Scientific challenges in chemical data assimilation

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Royal Netherlands Meteorological Institute,
De Bilt, the Netherlands

Topics:
- Ozone
- Tropospheric chemistry:
  * satellite trace gas observations
  * 4D-Var

Ozone assimilation at numerical weather centres

NWP and ozone

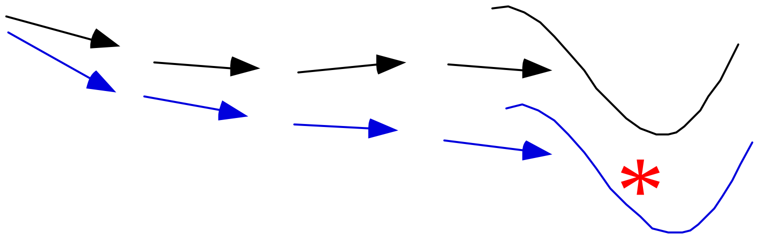
Benefits for atmospheric chemistry science community:

Multi-year data base of 4D ozone fields, consistent with the available satellite observations and atmospheric dynamics (ERA 40)

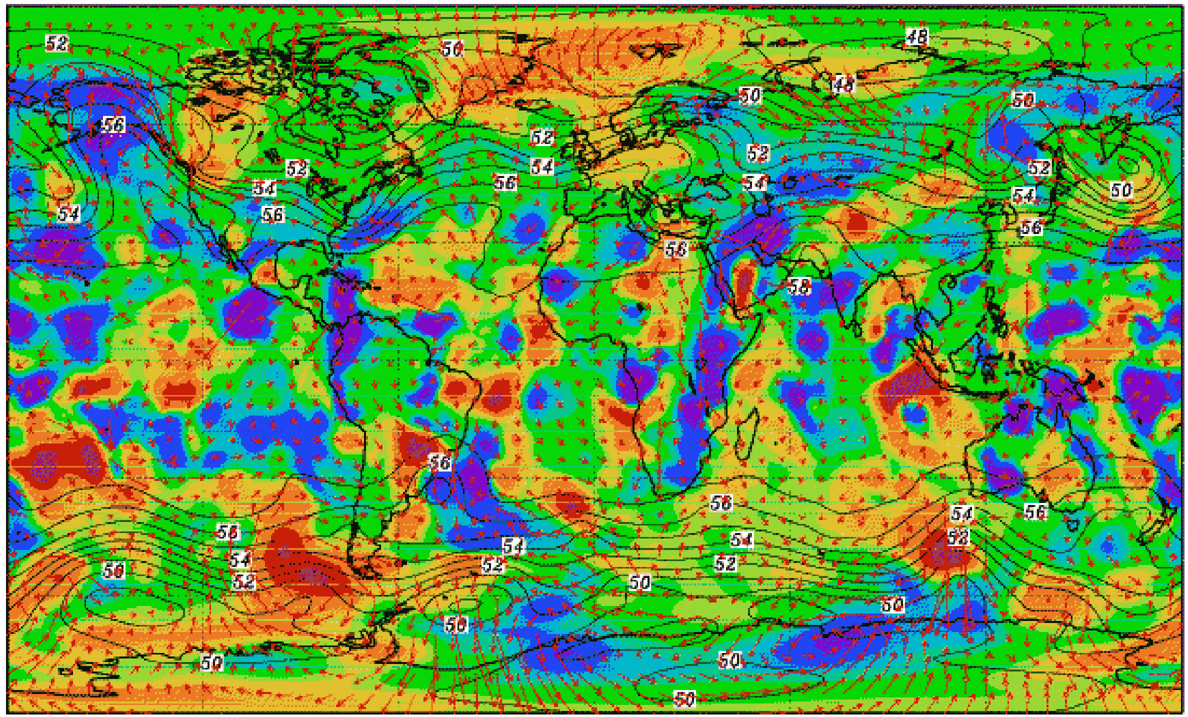
- Recovery ozone layer
- Chemistry - climate interaction

Benefits of accurate ozone observations to numerical weather prediction

- Radiation: ozone has significant influence on temperature (and wind)
- Satellite retrieval: TOVS
- Assimilated ozone observations lead to wind increments
- UV forecast



Impact of ozone on NWP winds



Wind increments due to TOVS ozone observations

ECMWF model

Elias Holm
EU SODA project

Wind increments ~ 0.5 m/s

Ozone satellite observations

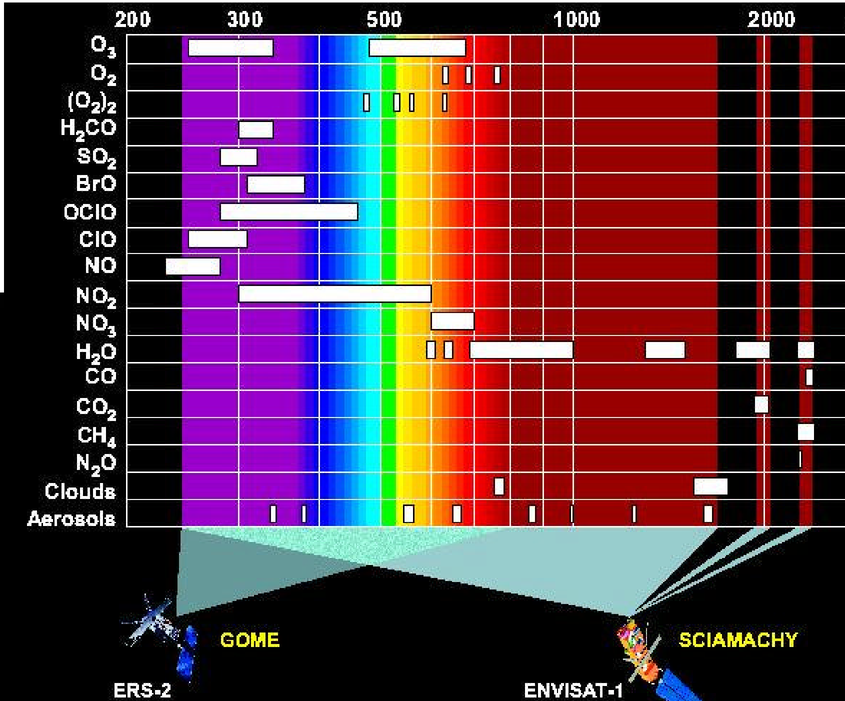
Satellite instruments measuring ozone

UV-Vis nadir
- TOMS (1978-present), SBUV, SBUV-2, GOME, SCIAMACHY, OMI

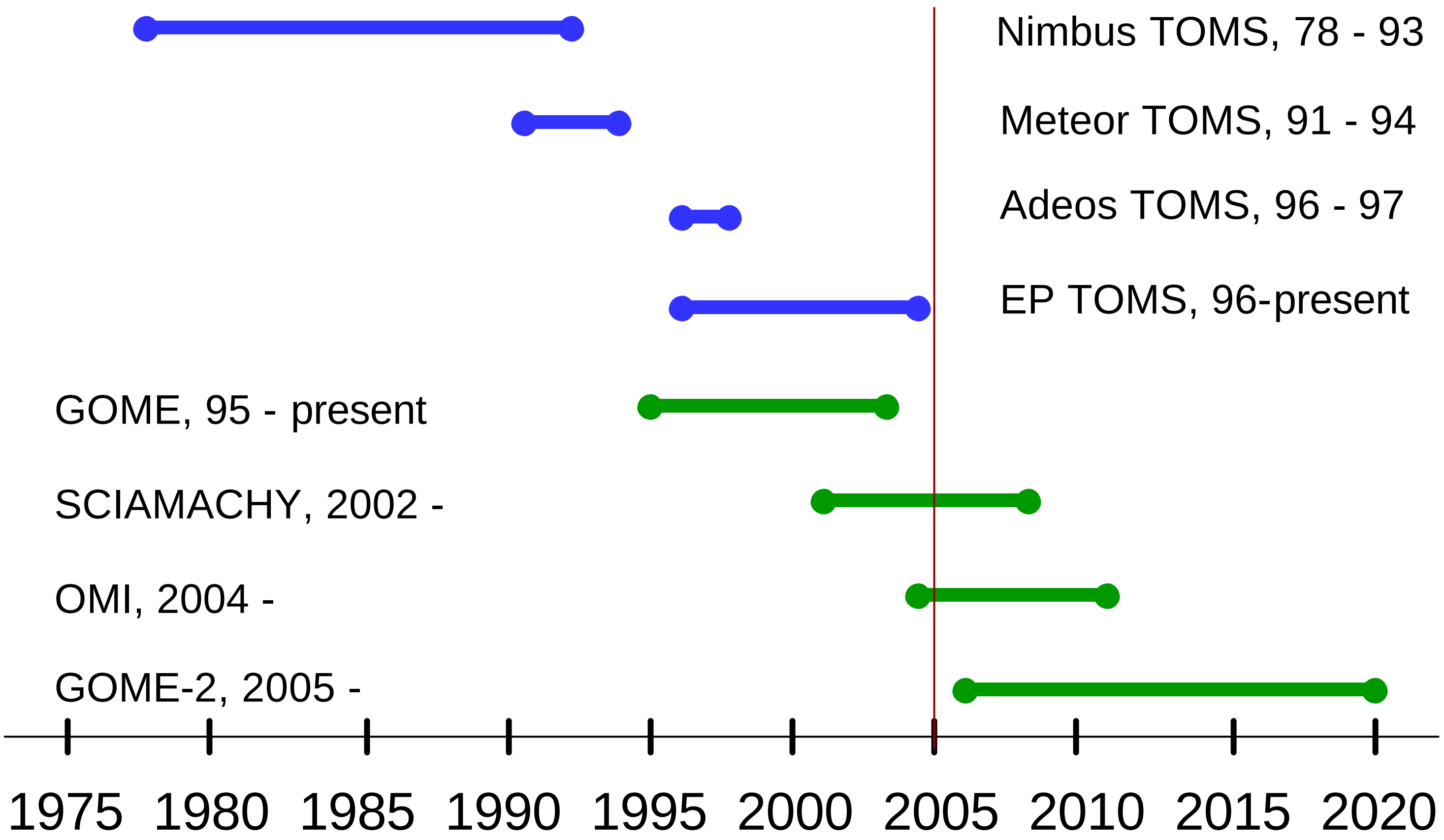
Limb (IR, MW, UV-Vis)
- MLS on UARS, MIPAS, OSIRIS, SMR, MLS-Aura

Occultation
- HALOE, SAGE, POAM, GOMOS

Nadir (IR)
- TOVS, AIRS



Ozone column measurements: 1978-2005



SCIAMACHY total ozone (KNMI retrieval)

KNMI

QuickTime™ en een
TIFF (ongecomprimeerd)-decompressor
zijn vereist om deze afbeelding weer te geven.

currently
assimilted
in IFS

Stratospheric ozone assimilation

Ozone assimilation at KNMI

Chemistry-transport assimilation model:

- TM model: 2x3 degree lat-lon resolution, 44 layers
- ECMWF analyses of winds, temperatures
- Second moments advection
- Stratospheric chemistry parametrizations
  - Gas-phase
  - Heterogeneous
- GOME/SCIAMACHY ozone columns
- Sub-optimal Kalman filter data assimilation scheme

Eskes et al. Q. J. R. Meteorol. Soc., ***129****, 1663-1681, 2003*

Stratospheric chemistry parameterization

Gas-phase chemistry

Cariolle, Déqué, JGR 91, 10825, 1986

$$\frac{d\chi}{dt} = \langle S \rangle + \left\langle \frac{\partial S}{\partial \chi} \right\rangle (\chi - \langle \chi \rangle) + \left\langle \frac{\partial S}{\partial T} \right\rangle (T - \langle T \rangle) + \left\langle \frac{\partial S}{\partial \Phi} \right\rangle (\Phi - \langle \Phi \rangle)$$

- χ ozone concentration
- S sources - sinks
- Φ ozone column above point

Stratospheric chemistry parameterization

Heterogeneous chemistry

(Peter Braesicke, CAS, Cambridge Univ.)

$$\frac{d\chi}{dt} = -\frac{1}{\tau} A \chi$$

$$\frac{dA}{dt} = \frac{1}{\tau_p}(1 - A) - \frac{1}{\tau_l} A$$

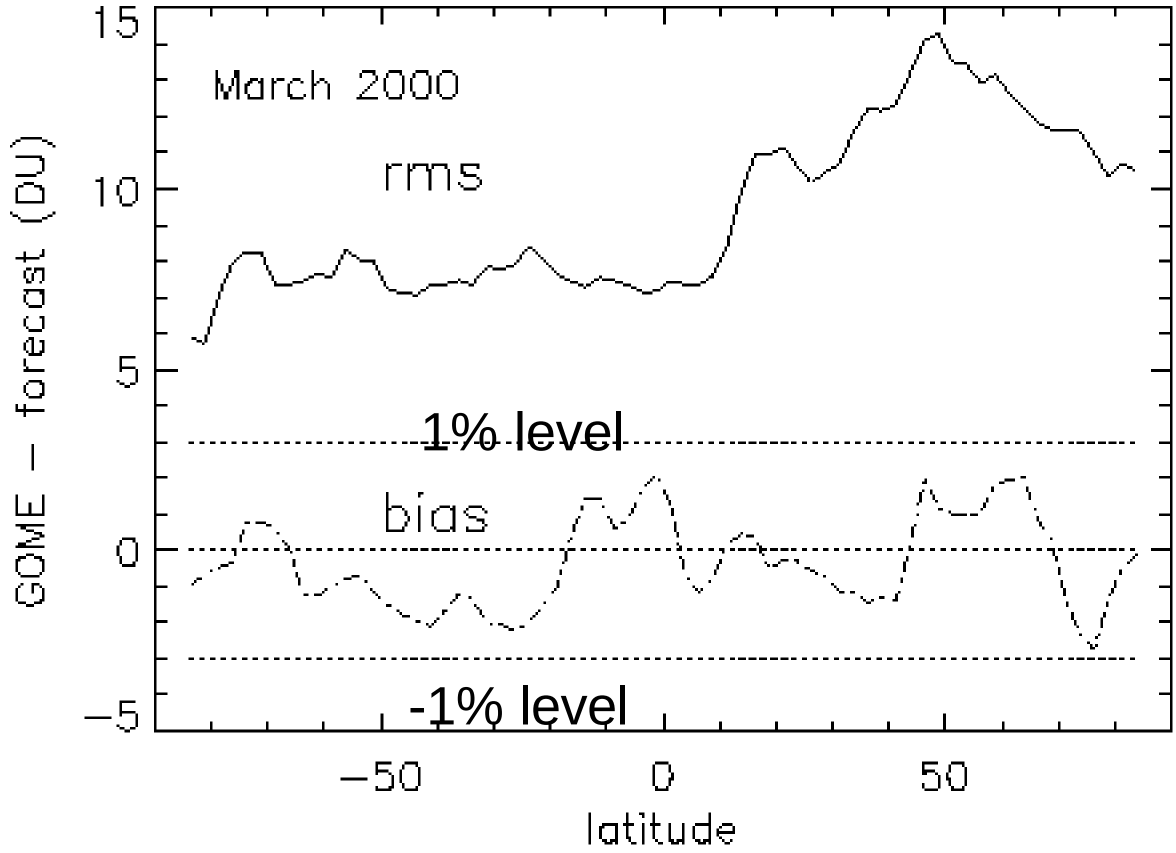
χ	ozone concentration
A	activation tracer field (cold tracer)
τ	ozone depletion time scale
τ_p	activation time scale
τ_l	cold tracer life time

Typical forecast performance: OmF

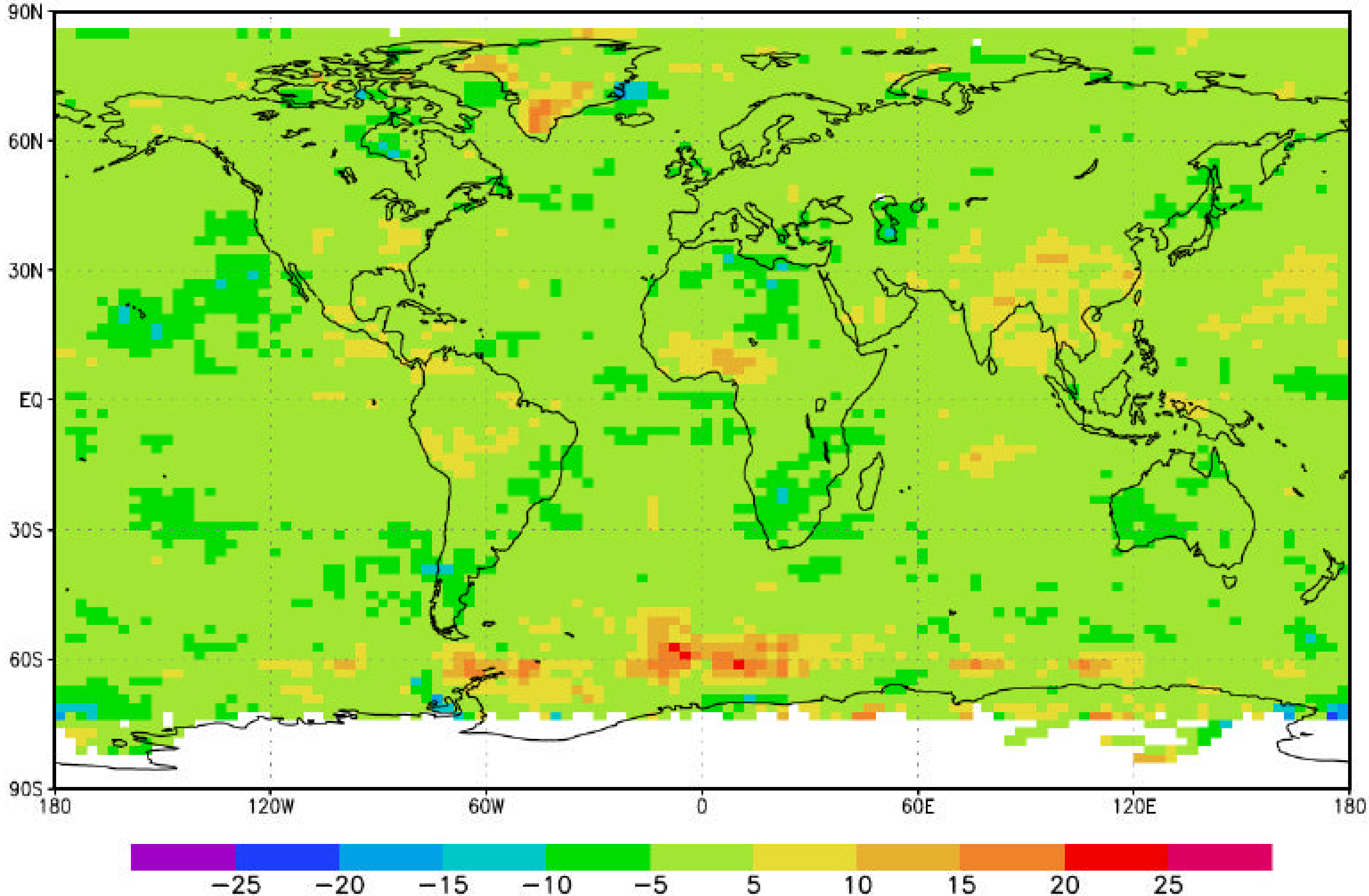
total ozone

rms(OmF)
typically 3%

bias within 1%



SCIAMACHY vs. assimilation



Ozone forecasts

Anomaly correlation

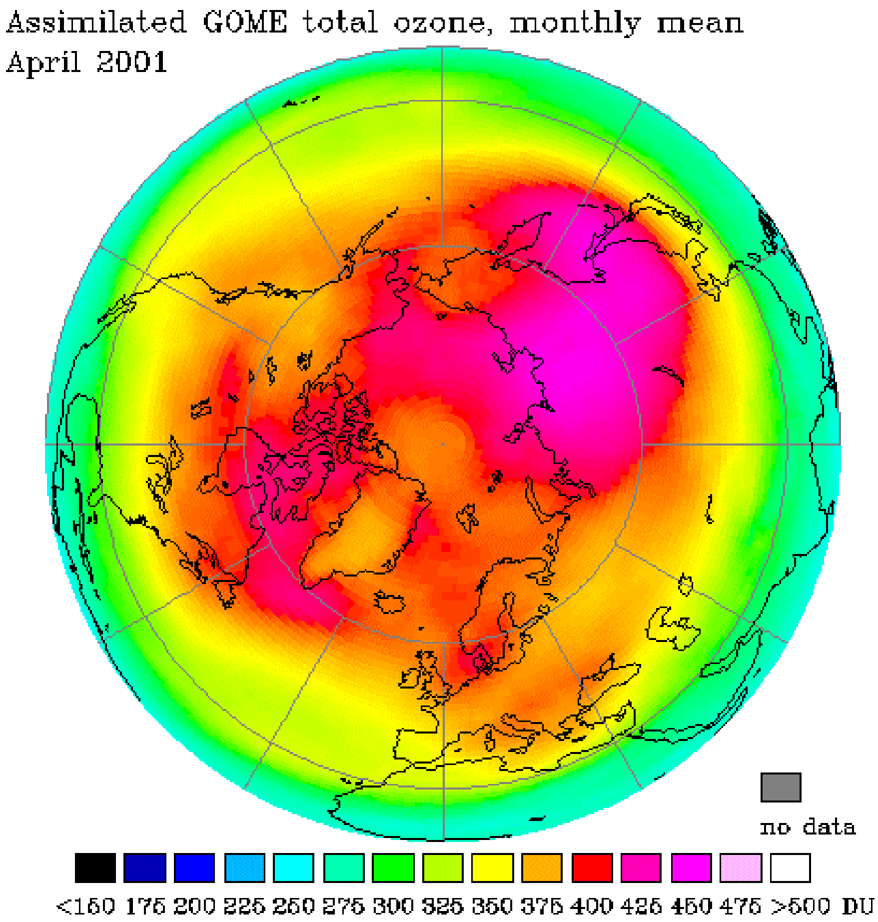
Anomaly correlation

$$C = < (f-c)(a-c) > \ / \ v<(f-c)^2> v<(a-c)^2>$$

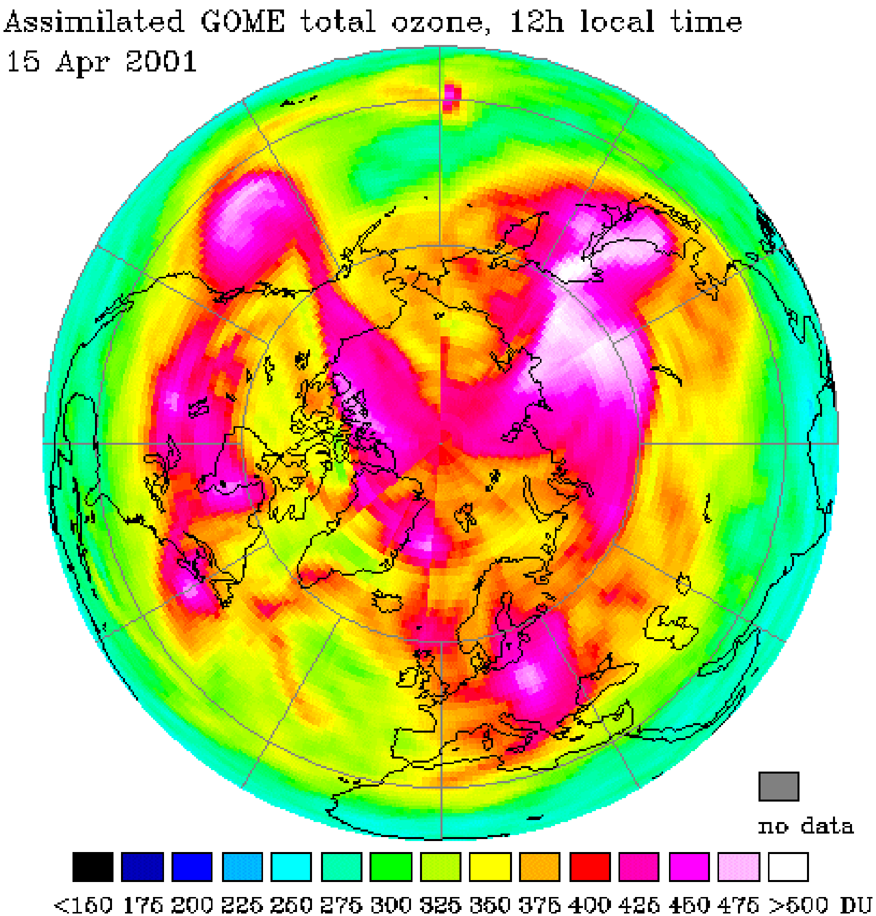
(f = forecast, a = analysis, c = climatology)

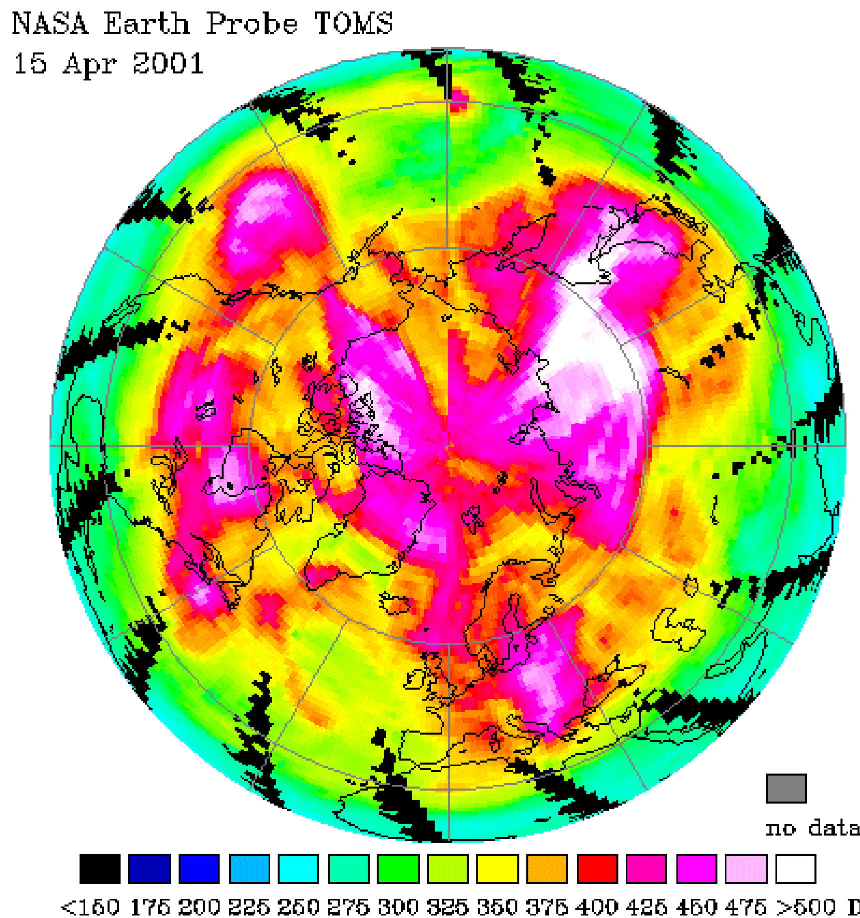
- Anomaly normallydefined w.r.t. climatology "c" :
  Not useful for ozone - artificially high scores
- Alternative: "c" = running monthly mean

Monthly-mean analysis: April 2001



Analysis vs TOMS: 15 April 2001

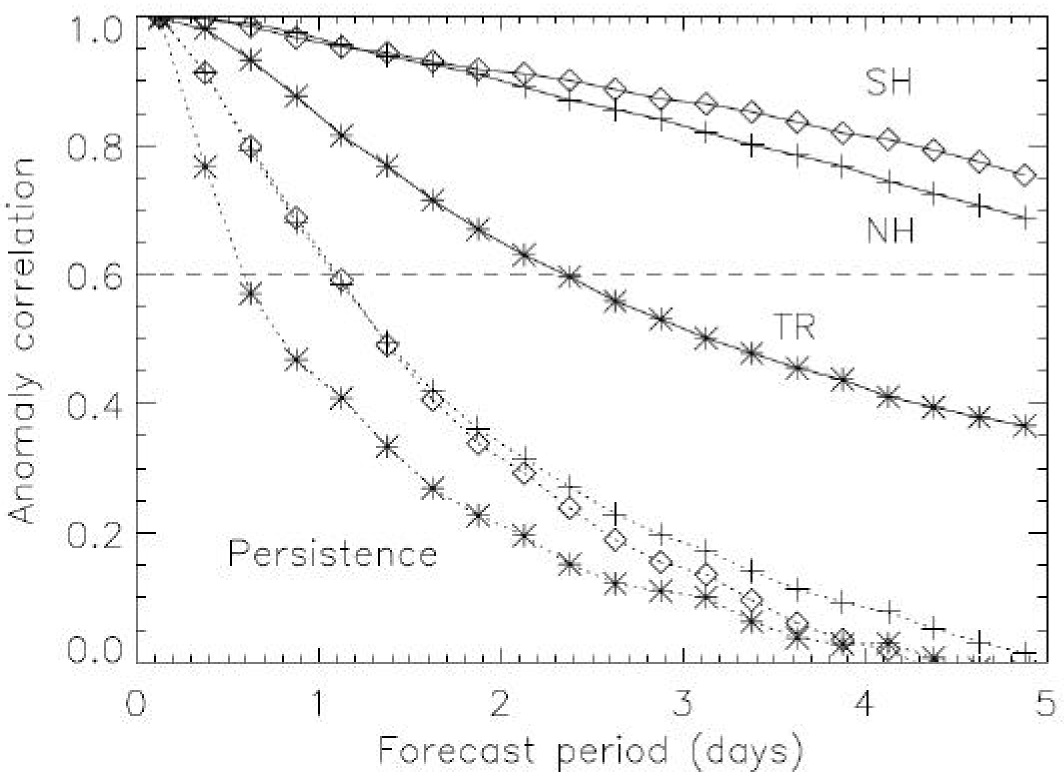




Total ozone anomaly correlation

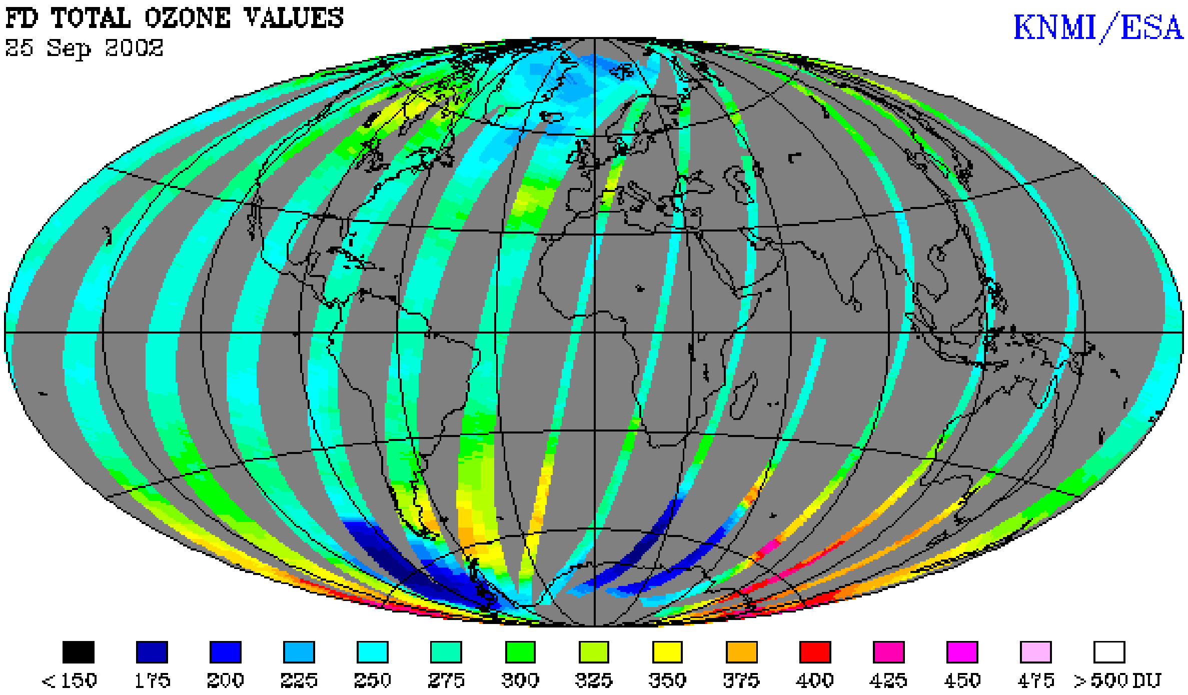
meaningful
forecasts up to
7 days
(outside the tropics)

Eskes et al.,
ACP, 2, 271, 2002



Forecast of the 2002 ozone hole split event

GOME measurements at 25 September 2002

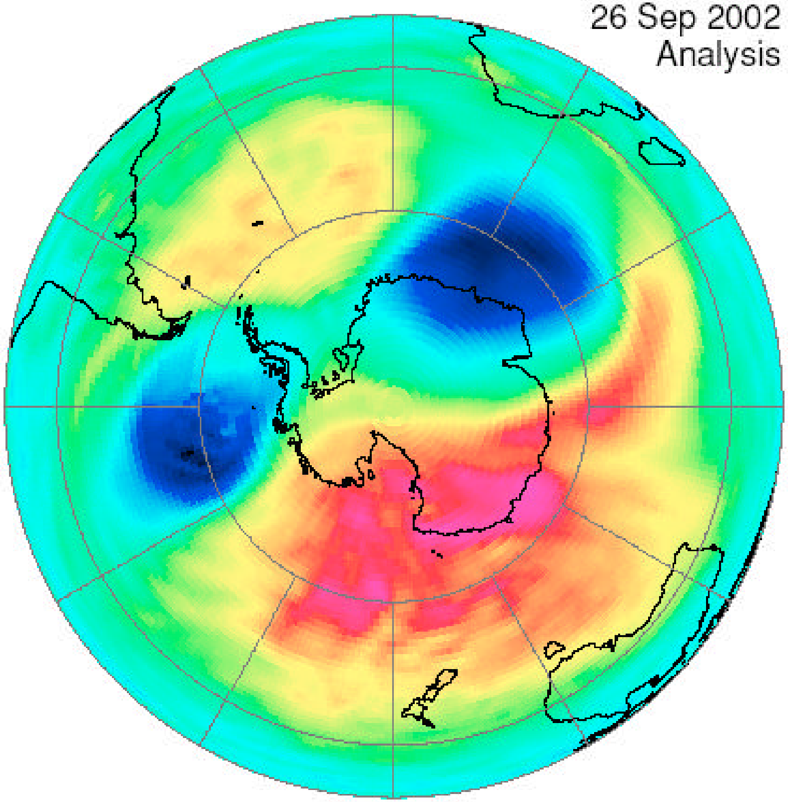


Vortex breakup, September 2002

26 September 2002
Analysis based on GOME

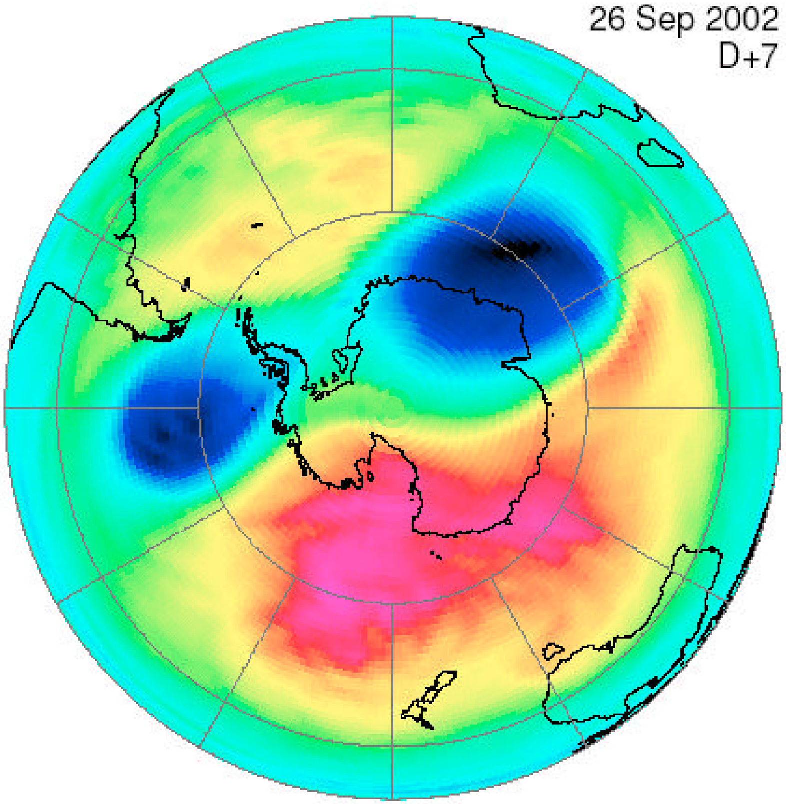
H. Eskes et al,
J.Atmos.Sci. 62, 2005

A. Simmons et al,
J.Atmos.Sci. 62, 2005



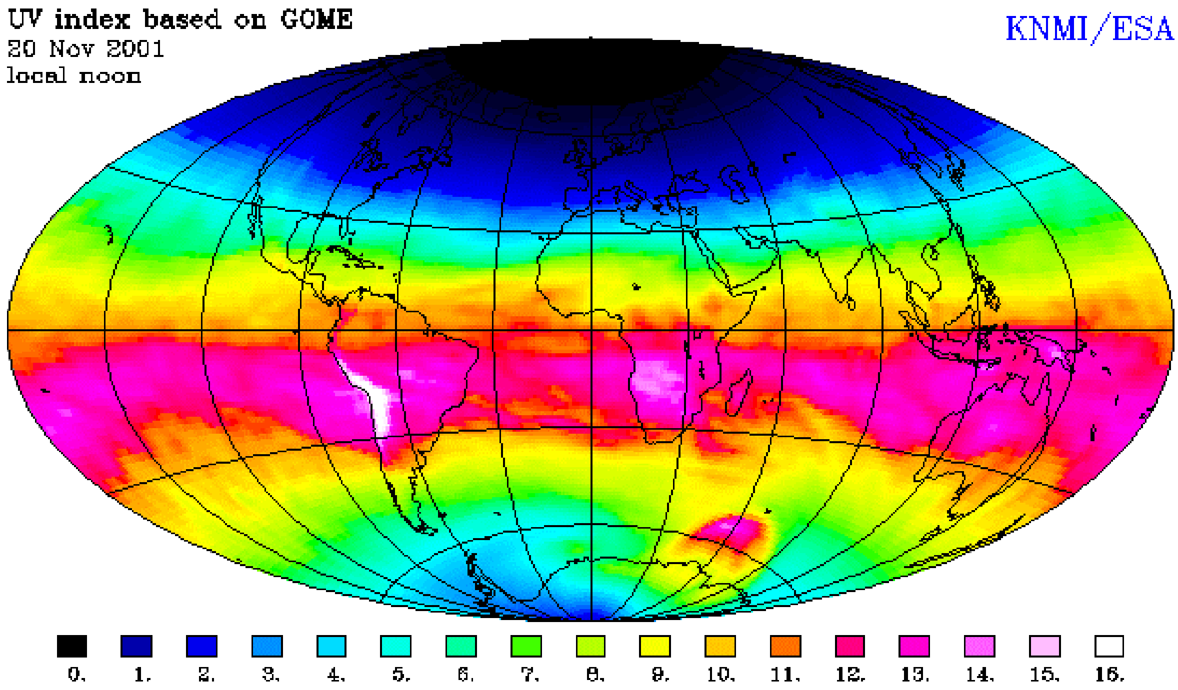
Vortex breakup, September 2002

26 September 2002
7-day forecast



Clear-sky UV forecast (UV-index)

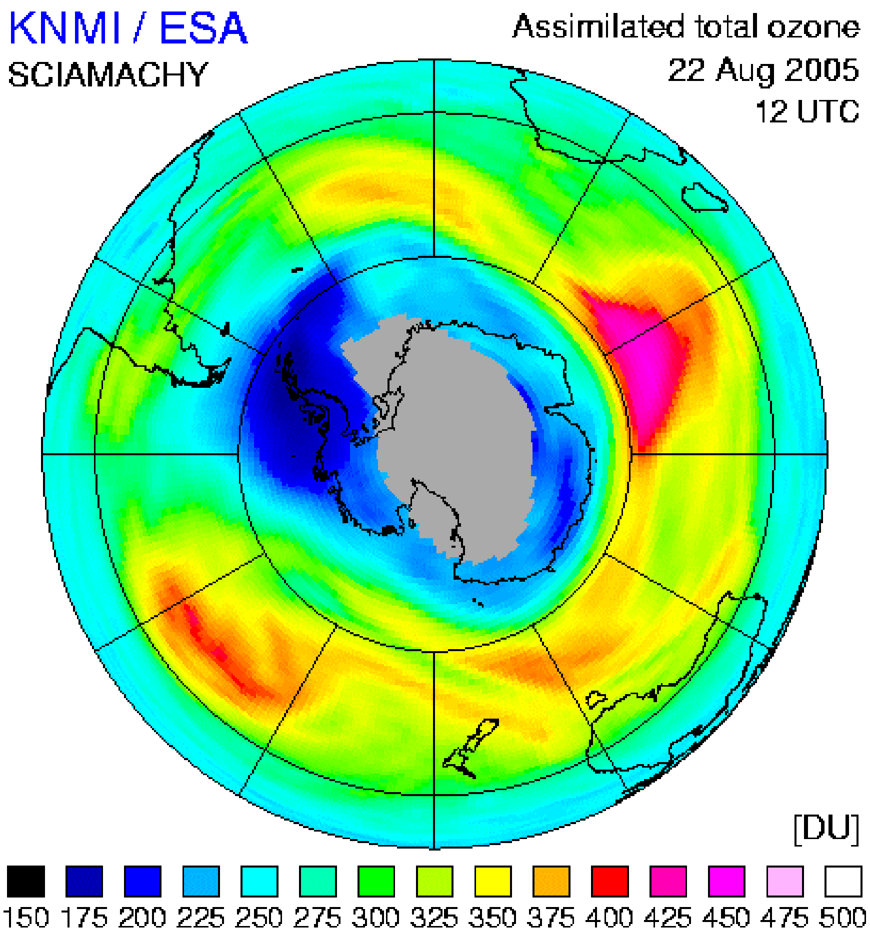
20 November 2001
(5-day forecast)



August 2005: very early start of ozone hole

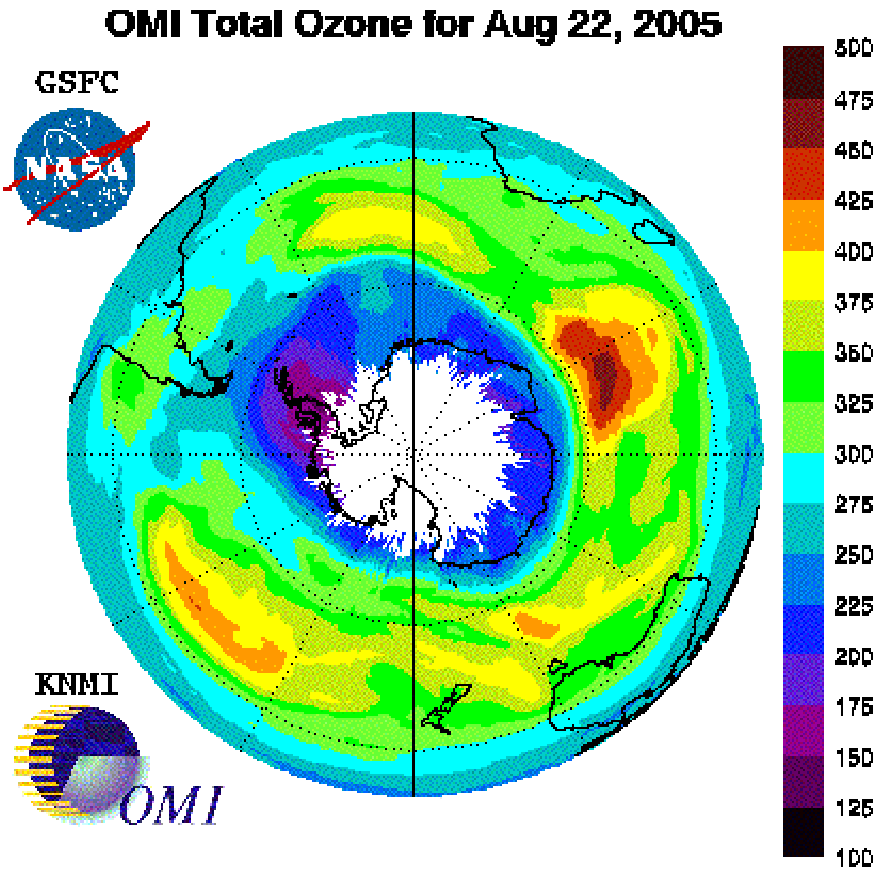
SCIAMACHY
assimilation

(grey:
large analysis error)



August 2005: very early start of ozone hole

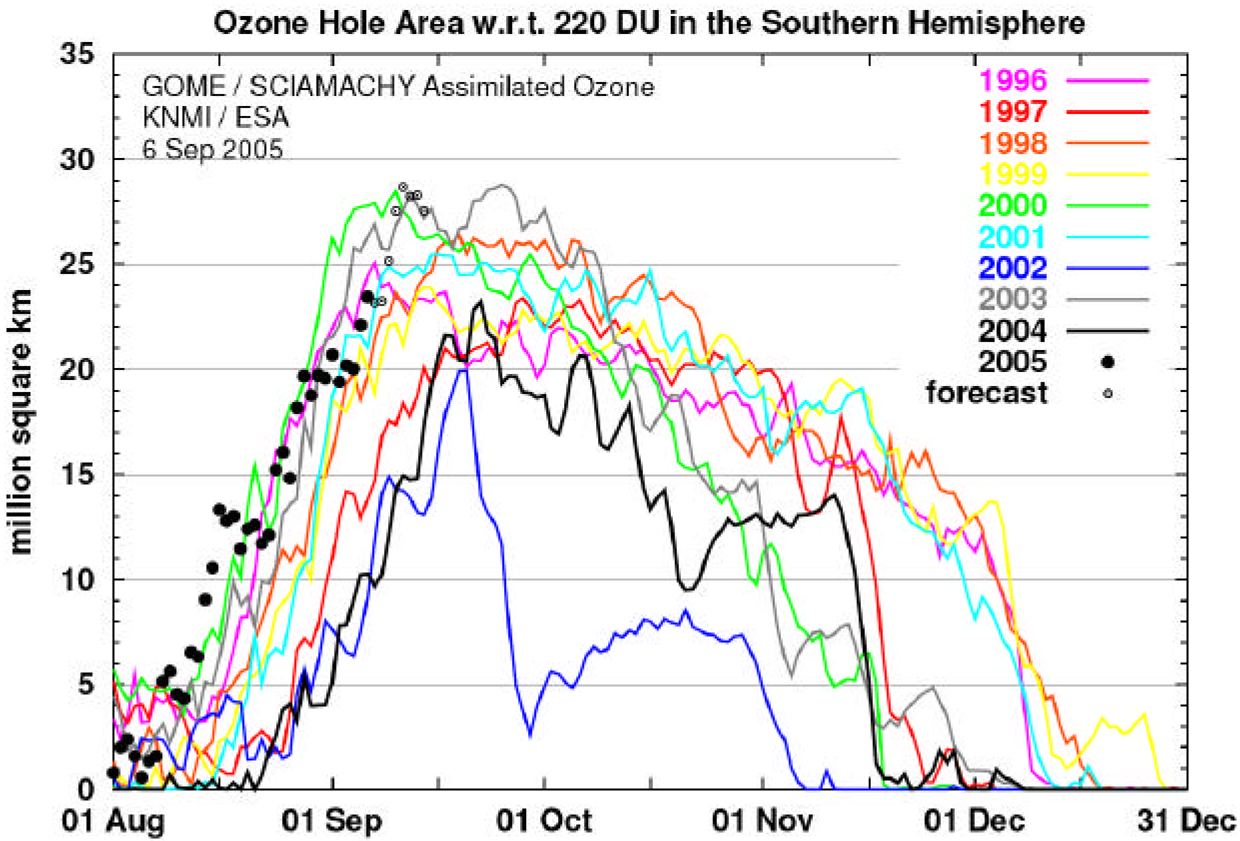
As seen by OMI ...



August 2005: very early start of ozone hole

Ozone hole size
GOME and
SCIAMACHY

plot generated on
6 Sep 2005



Residual transport

Residual circulation: Brewer-Dobson, STE

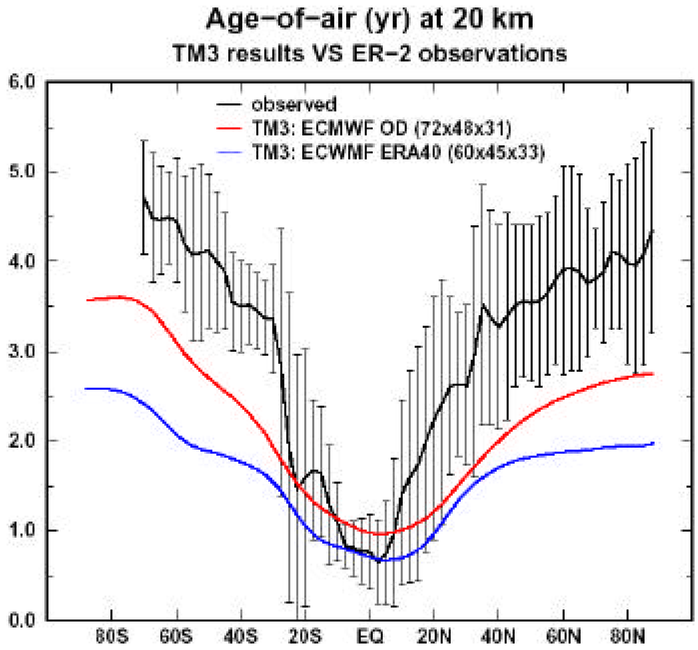
Issue:

The distribution and concentration of long-lives trace gases (CH4, N2O, O3, CO) is very sensitive to a correct description of slow overturning processes in the atmosphere:
mixing barriers subtropics - midlatitudes, stratosphere-troposphere, northern - southern hemispere

Example: Too much stratosphere-troposphere exchange has a profound influence on chemistry in the troposphere

Note: NWP models are especially well tested for medium-range time scales (10 days)

Residual circulation: Brewer-Dobson, STE

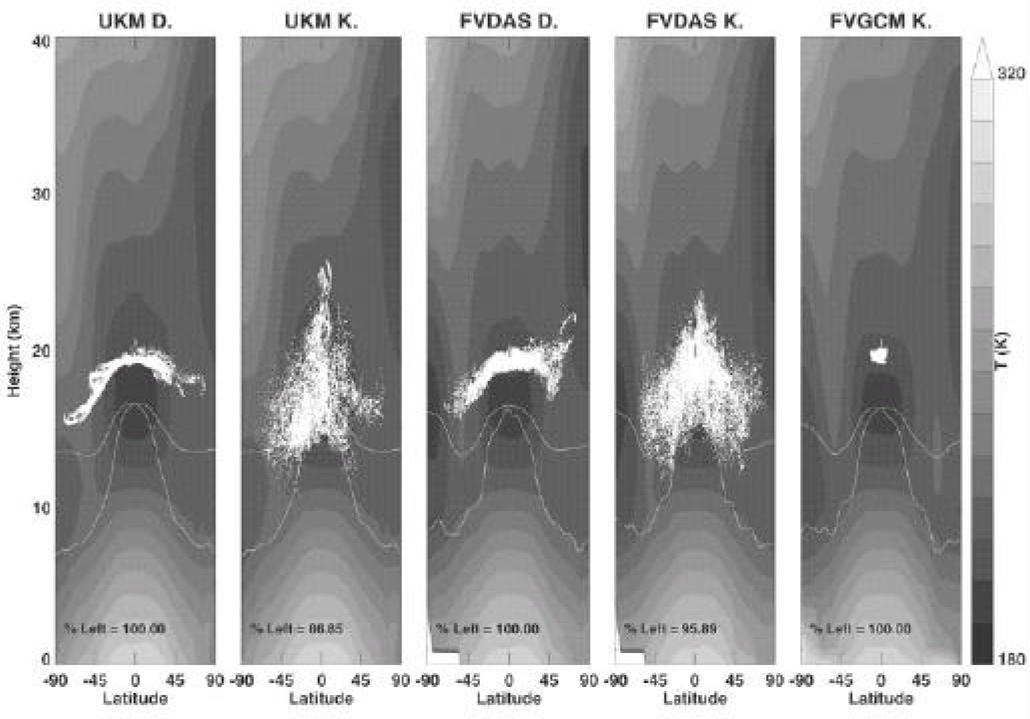


Bram Bregman

- Stratosphere-troposphere exchange enhanced:
  large ozone influx problem for tropospheric chemistry models
  Twan van Noije, J. Geophys. Res, 109, 2004

Residual circulation: Brewer-Dobson, STE

Trajectory study:
Schoeberl et al, jgr 108, 2003



Recent run at ECMWF with improved bias correction on temperature and with 4D-Var shows considerable improvement:
Adrian Simmons, GEMS kick-off

Ozone: Summary and challenges (1)

KNMI

Satellite ozone measurements and assimilation

- Long list of satellite instruments measuring ozone, but only small fraction is assimilated operationally: SBUV, TOVS, bit of MIPAS, GOME, SCIAMACHY, TOMS for reanalyses
- Total ozone measured accurately by UV-Vis spectrometers TOMS, GOME, SCIA, OMI: latest retrievals have accuracy order 2%
- Still lack of tropospheric satellite ozone measurements
- **Challenges:**
  1. Create operational analyses and re-analyses based on multiple-satellite observations: limb-nadir, trop-strat-meso 3D view
  2. Realistic tropospheric analyses, e.g. by combining total ozone observations, stratospheric profile observations and a well tuned data assimilation scheme. Improve retrievals specifically with respect to troposphere.

Ozone: Summary and challenges (2)

Ozone modeling

- Dynamical features in the lower stratosphere (and total column anomalies) modelled well in much detail
- Ozone and clear-sky UV forecast work well
  useful up to D+7, also for extreme events like sudden warmings
- **Challenge:**
  Find efficient way to accurately represent ozone chemistry
  in NWP models
  GEMS: coupling IFS and CTMs with comprehensive chemistry

Ozone: Summary and challenges (3)

KNMI

Ozone assimilation

- rms(OmF) of total ozone data assimilation typically 3%
- **Challenge:**
  Demonstrate positive impact of ozone assimilation on wind field

Age of air, strat-trop exchange

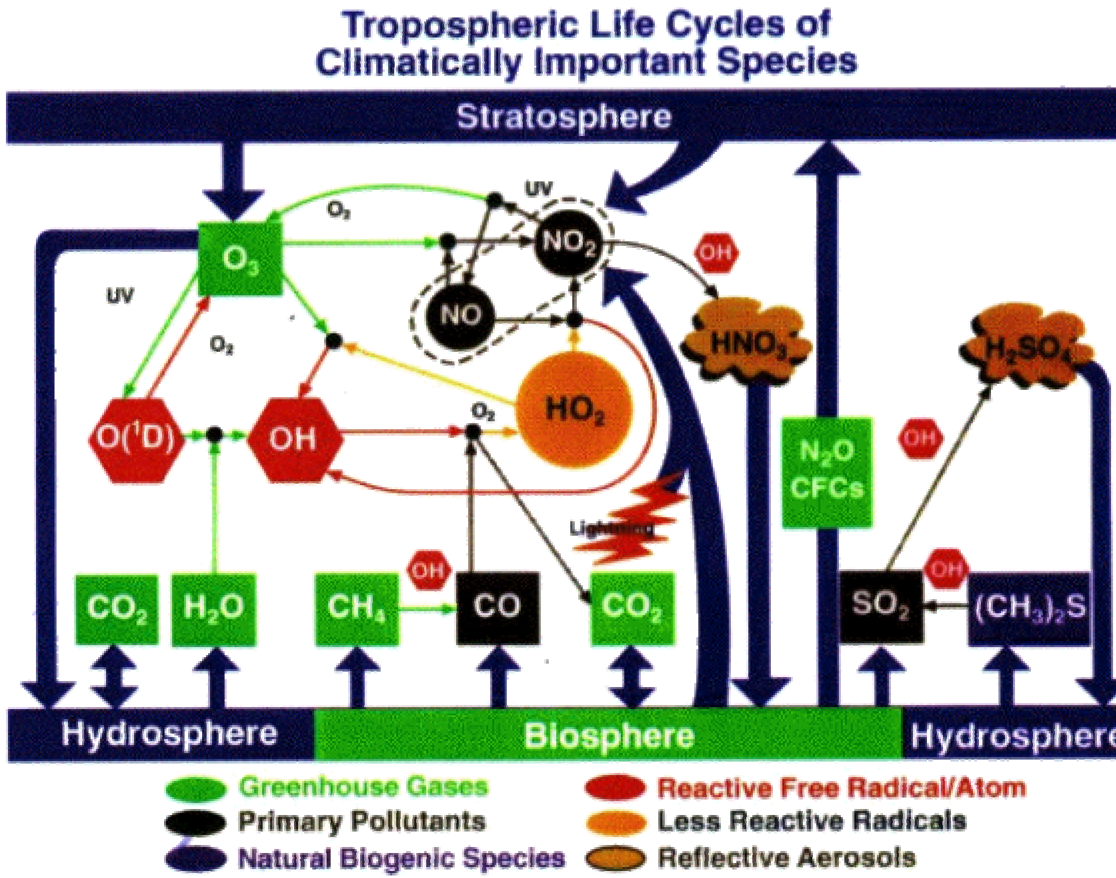
- Assimilation models typically show too strong mixing
  between tropics-extratropics (M. Schoeberl),
  stratosphere-troposphere exchange too fast
  These issues crucial for trace gas modelling
- **Challenge:**
  Identify problems and improve
  e.g. bias corrections of satellite temperature observations in
  higher stratosphere (ECMWF)

Satellite observations of tropospheric chemistry / air quality

GEMS: Focus on O_3, CO, CH_4, NO_2, CH_2O, SO_2

Why these gases ?

- Crucial compounds for chemistry of free troposphere
- Crucial compounds in air-quality O_3, NO_2, CO, SO_2 (and aerosols) all subject to regulations
- CH_2O related to total hydrocarbon release
- CH_4 greenhouse gas
- Satellite data has recently become available !



W.W. McMillan et al, JGR 2005

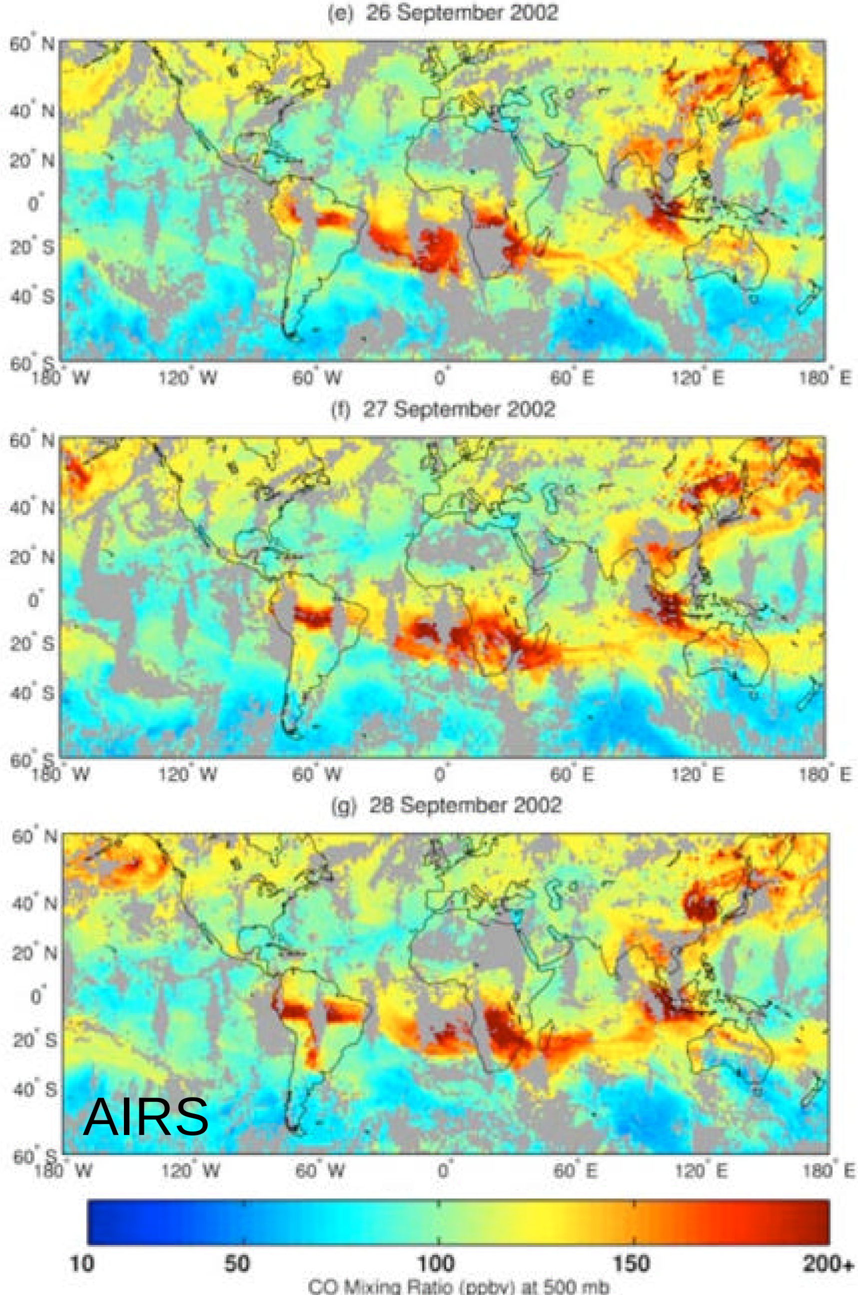
Carbon monixide

Satellite sensors:

- MOPITT
- AIRS
- IASI
- TES Aura
- SCIAMACHY
- IMG
- MIPAS
- SMR - Odin
- ACE-FTS
- MLS-Aura

Note:

- Infrared instruments especialy sensitive to middle troposphere
- Near infrared sensitive to surface



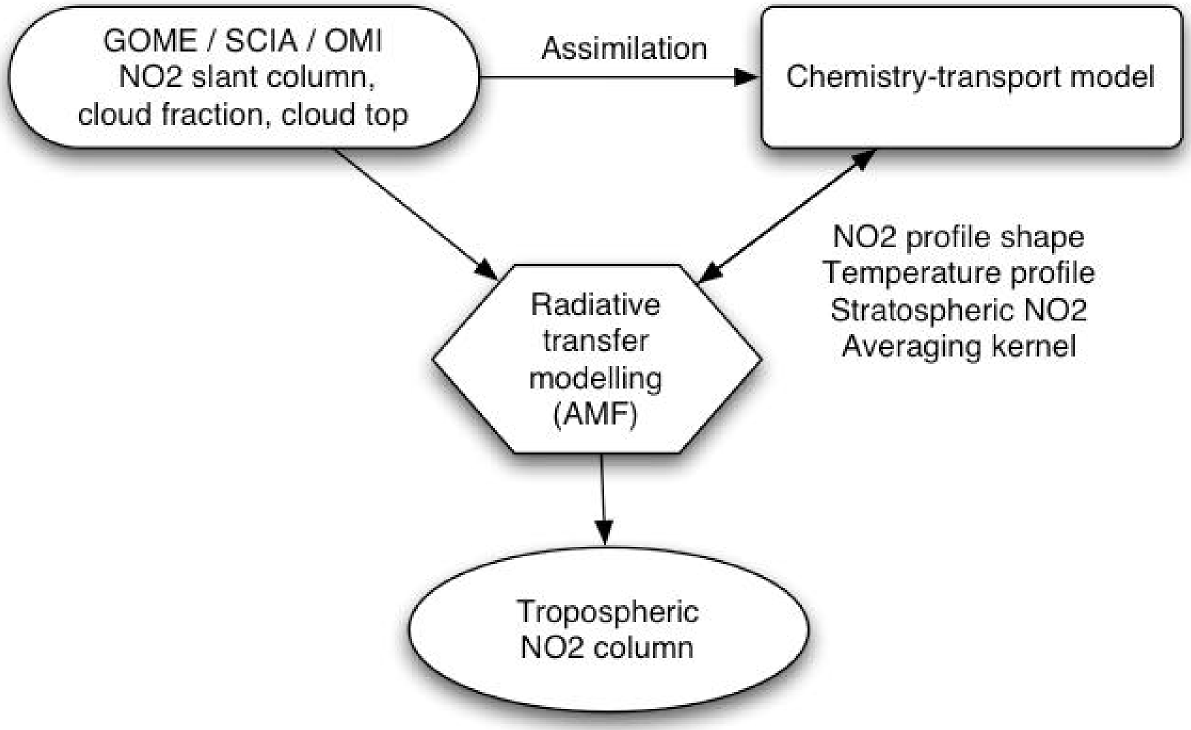
NO_2: combined retrieval/modeling/assimilation

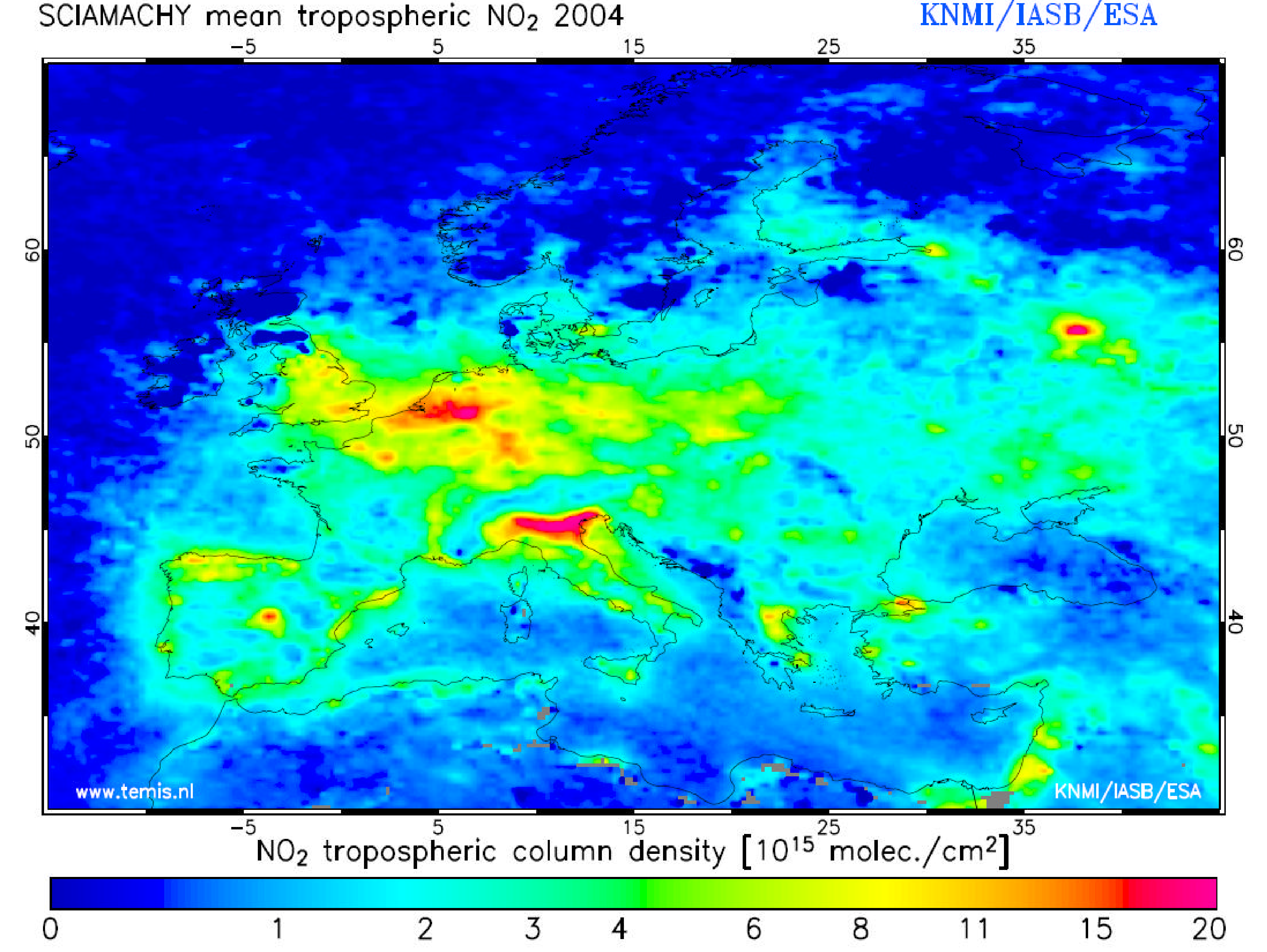
KNMI

Slant column retrieval by BIRA-IASB

Tropospheric column retrieval by KNMI

Accounting for:
- Clouds
- Surface albedo
- Profile shape
- Stratosphere
- T-dep cross sections



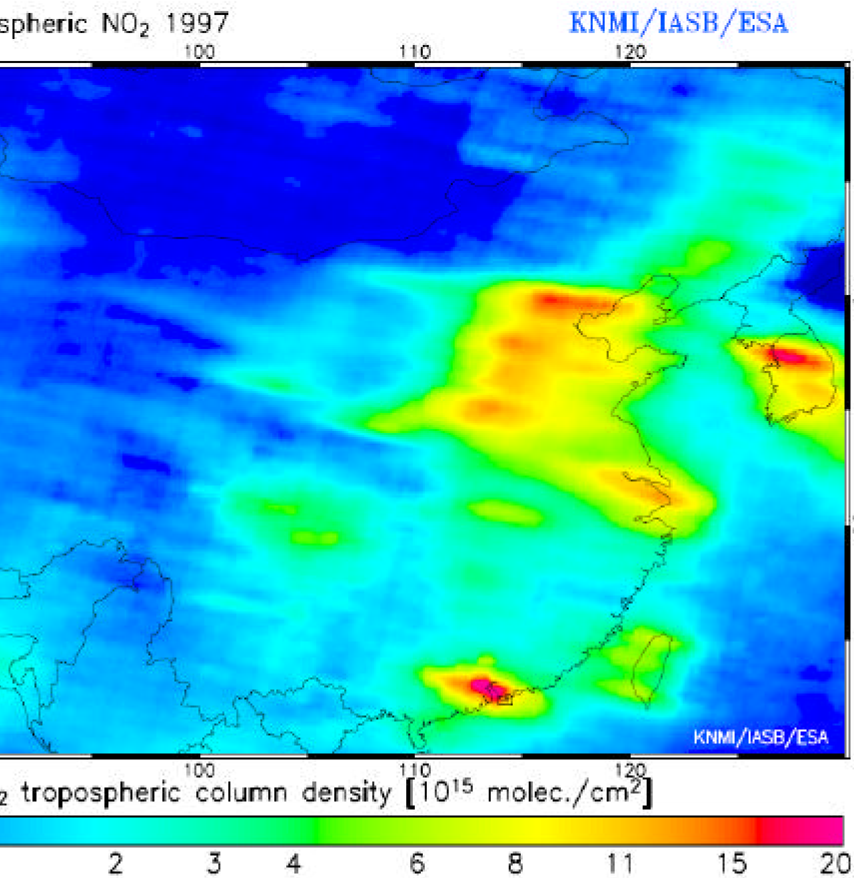


SCIAMACHY mean tropospheric NO2 2004
KNMI/IASB/ESA
−5
5
15
25
35
60
50
40
www.temis.nl
KNMI/IASB/ESA
NO2 tropospheric column density [10^15 molec./cm^2]
0
1
2
3
4
6
8
11
15
20

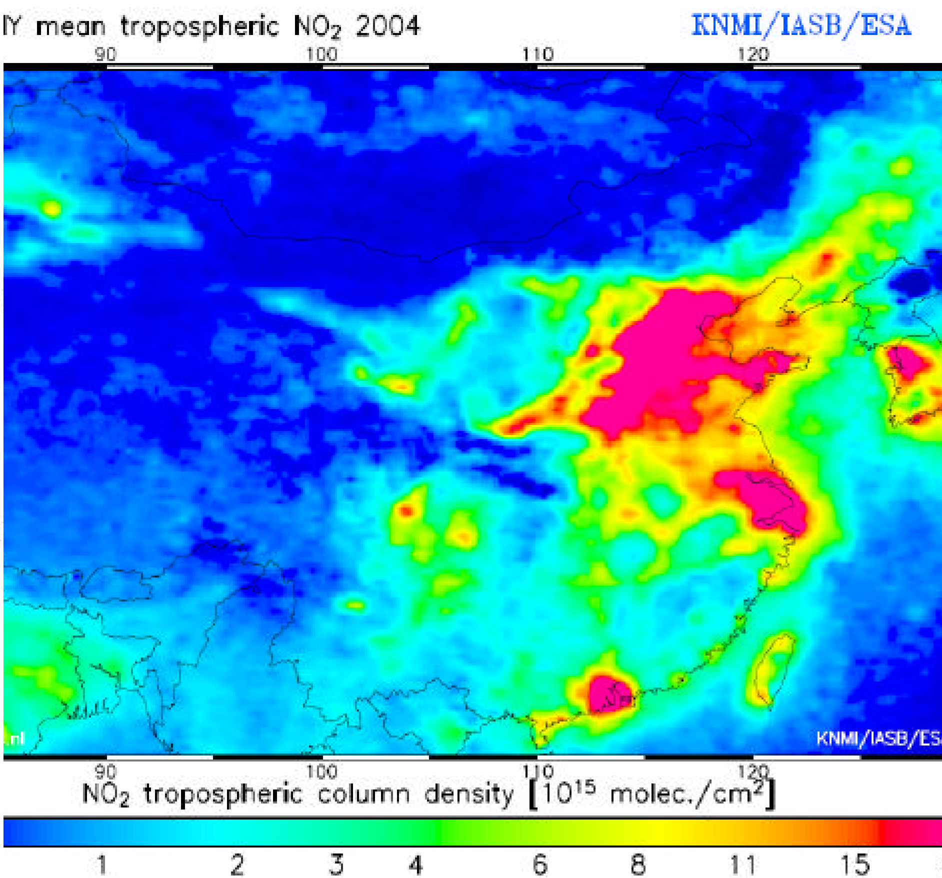
NO_2 trend over China

KNMI

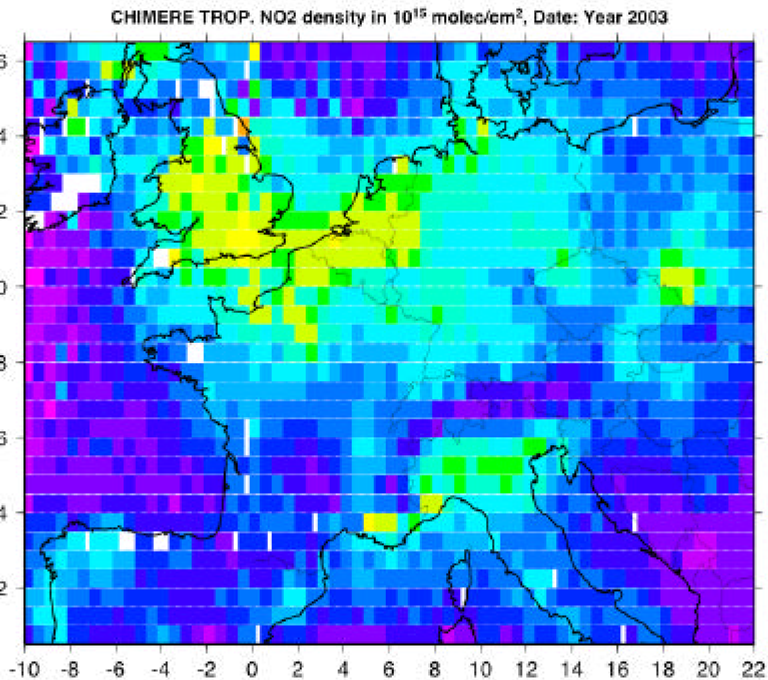
GOME, 1997

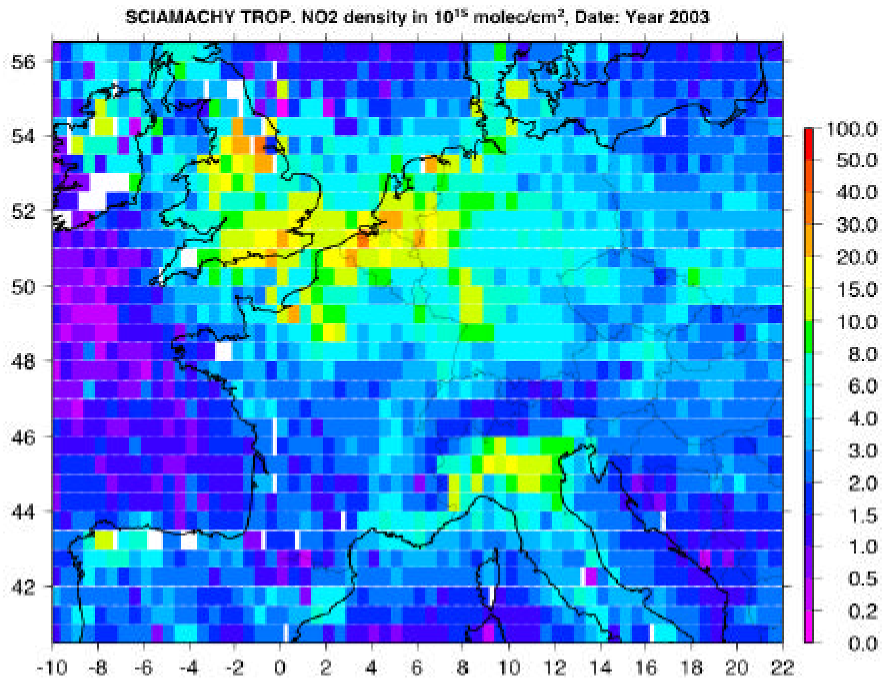


SCIA, 2004



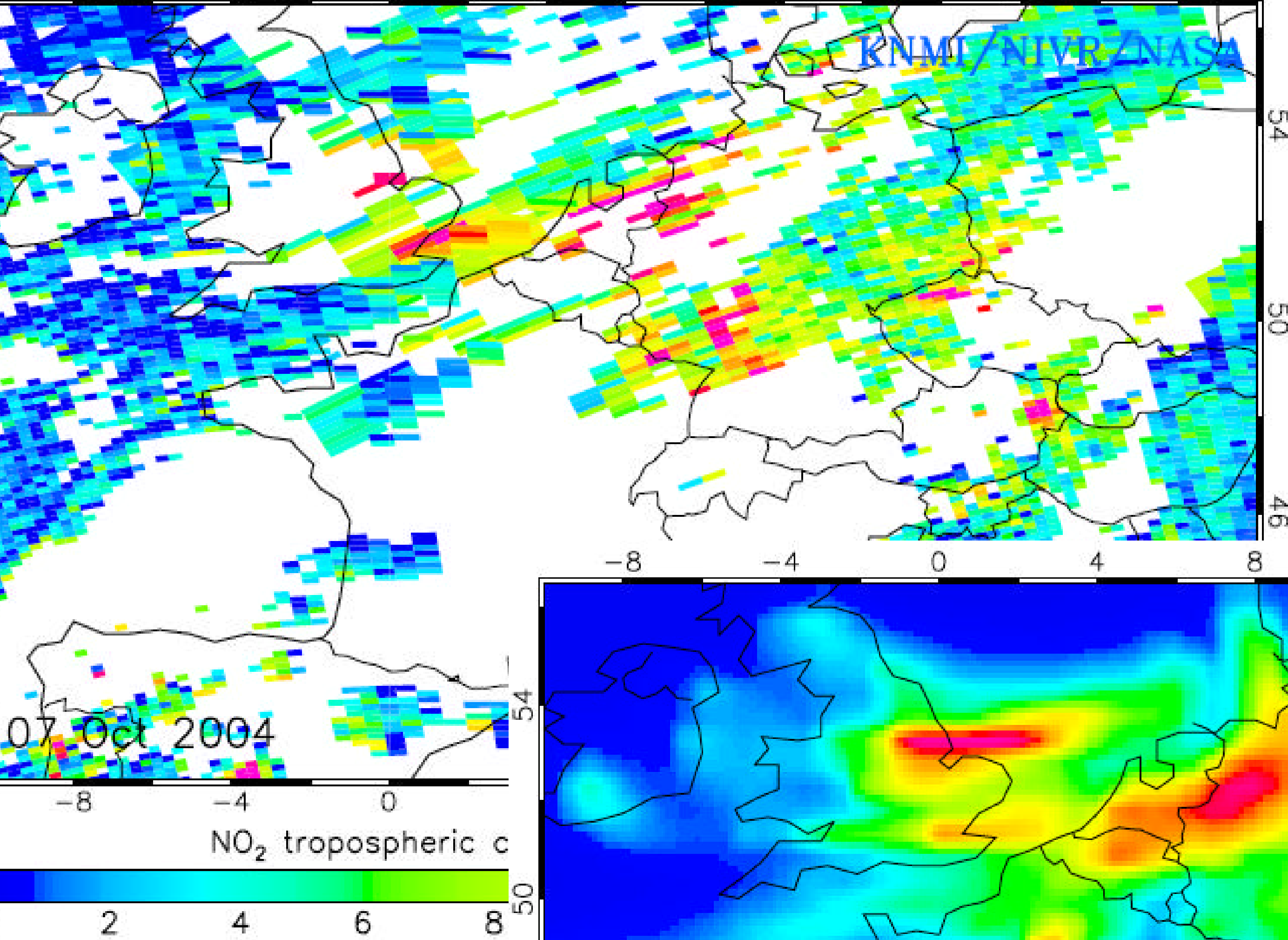
SCIAMACHY vs CHIMERE: 2003 yearly mean

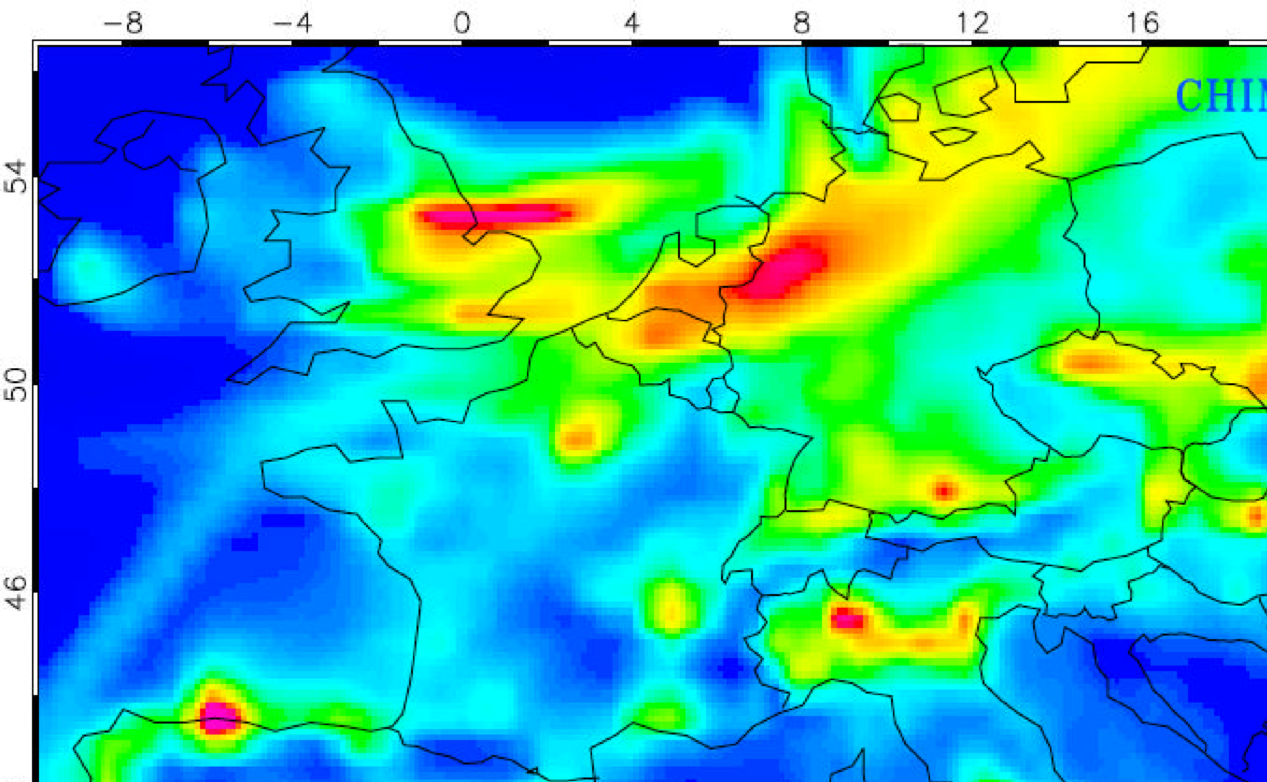




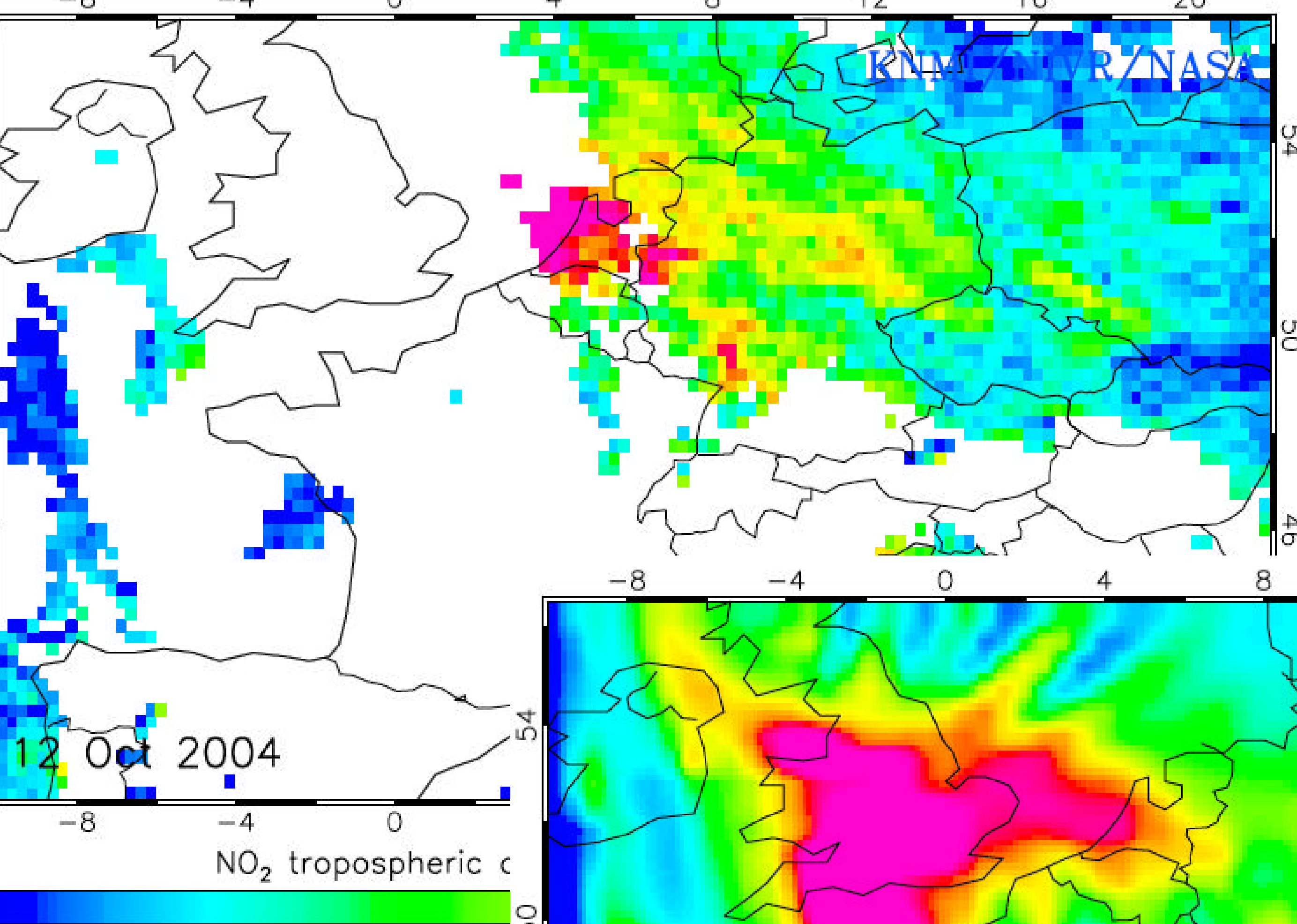
Yearly-mean bias = 0.2 10^{15} molec cm^{-2}, RMS 2.9, correl.coeff. 0.73
Cloud-free pixels

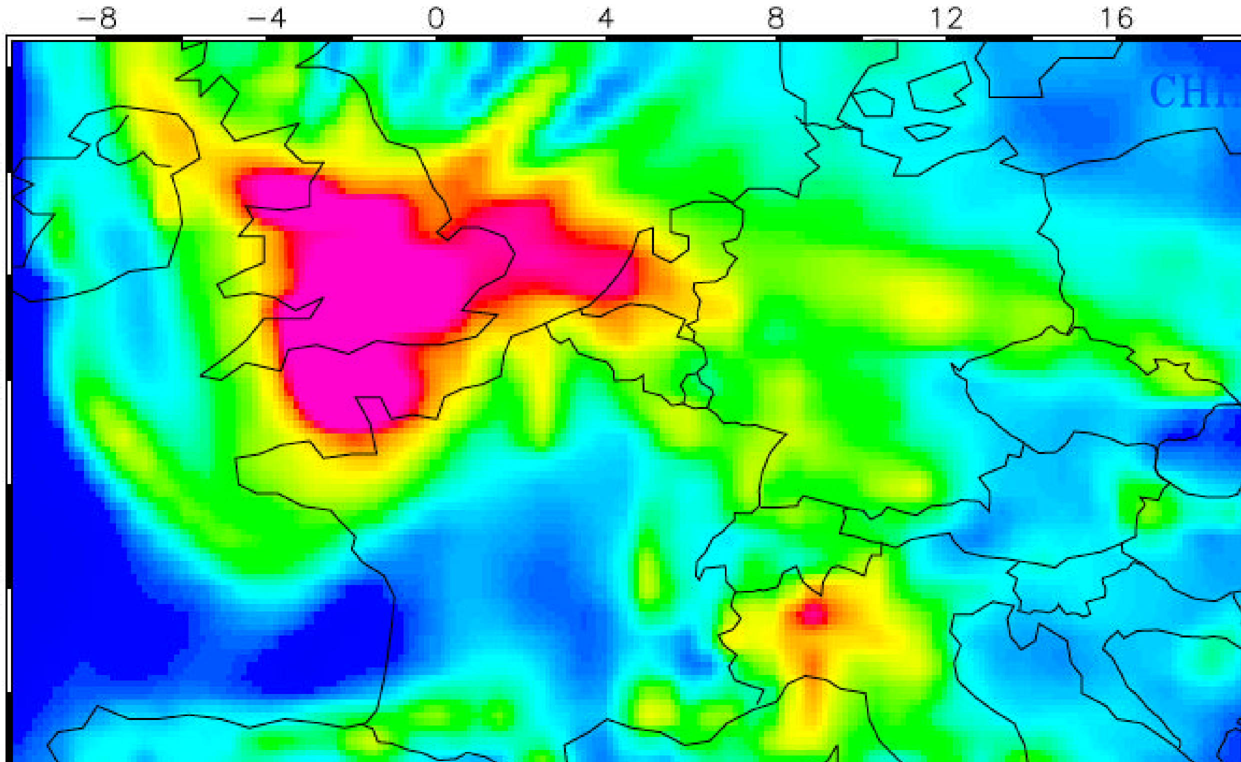
NO_2
OMI vs. Chimèr





NO_2
OMI vs. Chimèr

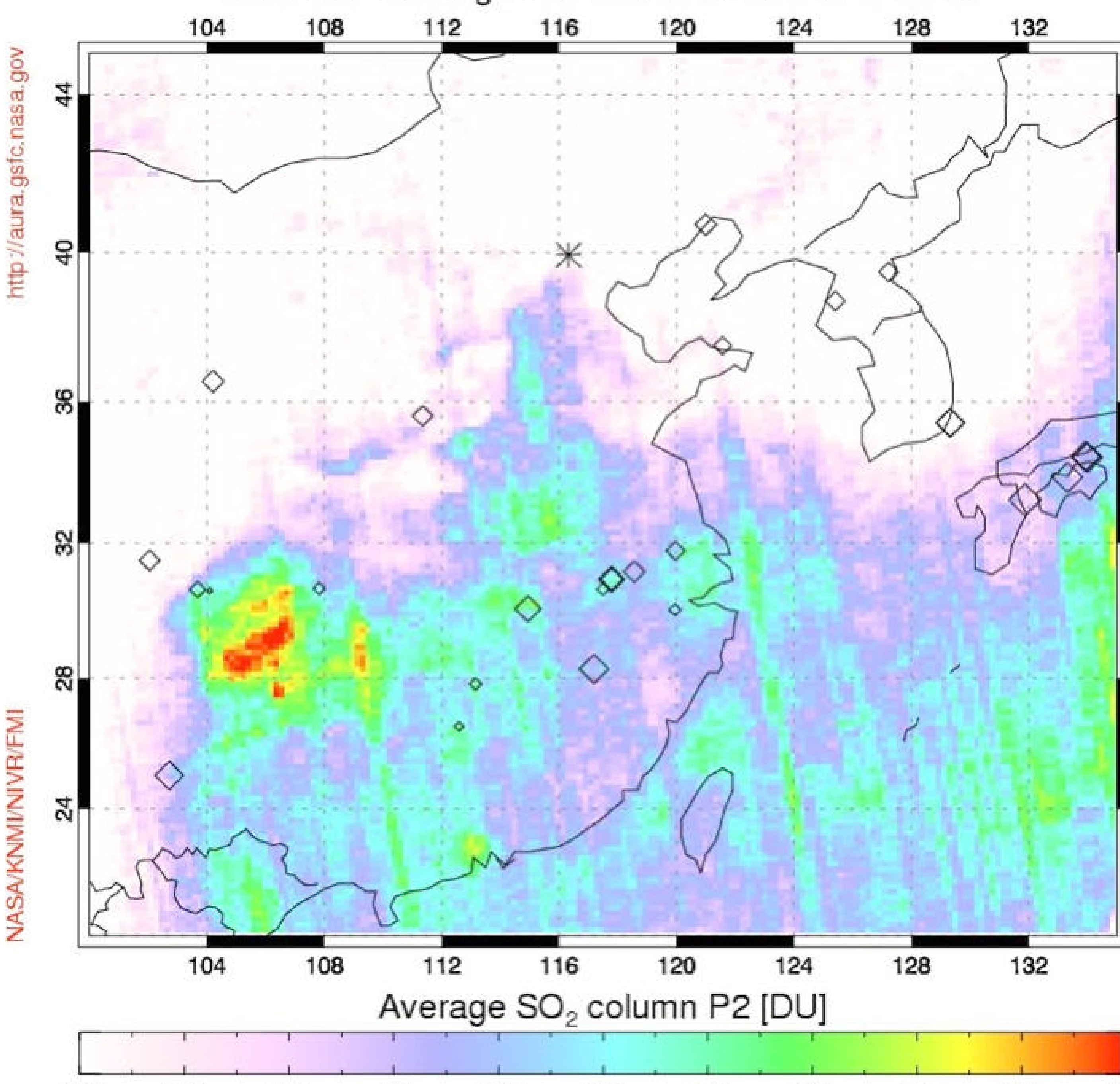




OMI SO_2

Source:
A. Krueger
S. Carn
(UMBC)

Presented at
OMI Science
Team meeting,
KNMI,
June 2005

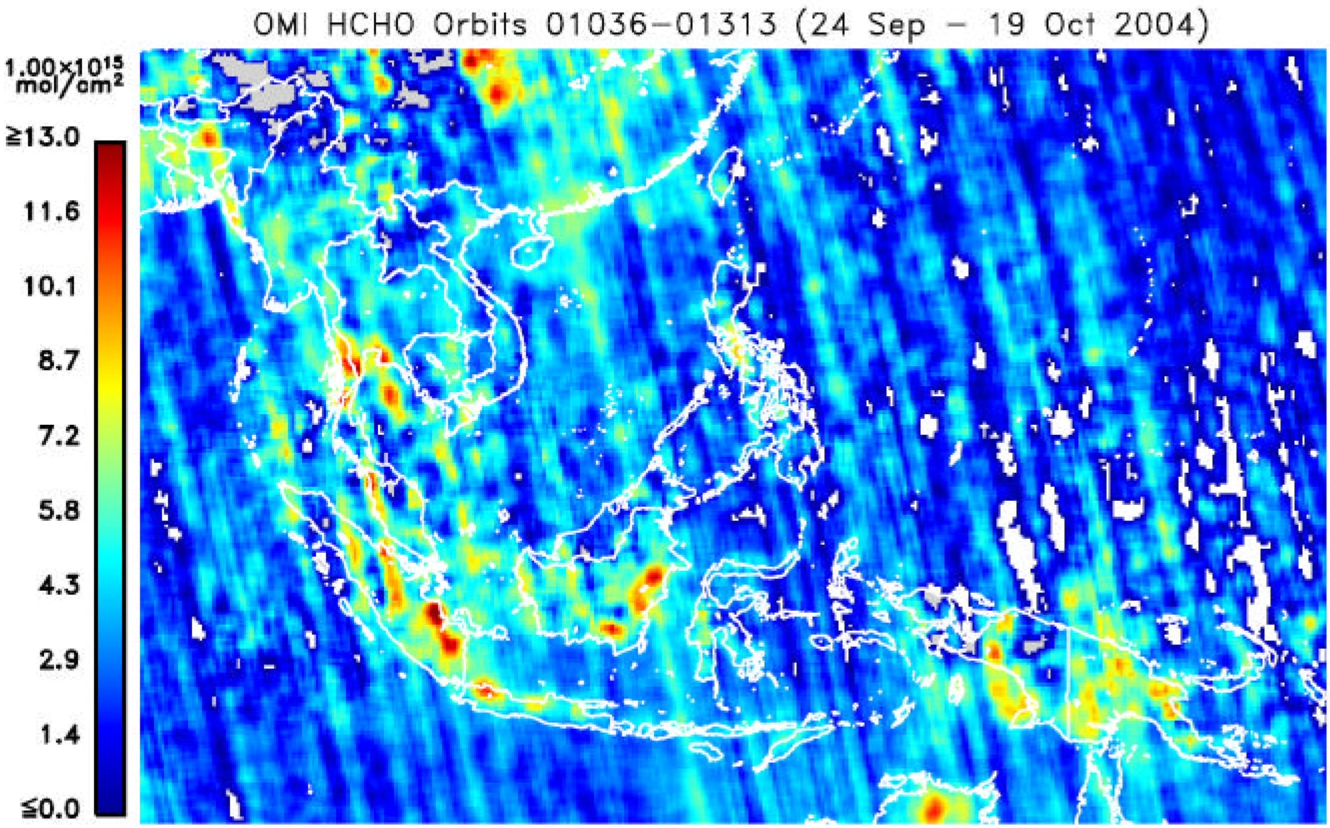


••••

OMI CH_2O

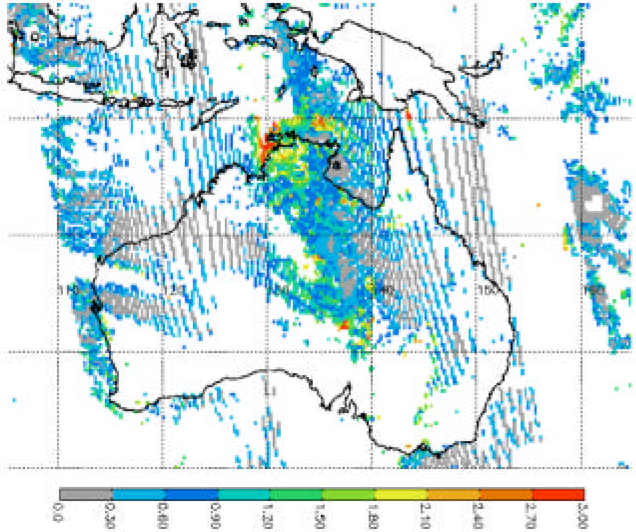
Source:
K. Chance
T. Koruso

Presented at
OMI Science
Team meeting,
KNMI,
June 2005

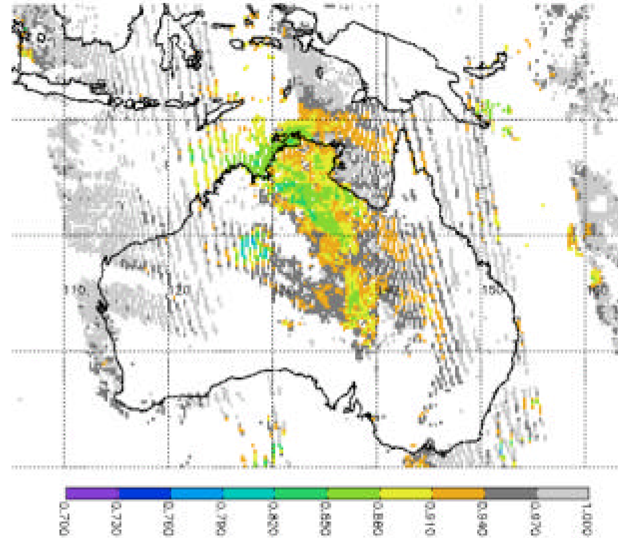


OMI aerosol

Aerosol optical depth



Single scattering albedo

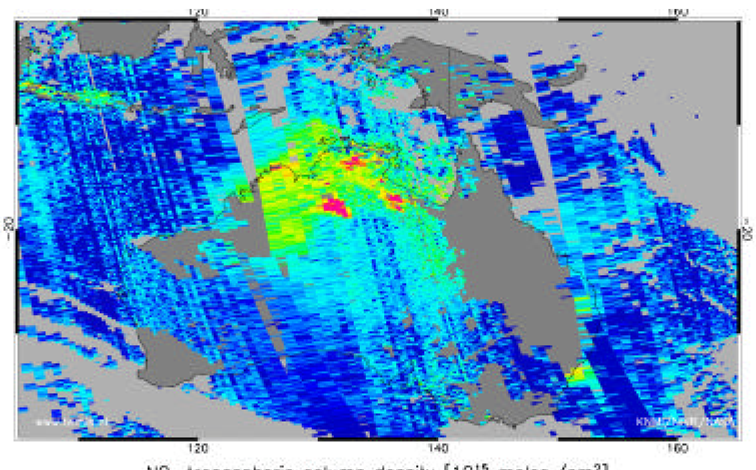


11 Oct 2004

Courtesy O. Torres
NASA-GSFC &
UMBC-JCET

Levelt et al,
IEEE special issue
on EOS-Aura, 2005

NO_2



Combined 4D-Var source and initial state assimilation of methane

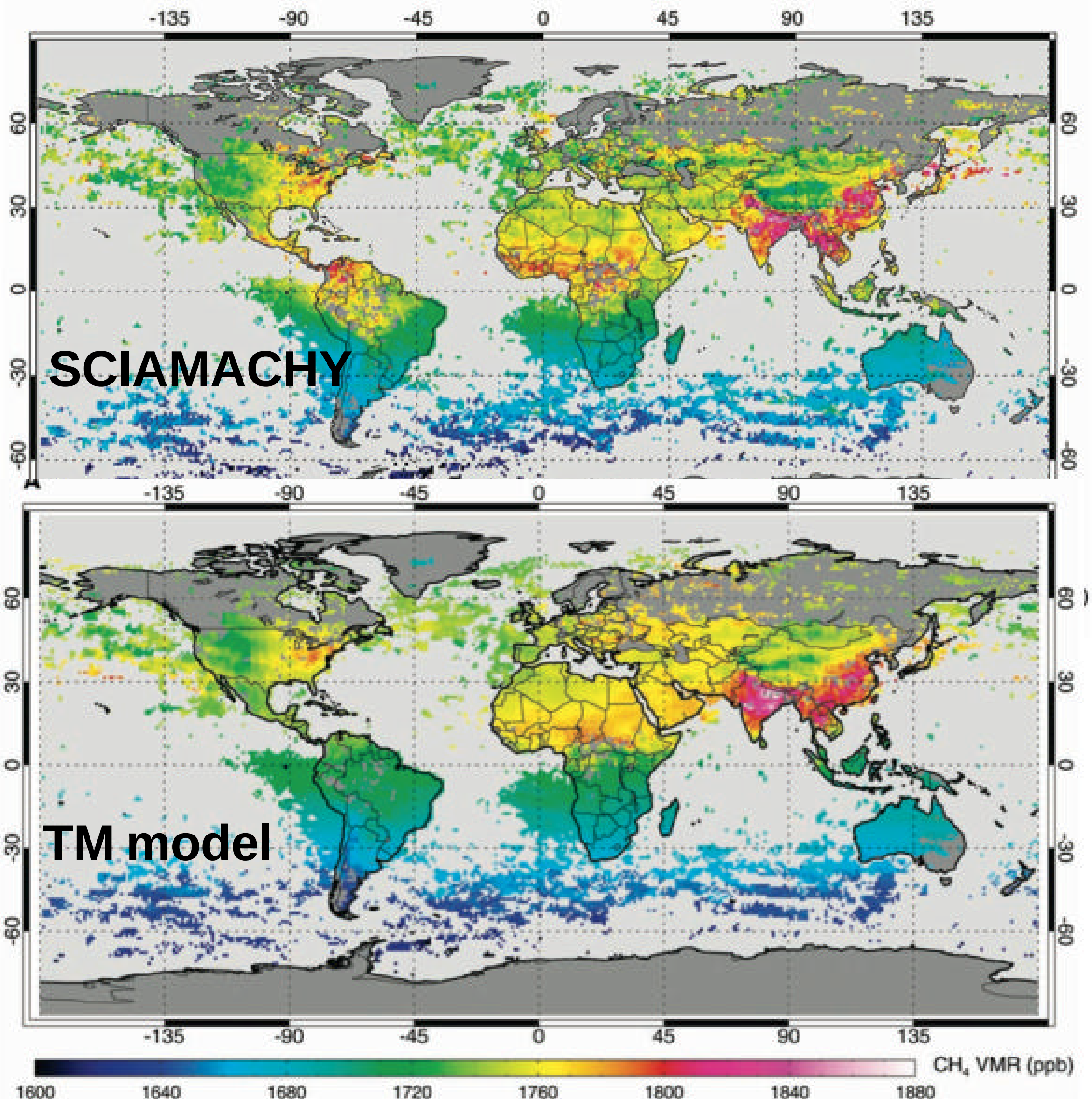
SCIAMACHY methane

SCIAMACHY

vs

TM model

C. Frankenberg
Science 308,
May 2005



SCIAMACHY methane OSSE

4D-Var:

joint optimalisation of 2D emissions + 3D initial field $\boldsymbol{v} = (\boldsymbol{s}, \boldsymbol{c}_0)$

1 month time window

$$J(\boldsymbol{v}) = \frac{1}{2}(\boldsymbol{v}_b - \boldsymbol{v})^T \mathbf{B}^{-1}(\boldsymbol{v}_b - \boldsymbol{v}) + \\ + \frac{1}{2}\sum_{i=0}^{n}(\mathbf{H}_i\boldsymbol{x}_i - \boldsymbol{y}_i)^T \mathbf{R}_i^{-1}(\mathbf{H}_i\boldsymbol{x}_i - \boldsymbol{y}_i).$$

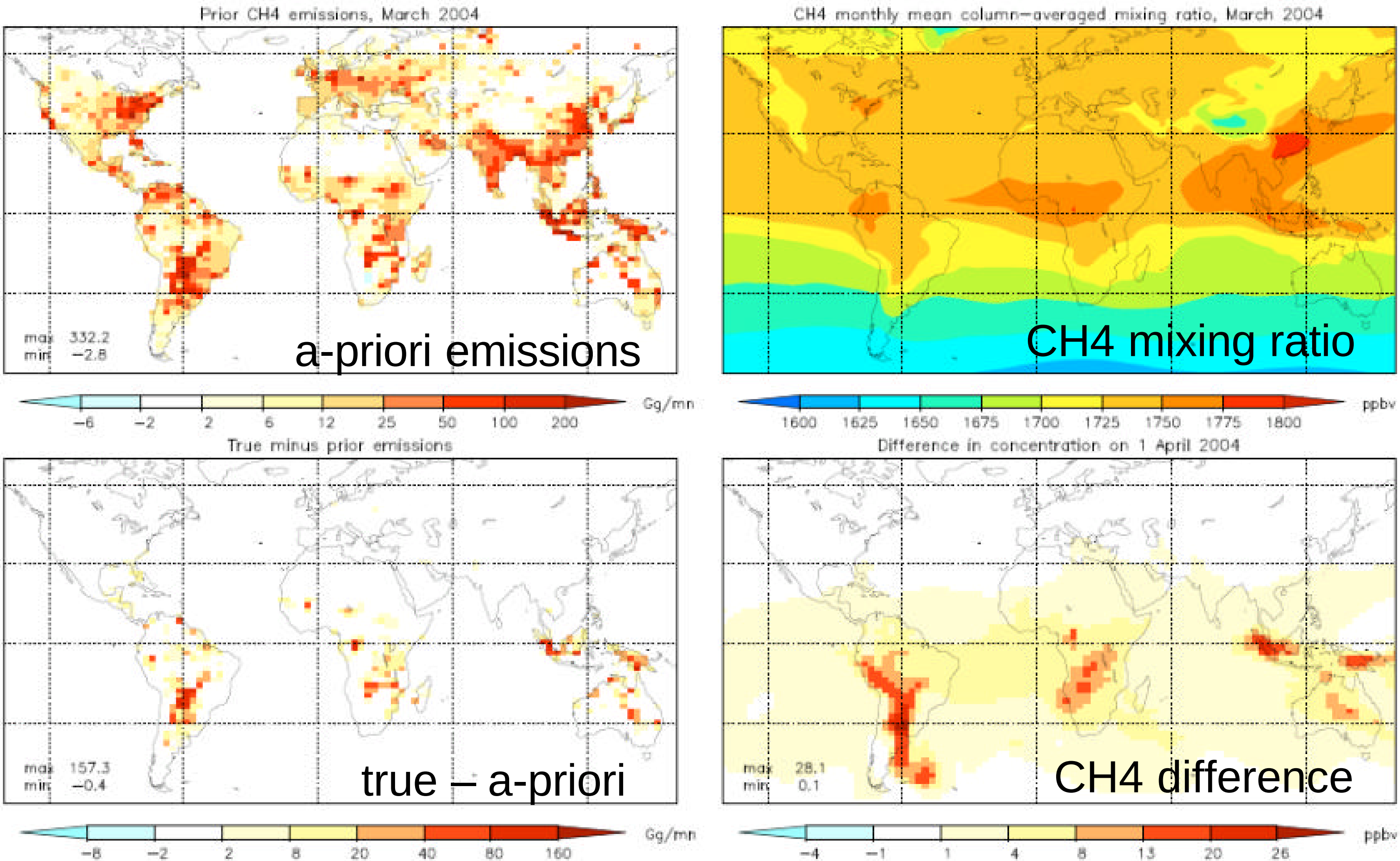
Model:

Single tracer. Detailed CH_4 emissions. Sink: OH from full chemistry run

SCIAMACHY simulated CH_4 observations, real cloud retrieval

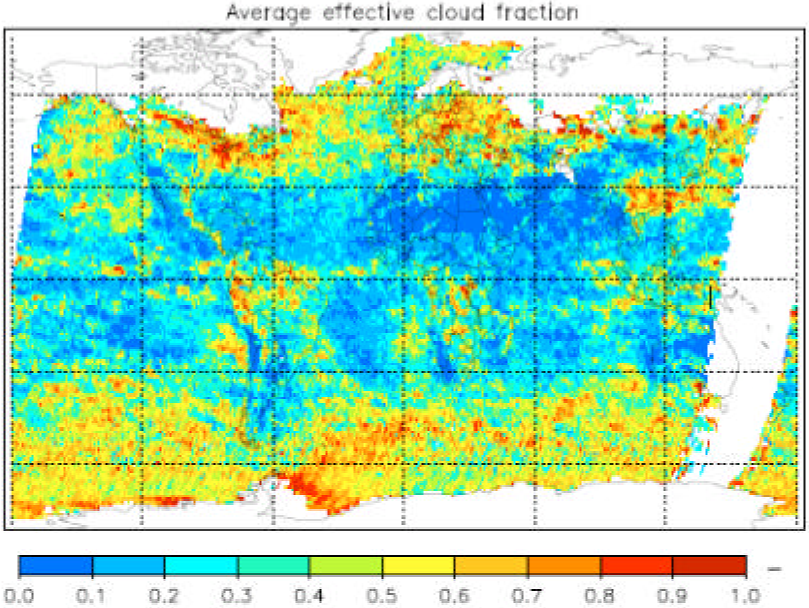
Meirink et al, submitted to ACP, 2005

SCIAMACHY methane OSSE: experiment setup

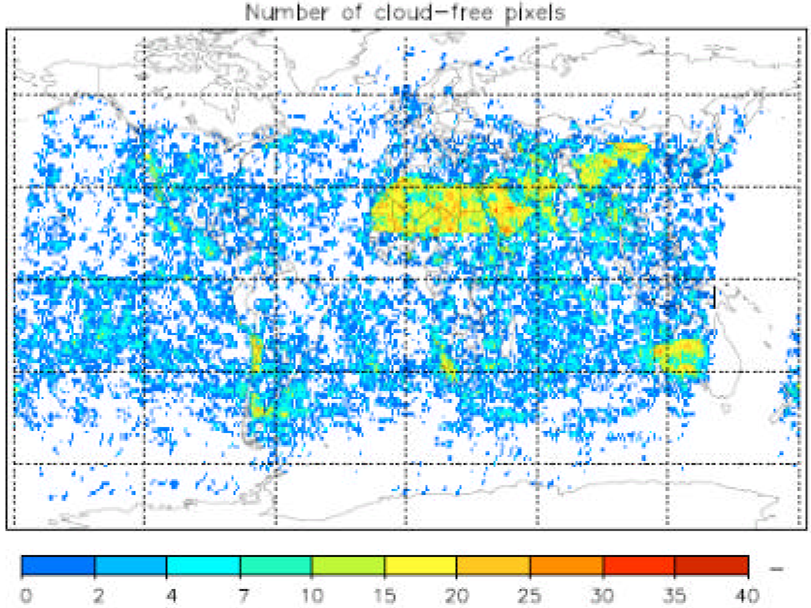


SCIAMACHY methane OSSE: cloud

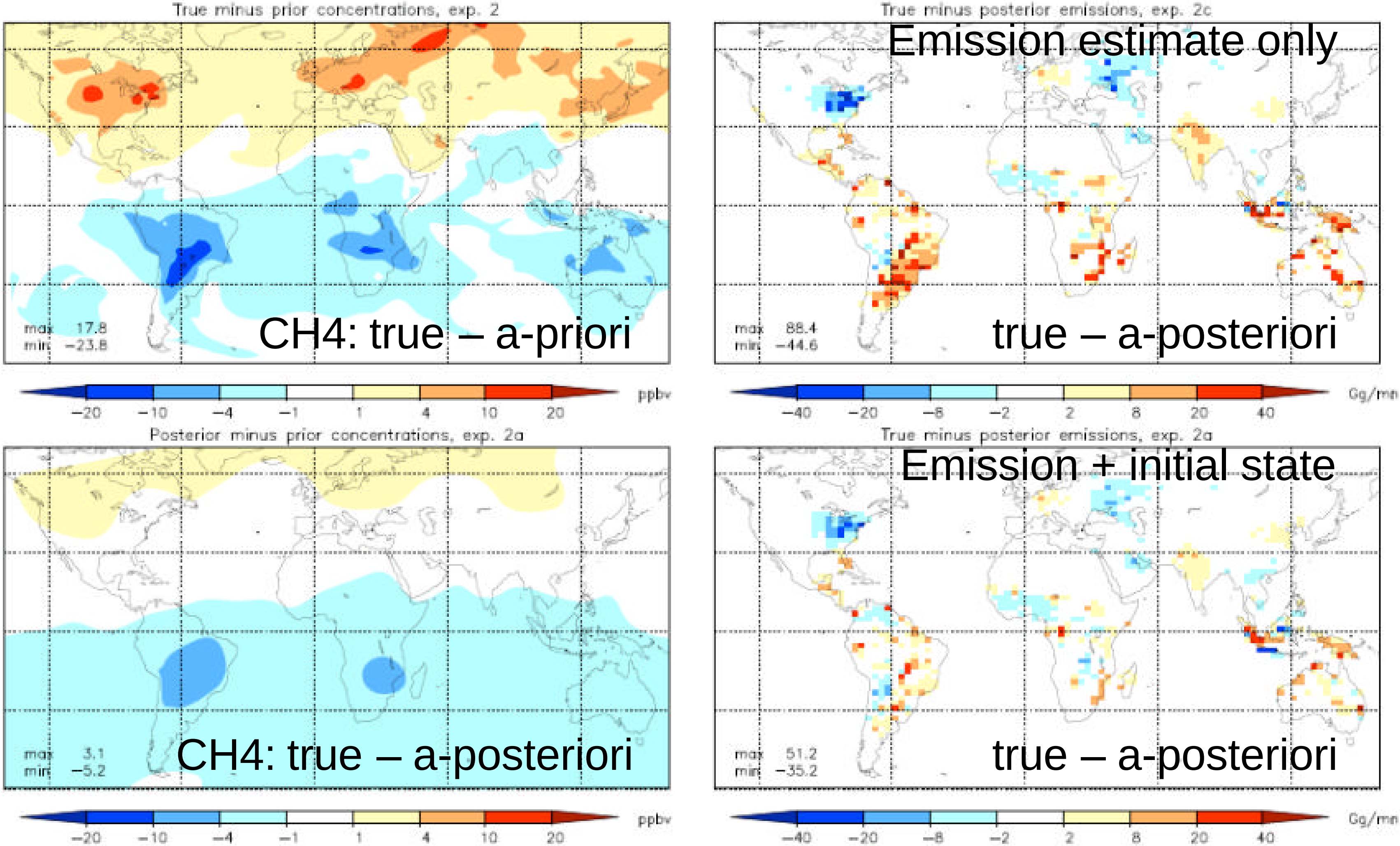
Mean cloud fraction



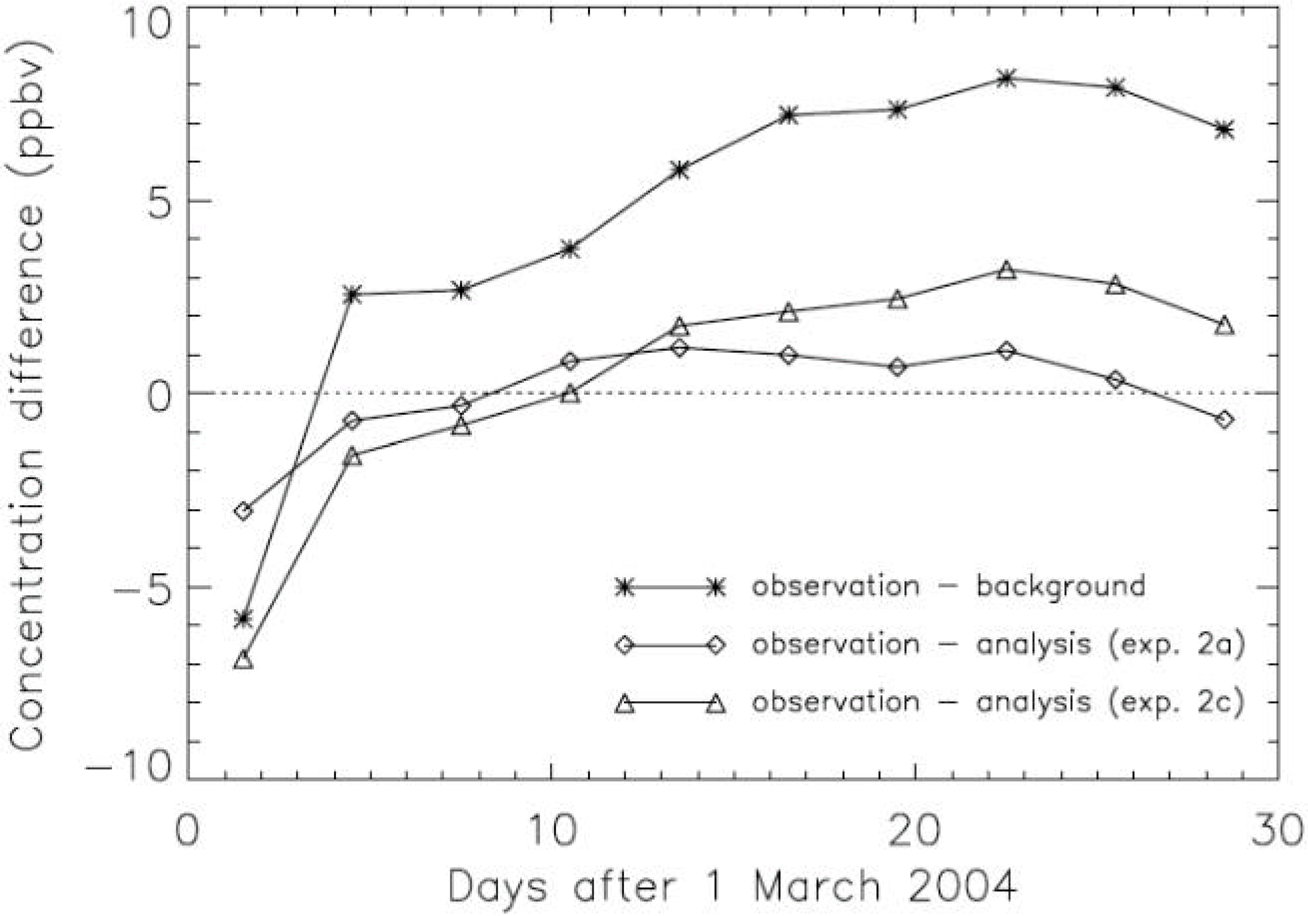
of cloud-free pixels



SCIAMACHY OSSE: emission and initial state opt



SCIAMACHY OSSE: emission and initial state opt



SCIAMACHY methane OSSE

Conclusions:

- A combined state + emission 4D-Var assimilation system is potentially able to extract meaningful information on emissions, on a monthly time scale and 500km spatial scale.
  With a 1 month time window the system can efficiently distinguish emission errors from initial state errors.
- A SCIAMACHY retrieval precision of 1-2 % will enable improved source estimations (Heidelberg retrievals reach 1.5-2%)
- The use of cloudy pixels is essential, despite their larger uncertainty. Cloud and albedo parameters should be retrieved as accurately as possible, averaging kernels should be provided with the observations.

Tropospheric chemistry: Summary and challenges

KNMI

Tropospheric observations of CO, CH_4, NO_2, CH_2O, SO_2

- New satellite instruments, new retrievals and data sets have become available for the troposphere in the past couple of years
- Tropospheric retrievals are difficult (compared to e.g. the stratosphere)
- Retrievals in troposphere difficult due to inteference from clouds, aerosols, surface properties
- New instruments like OMI with high coverage / small pixels allow day-to-day monitoring of individual events: fires, volcanoes
- **Challenge:**
  Improvement and characterisation of retrievals, validation

Tropospheric chemistry: Summary and challenges

KNMI

Assimilation, inverse modelling

- Very few studies up to now. Focus on CO from MOPITT.
- Joint state + emission 4D-Var:
  promising approach for all tropospheric tracers.
- **Challenge:**
  Set up assimilation/inverse modelling approaches for tropospheric chemistry. Use of satellite observations to improve tropospheric chemistry models, emission inventories, air-quality forecasts.