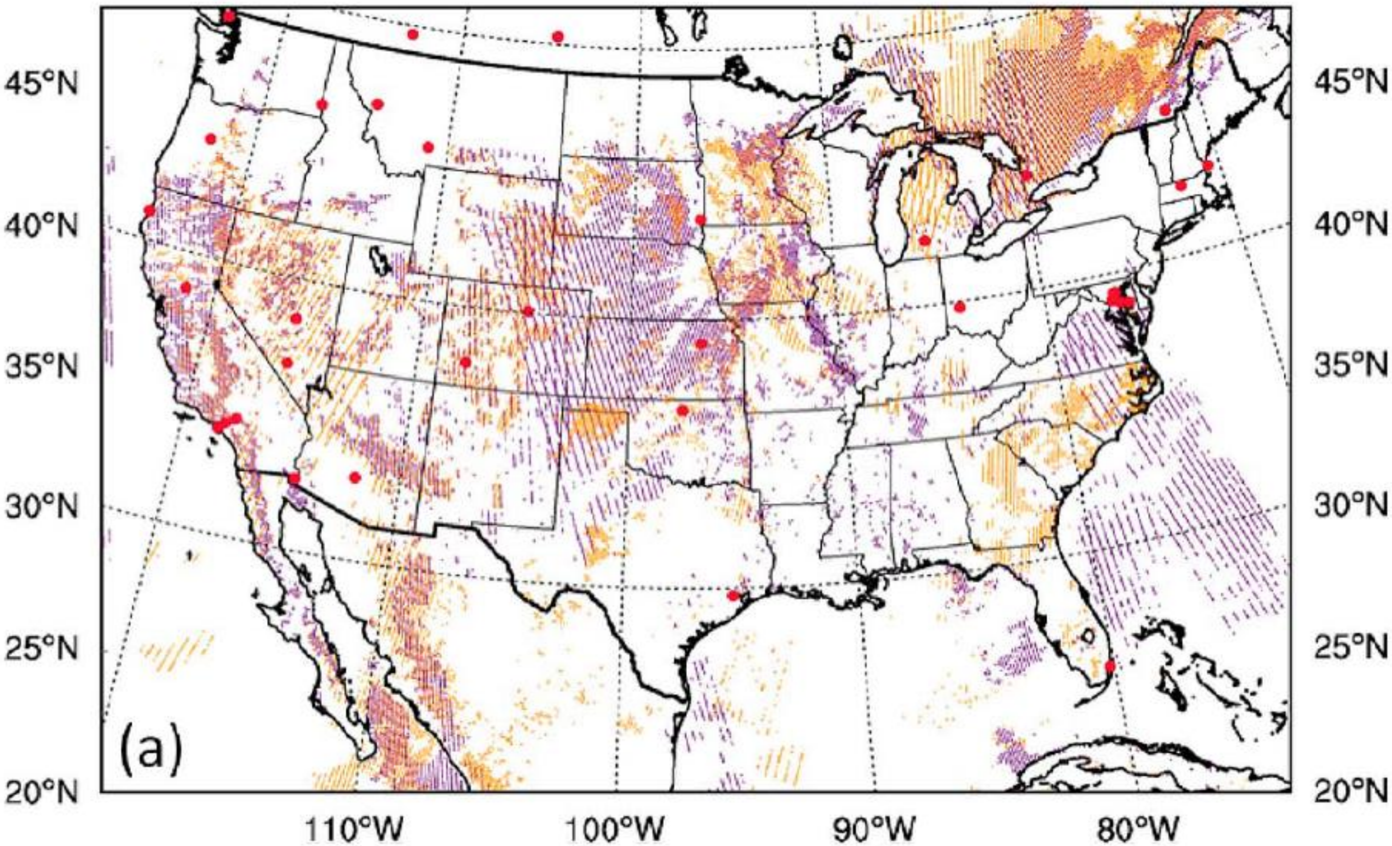
Validation with CALIPSO.

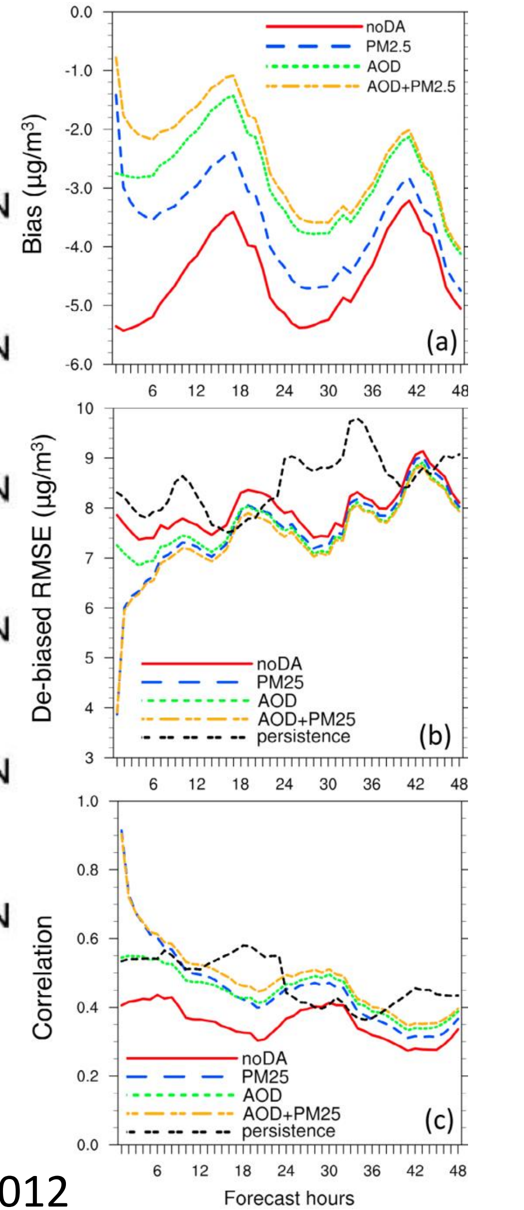



alongtrack assimilation control

**Zhiquan Liu, Quanhua Liu, Hui-Chuan Lin,1Craig S. Schwartz, Yen-Huei Lee, and Tijian Wang, 2011**

# MODIS AOD assimilation




Craig S. Schwartz, Zhiquan Liu,Hui-Chuan Lin, and Stuart A. McKeen, 2012

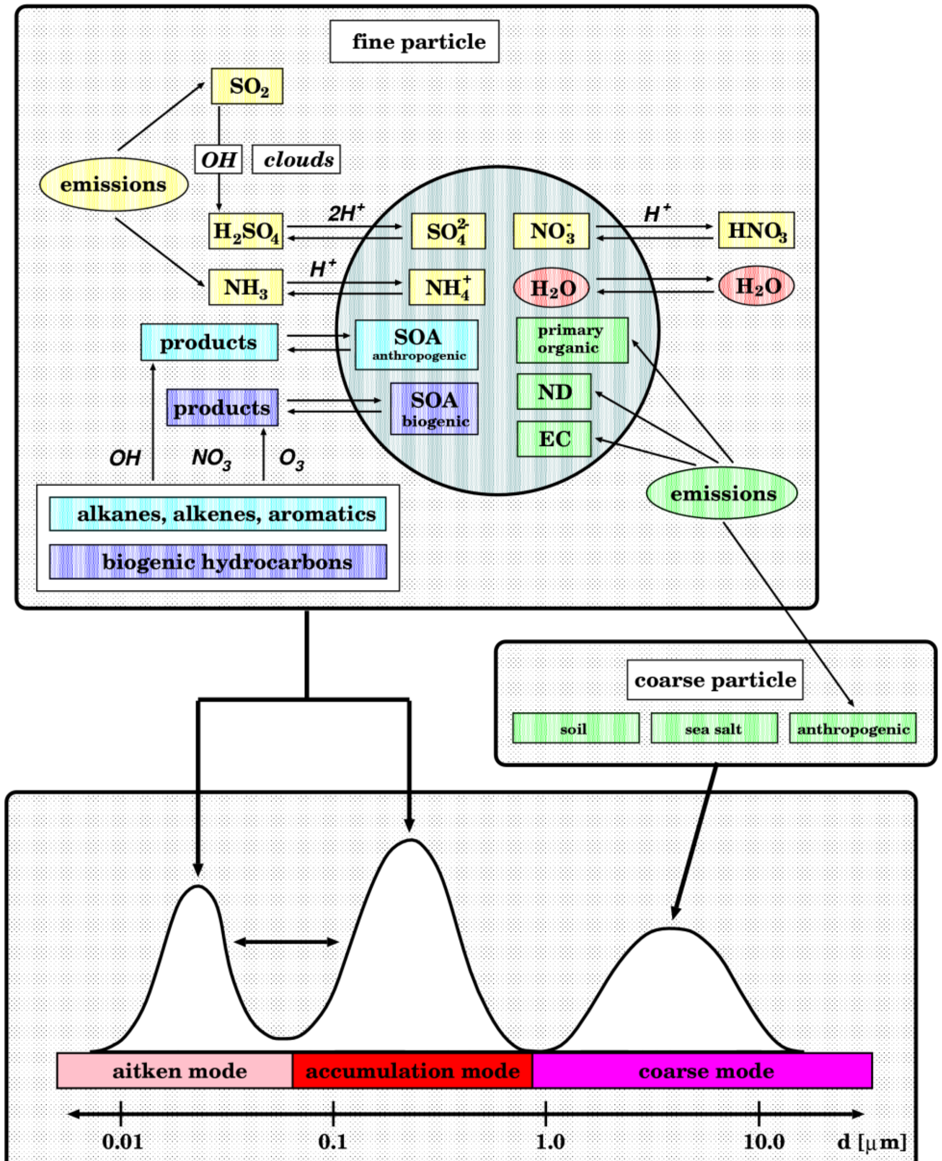
# Can we bridge from optical to chemical information?

Example:
Aerosol Chemistry in
**MADE**
**M**odal **A**erosol **D**ynamics for
**E**URAD/**E**urope
(Ackermann et al., 1998,
Schell 2000)

$$dM_i^k/dt = nuk_i^k + coag_{ii}^k + coag_{ij}^k + cond_i^k + emi_i^k$$

$M_i^k$:= $k^{th}$ Moment of $i^{th}$ Mode

assimilation of aerosol
By satelite retrievals: e.g.
MERIS MODIS
**AATSR+SCIAMACHY**,...



# Assimilation of Aerosol observations

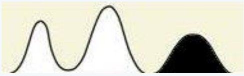
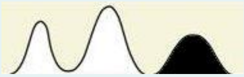
- In situ:

  EEA Airbase: Database of groundstations of EU member countries & states:
  - 450 stations for $PM_{10}$ (2003)
  - No $PM_{2.5}$. (4 stations in UK only)
- Satellite measurements:

  SYNAER (SYNergetic AErosol Retrieval, DLR-DFD, [Holzer-Popp, 2001])*
  - combines GOME&ATSR-2, SCIAMACHY&AATSR measurements aboard ERS-2/ENVISAT
  - ATSR-2/AATSR:
    dark field detection, BLAOT (Boundary Layer Aerosol Optical Thickness) and albedo are calculated
  - GOME/SCIAMACHY:
    Provides $PM_{0.5}$, $PM_{2.5}$ and $PM_{10}$ columns and its composition (6 intrinsic species)

# SYNAER retrieval algorithm

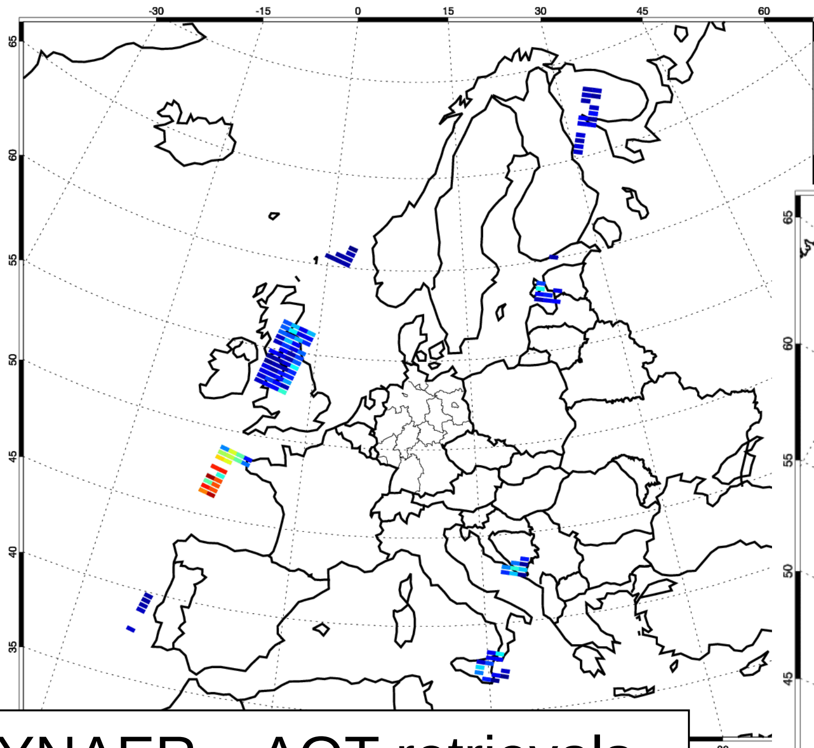
## Species Mapping

| EURAD-IM [µg/m³] | SYNAER - AOT |
|---|---|
| $SO_4$, $NH_3$, $NO_3$, $H_2O$, SOA  | WASO (WAter SOluble) |
| Unidentified PM  | INSO (water INSOluble) |
| Elemental Carbon  | SOOT |
| Sea Salt  | SEAS |
| Mineral Dust  | DUST |

radiative transfer model →

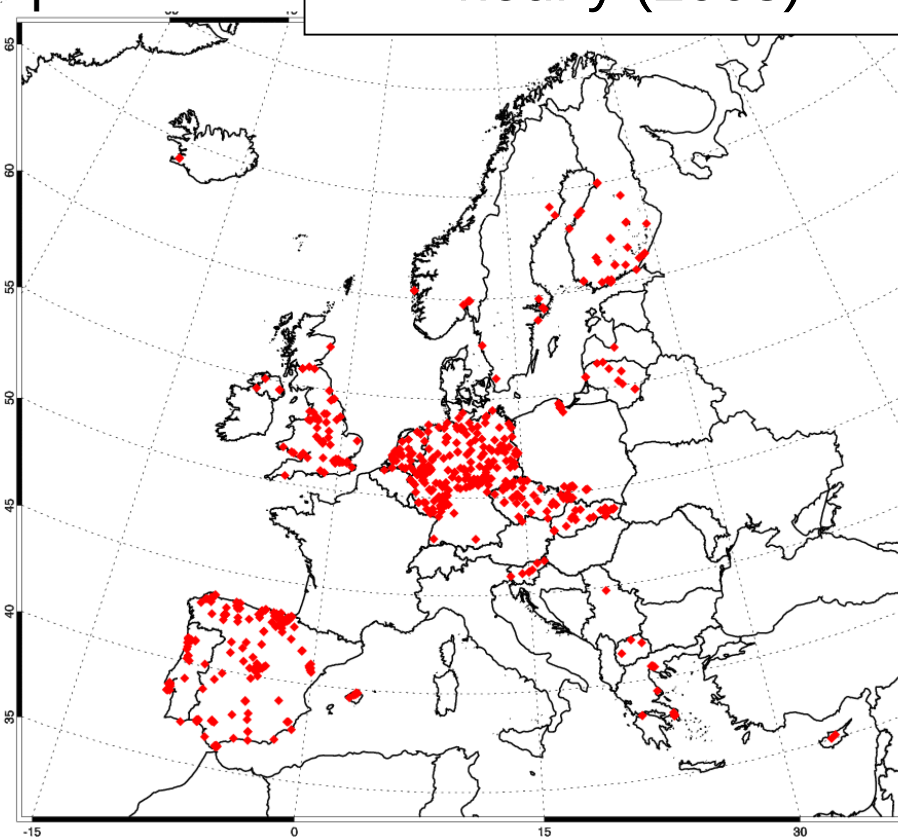
← adjoint radiative transfer model

# Model Domain and Observations



SYNAER – AOT retrievals
2 – 3 traces per day

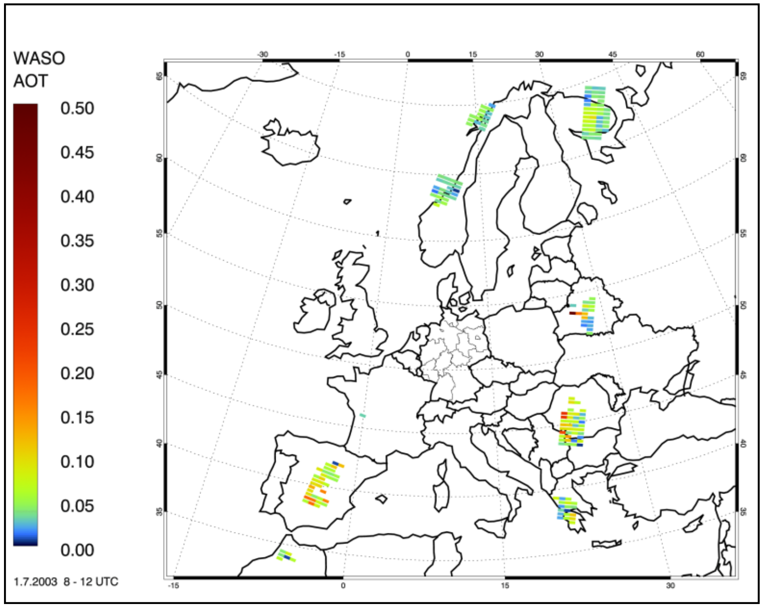
13 July 2003

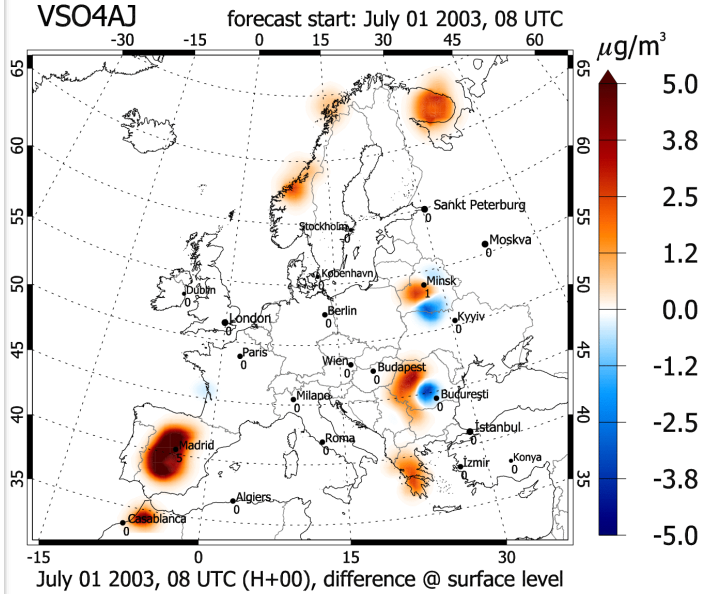


EEA in-situ $PM_{10}$
hourly (2003)

# Analysis and increments for acc. $SO_4^{2-}$ July 1, 8 UTC

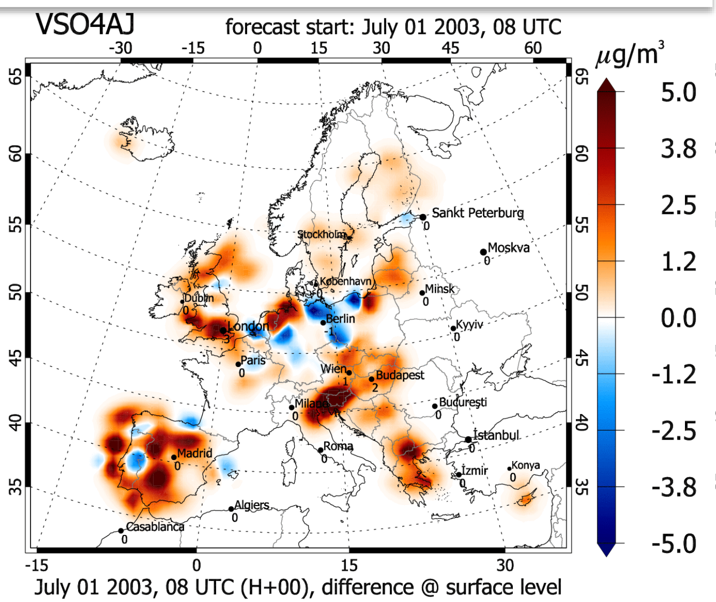
SYNAER AOT-WASO

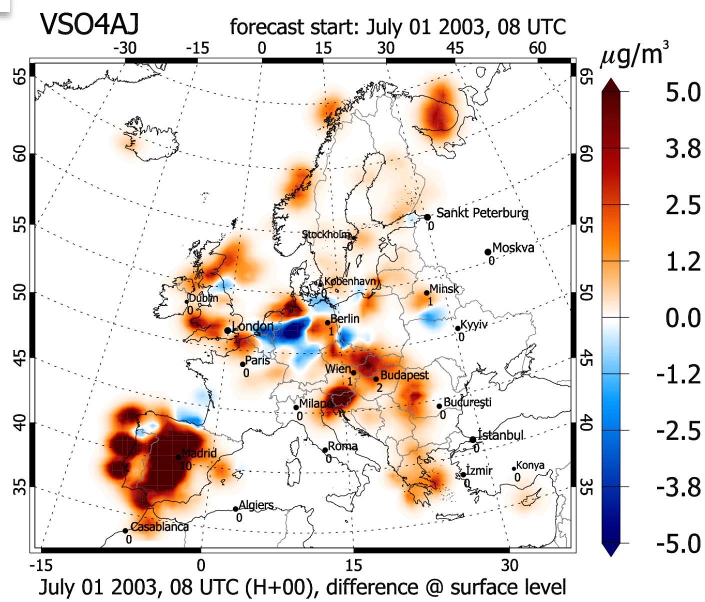



Analysis – Background SYNAER only

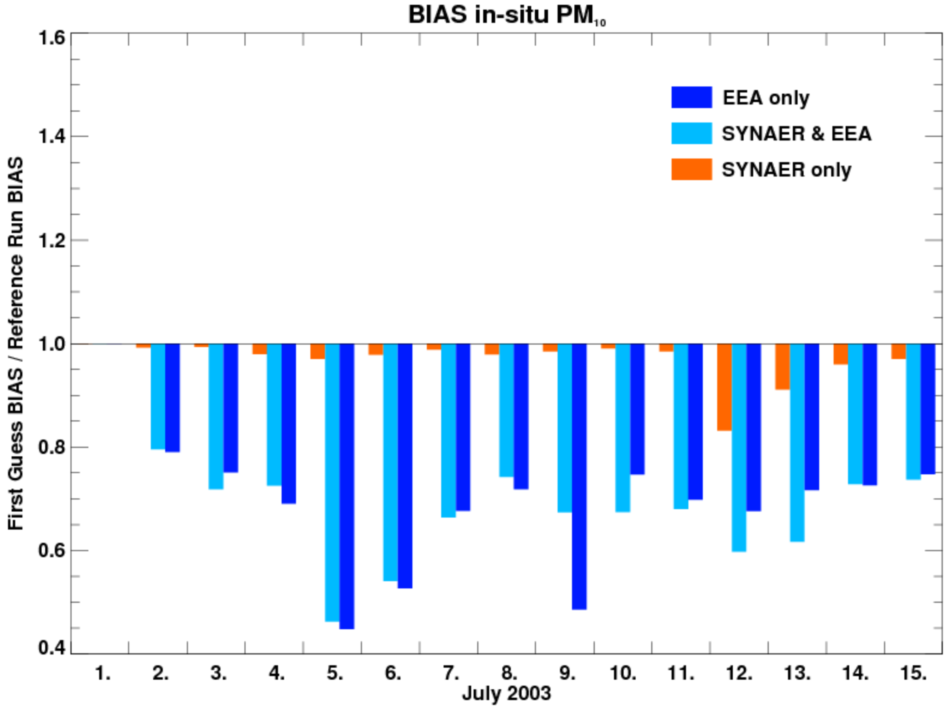
Analysis – Background EEA only



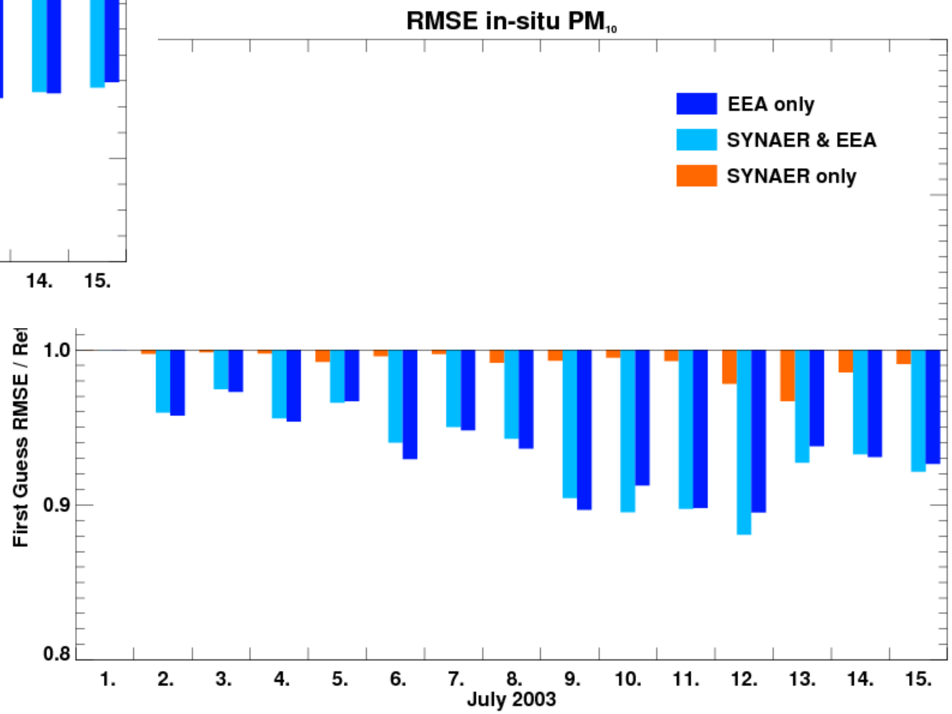

Analysis – Background SYNAER & EEA

# Developement of forecast performance




**Overall BIAS reduction**

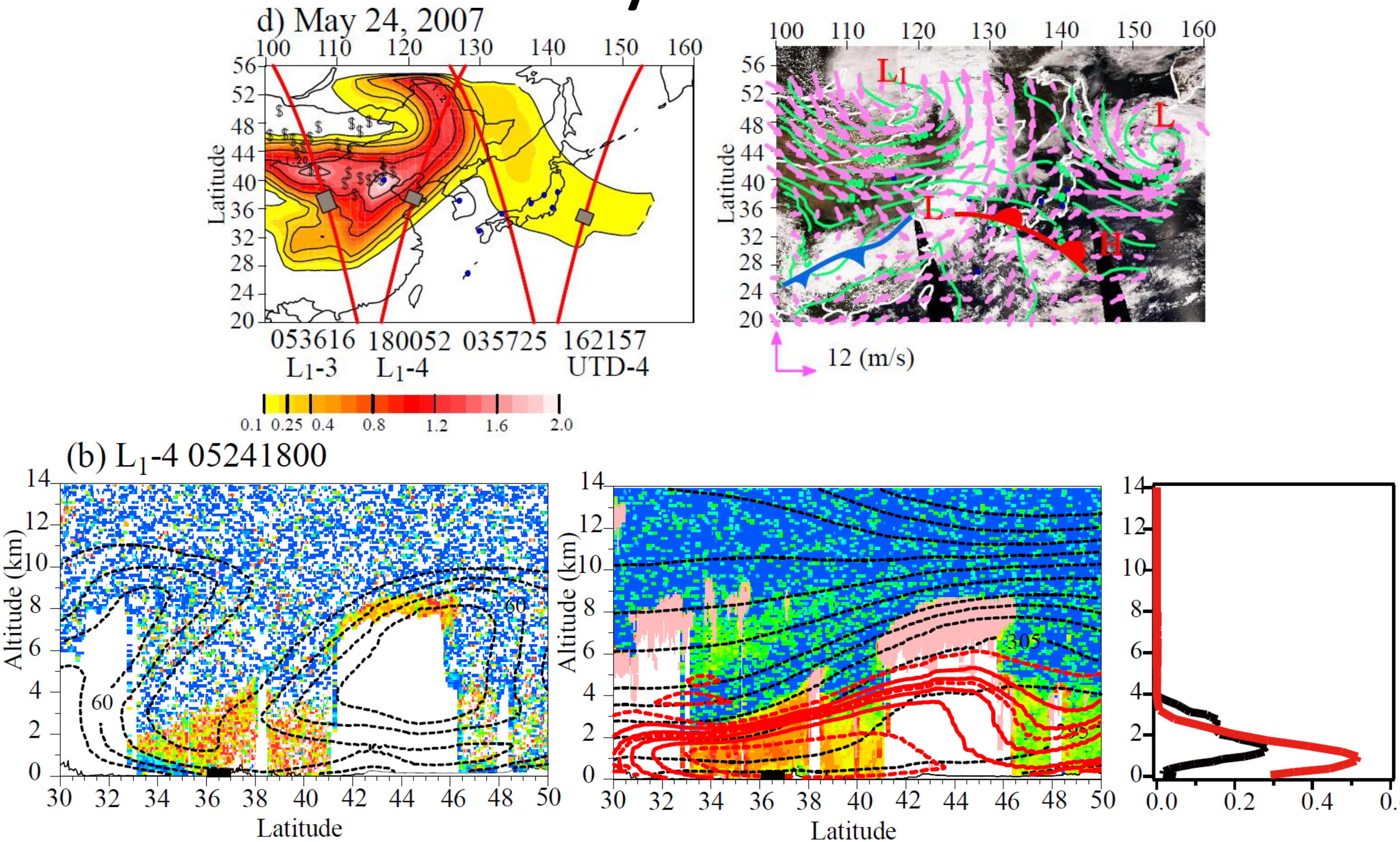
| | |
|---|---|
| SYNAER | 0.96 |
| SYN & EEA | 0.67 |
| EEA | 0.67 |




**Overall RMSE reduction**

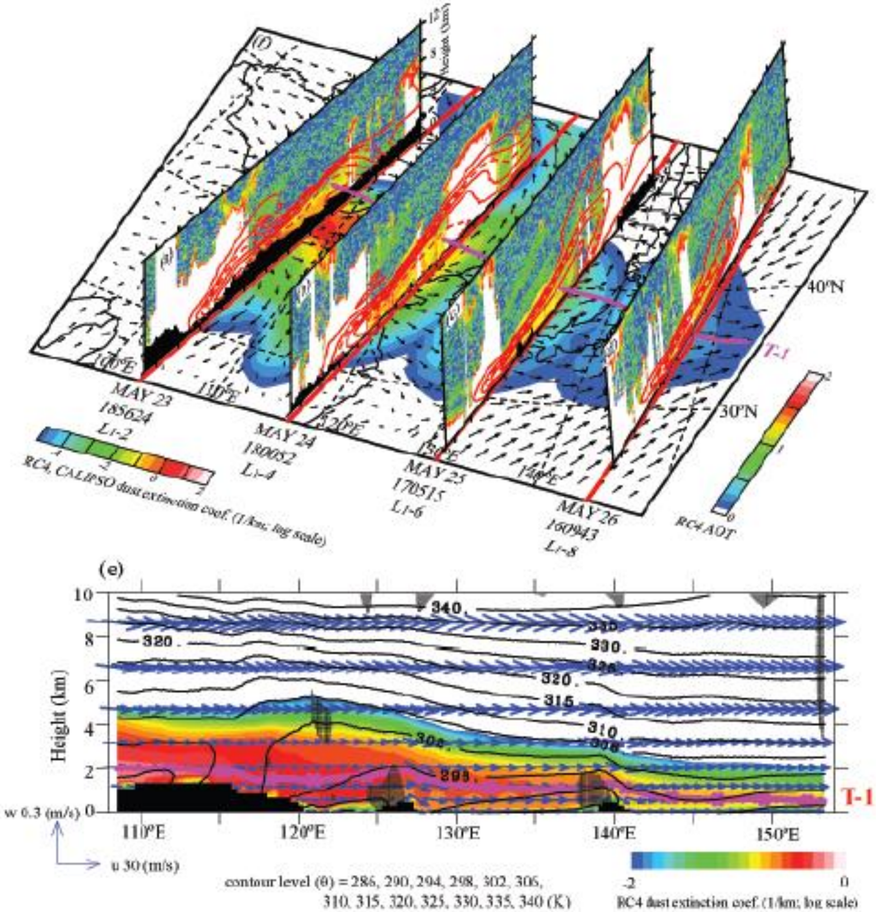
| | |
|---|---|
| SYNAER | 0.99 |
| SYN & EEA | 0.93 |
| EEA | 0.92 |

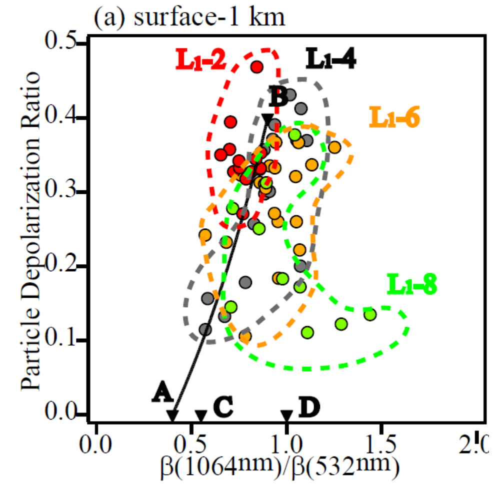
# Asian Dust by 4D-var CALIOP DA

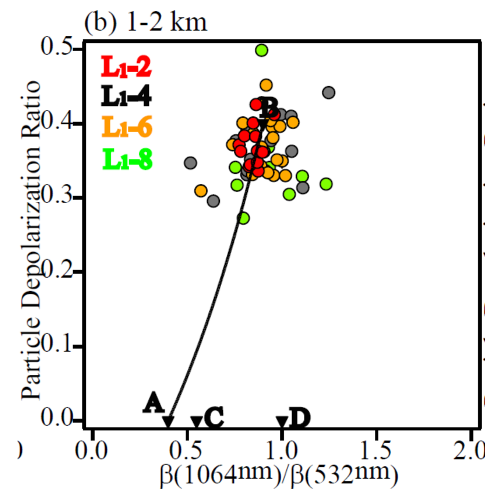



Y. Hara, K. Yumimoto, I. Uno, A. Shimizu, N. Sugimoto, Z. Liu, and D. M.Winker, 2009

# Asian Dust by 4D-var CALIOP DA



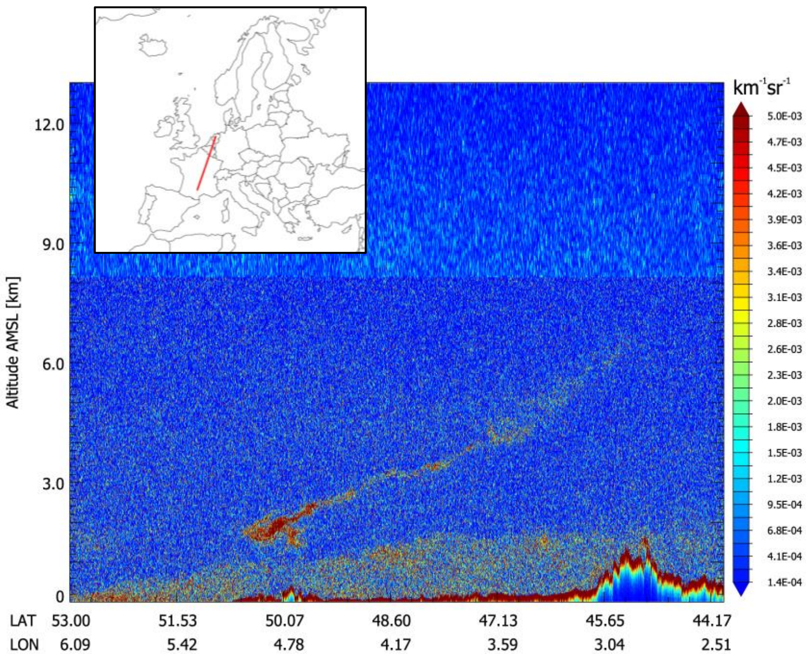

Y. Hara, K. Yumimoto, I. Uno, A. Shimizu, N. Sugimoto, Z. Liu, and D. M.Winker, 2009

# Example CALIOP
# Variational volcanic ash data Assimilation Module with selective background weakening for special events

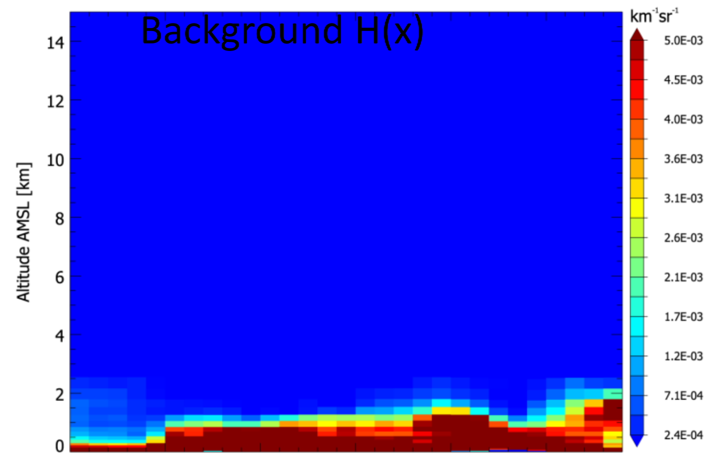
LiDAR 4D-var data assimilation for improved analysis of unexpected aerosol events
→ automatable online adaptation of background error covariace matrix

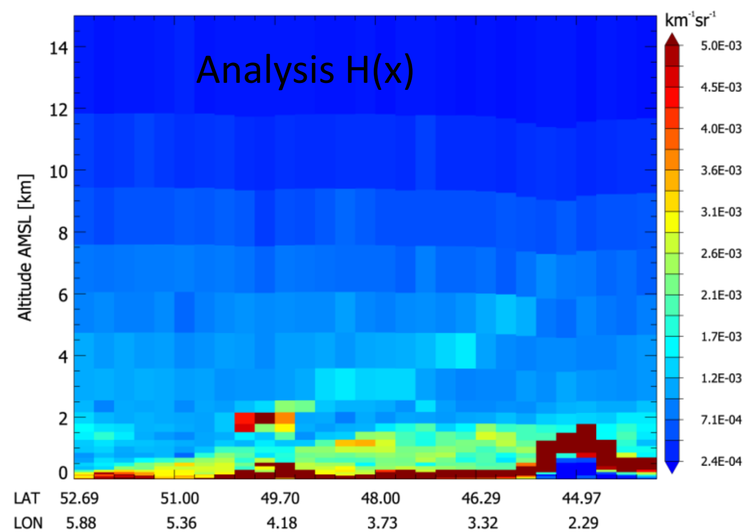
CALIOP observation of the Eyjafjallajökull ash cloud

17 April 2010, 02:01:19 - 02:14:53 UTC (Winker et al., 2012)




A. Lange, master thesis



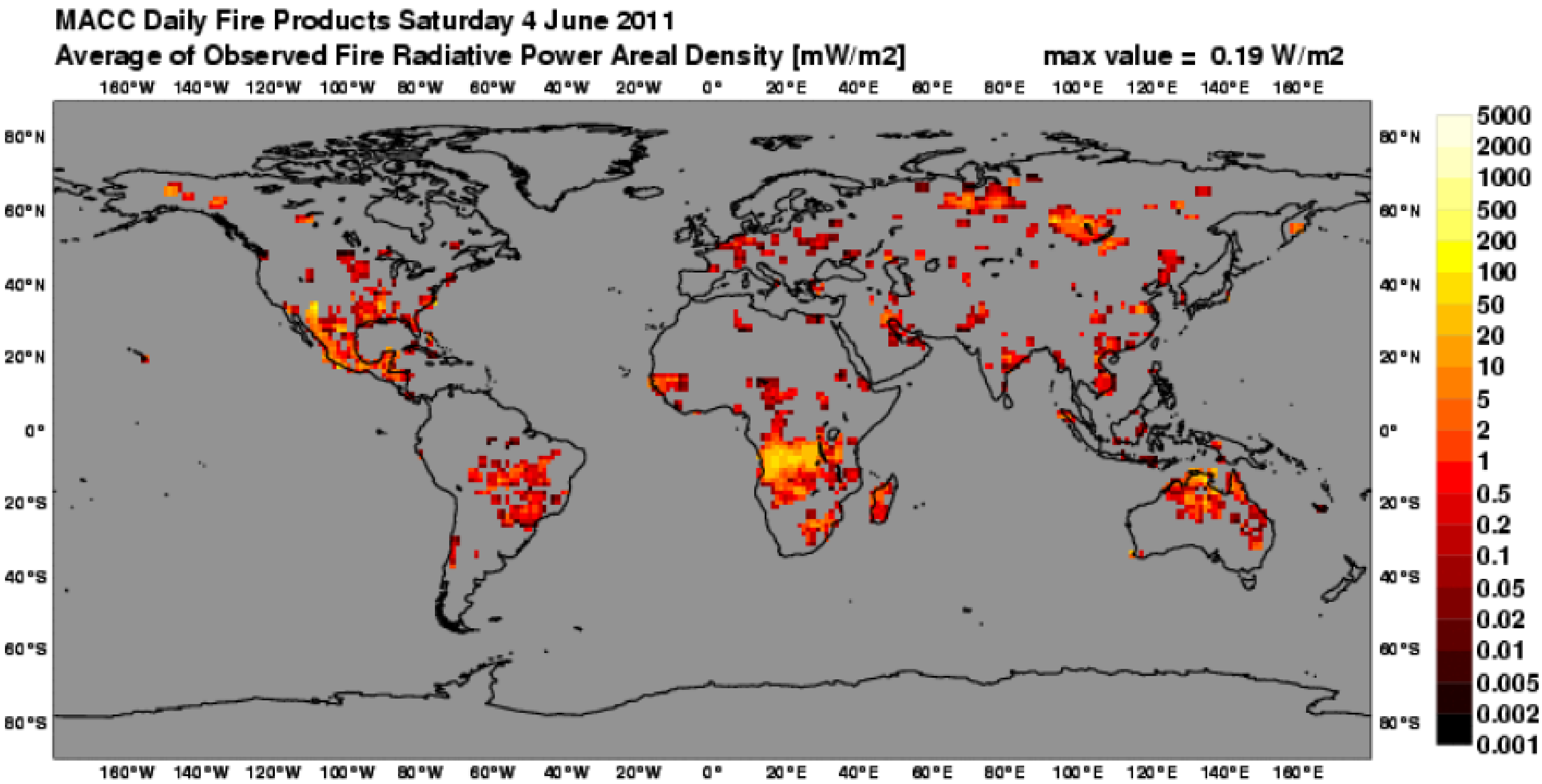



# FIRE SATELLITE DATA ASSIMILATION

# GFAS (Global Fire Assimilation System)

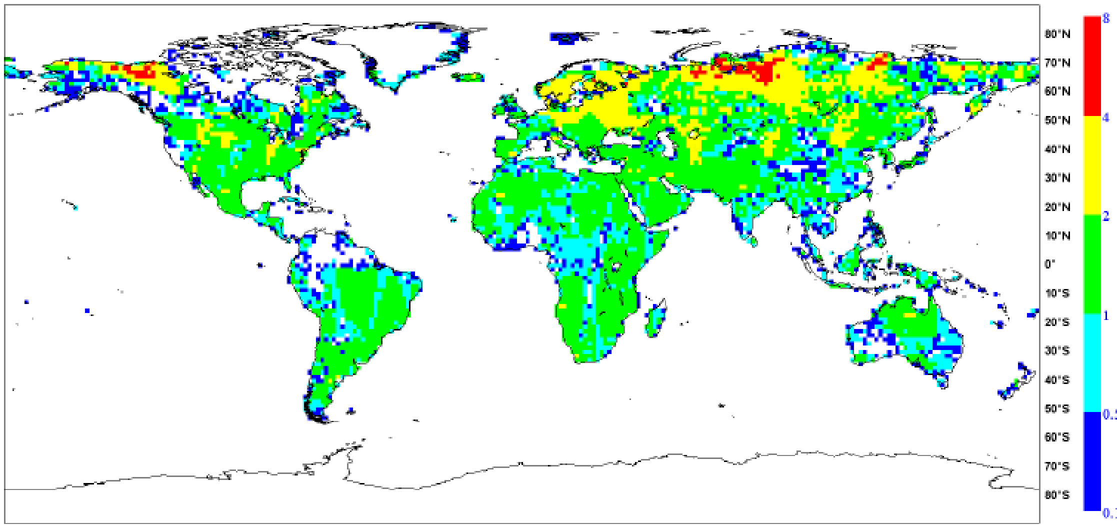
J. Kaiser and coworkers, ECMWF and MPI-C

implemented for CIFS and MACC regional modells

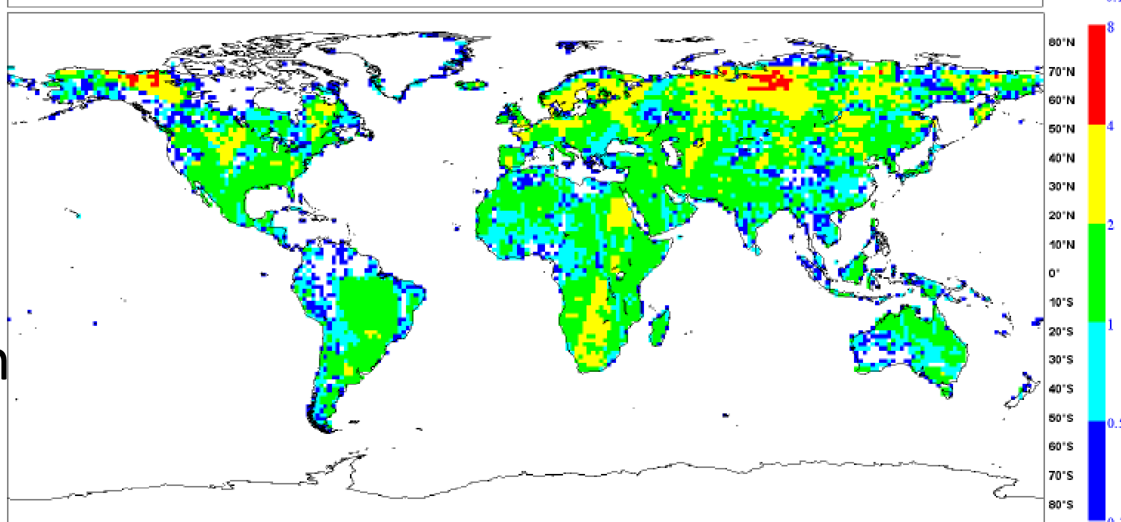


# Effective number of satellite observations of grid cells by **MODIS**

MODIS
on TERRA
morning
overpass



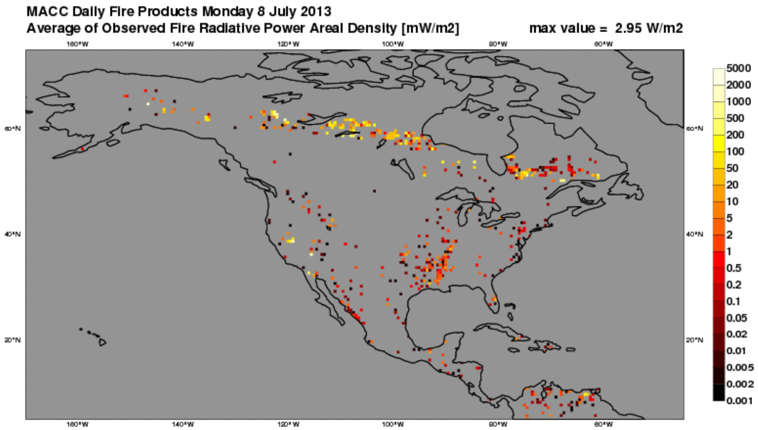

MODIS
on AQUA
afternoon
overpass

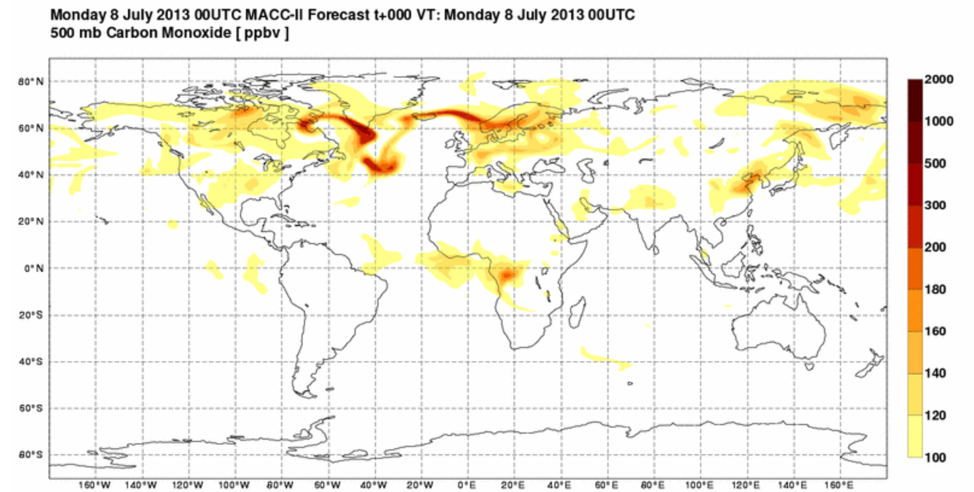


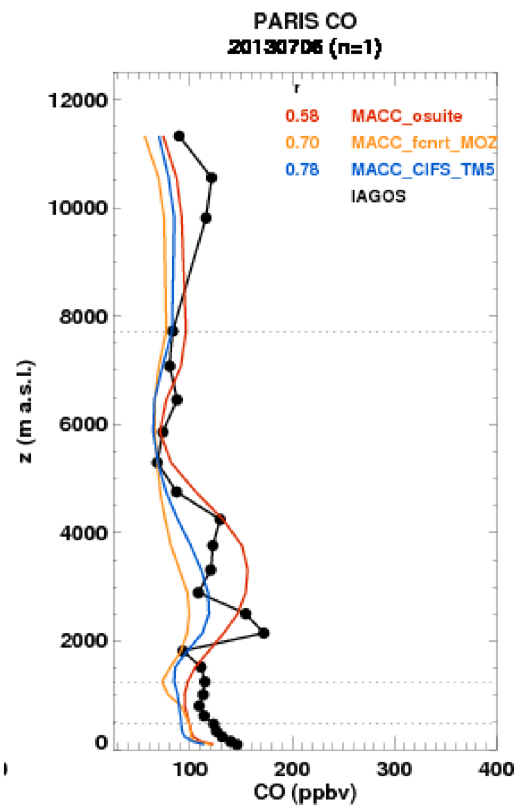

4 June 2011,
00:00–24:00 UTC

**Kaiser, Heil, Andreae, A. Benedetti, N. Chubarova, L. Jones, J.-J. Morcrette, M. Razinger, M. G. Schultz, M. Suttie, and G. R. van der Werf, 2012**

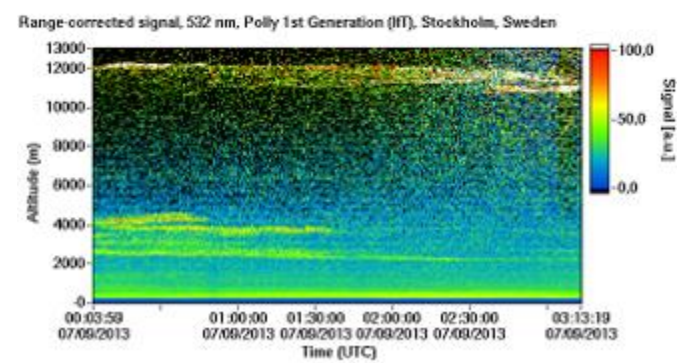
# Canadian smoke over Europe (July 2013)




The assimilation run (red, MACC o-suite) pick ups increased levels of pollutants, here Carbon Monoxide, between 2 and 4 km. Independent aircraft observations (black) confirm the presence of the plume, which is seen also by European lidars and ceilometers.

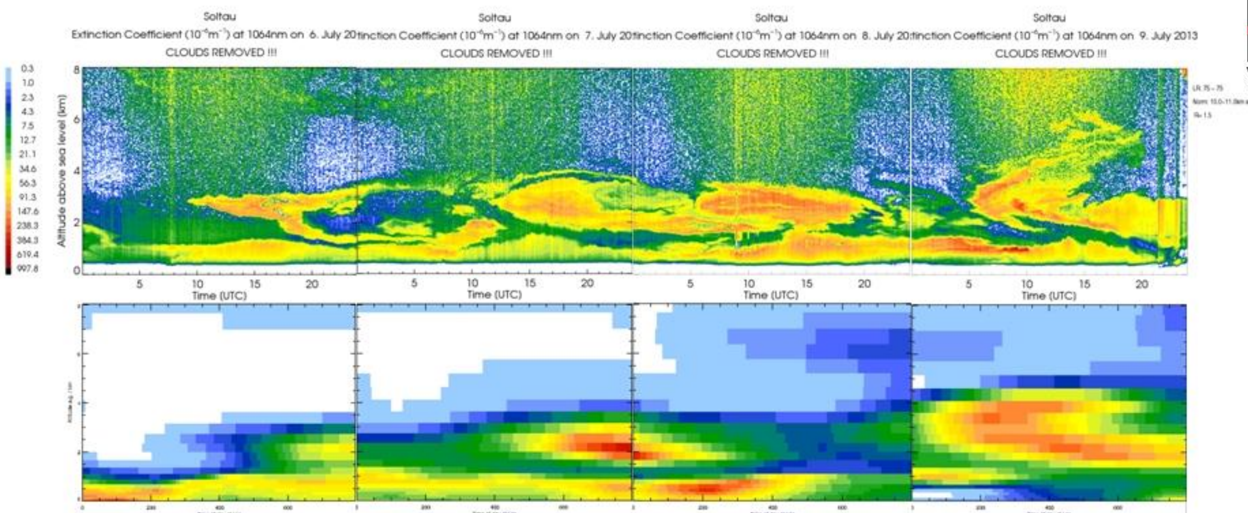



J. Kaiser

# Canadian Smoke in Europe
# July 2013

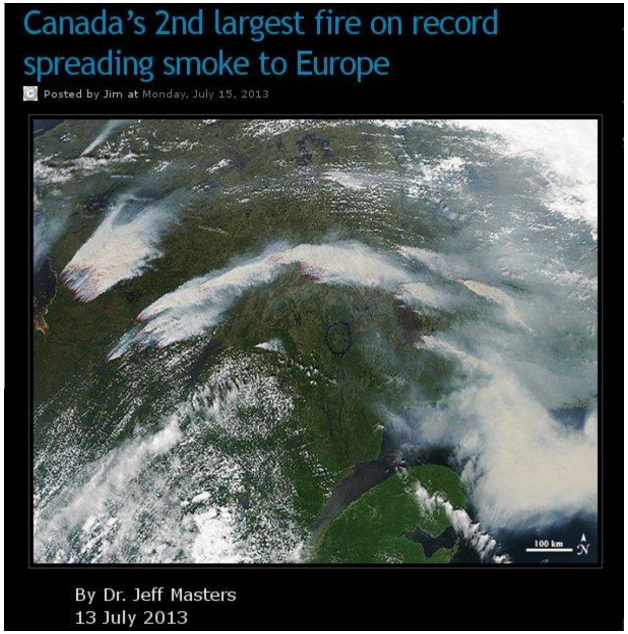
## Comparison of Canadian forest fire plume seen by Ceilometers over Soltau, North Germany
## 6 – 9 July 2013

MACC-2D plot is QUALITATIVE and linear scale in contrast to ceiloplot!!!
Shall just show the reproduction of the plume structure




Verification of MACC aerosol forecast with ceilometer data shows good performance for most plume occurrences (plots courtesy of Harald Flentje, DWD)


**Video 1.** Maxime Duperré, traveling in a truck near Nemiscau, Quebec, took this video of one of the massive fires burning in Quebec this July.

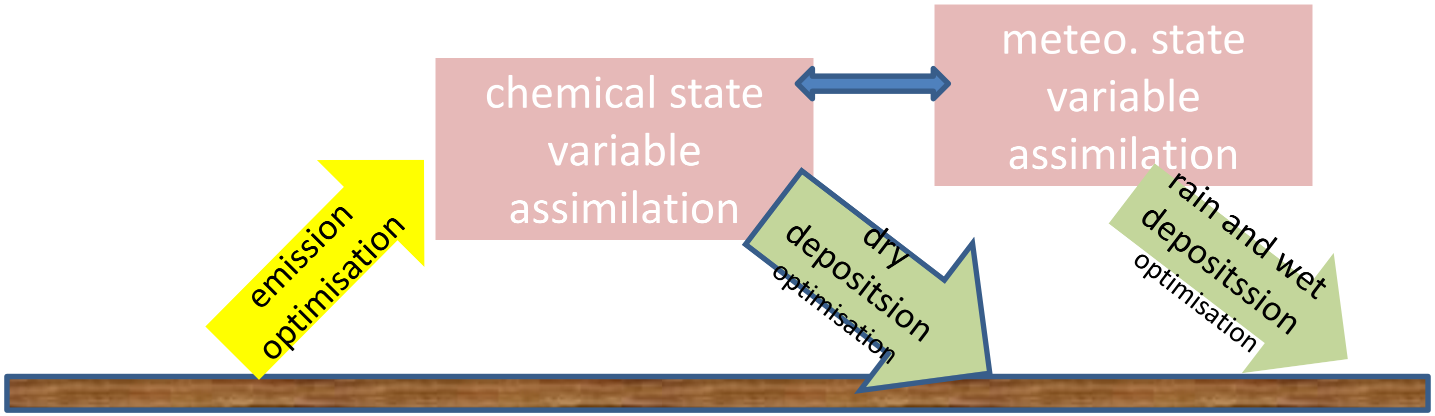



A. Benedetti

# FUTURE OBJECTIVES

# Future directions

1. boundary layer and air quality data assimilation must include coupling with surface processes (flux inversion):
   - related parameters for biogenic emissions and deposition (LAI, fPAR, … )




2. aerosols must be classified (lidar colour ratio, lidar ratio, depolarisation, T-matrix,…
3. joint assimilation/inversion to be extended to further multiple impacting parameters (e.g. radiative)
4. larger ensemble appoaches for non-normal errors

Thank You
for Your Attention