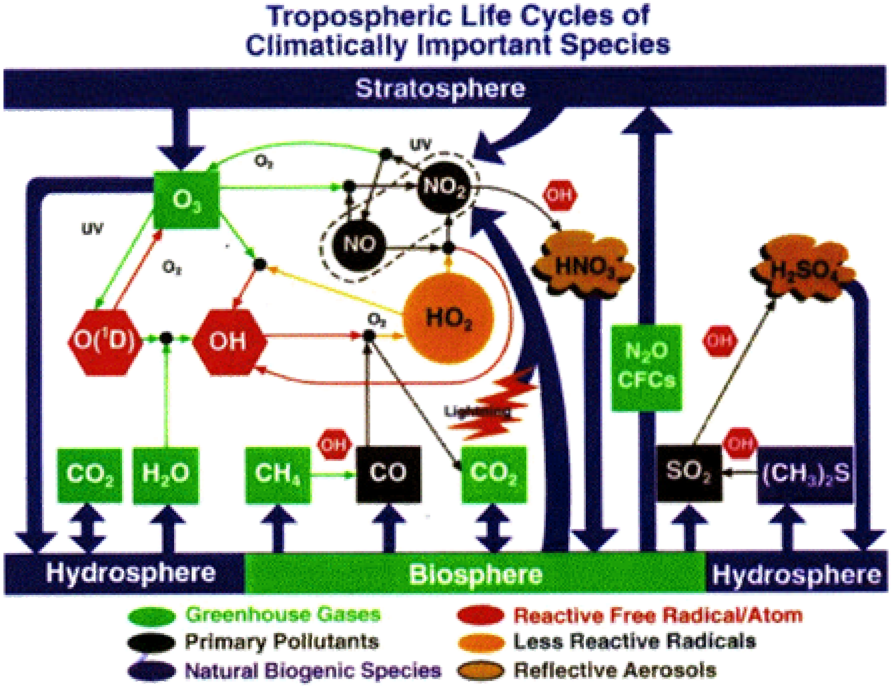
The role of data assimilation in atmospheric composition monitoring and forecasting

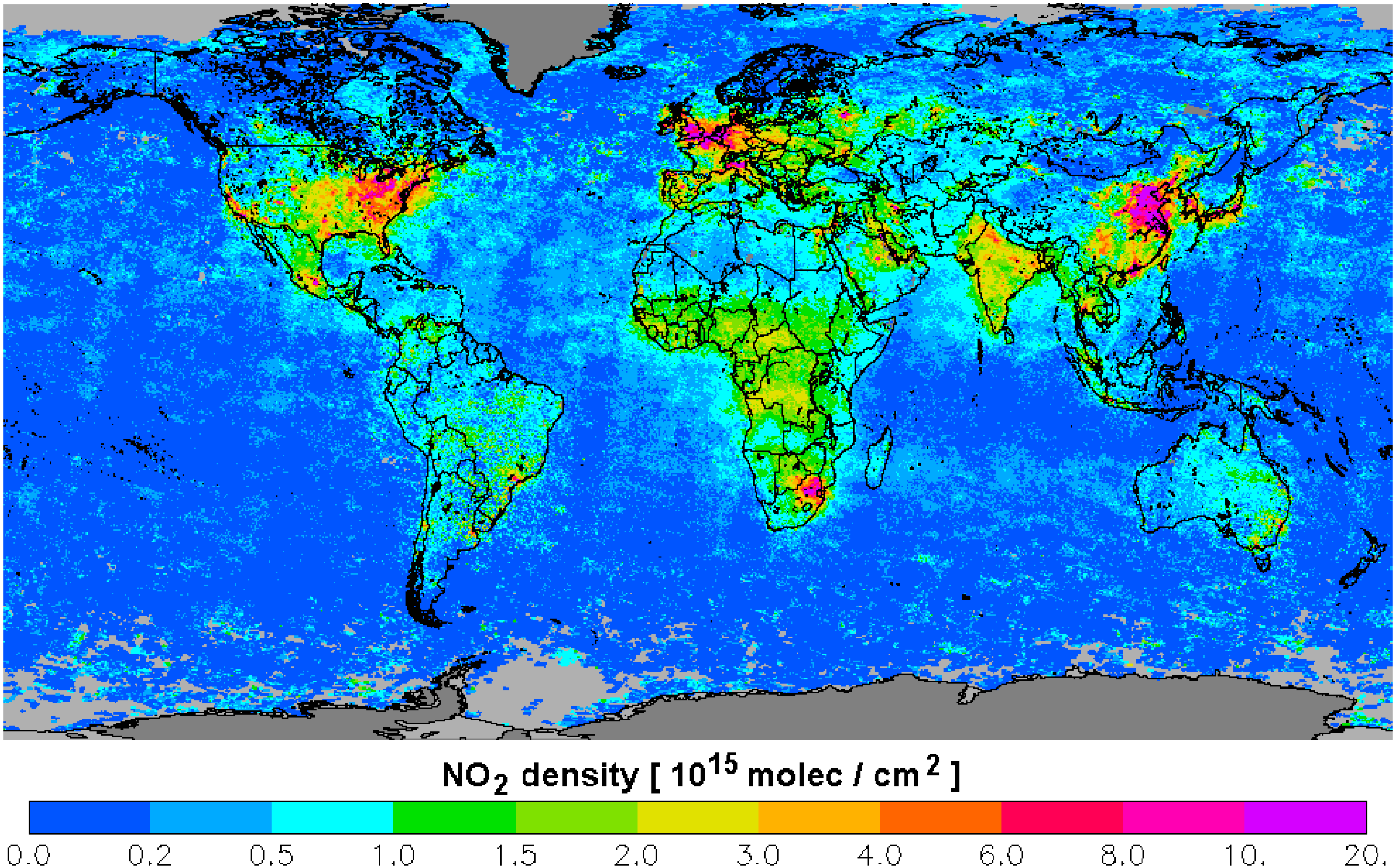
Why data assimilation ?

Henk Eskes
Royal Netherlands Meteorological Institute, De Bilt, The Netherlands

Atmospheric chemistry

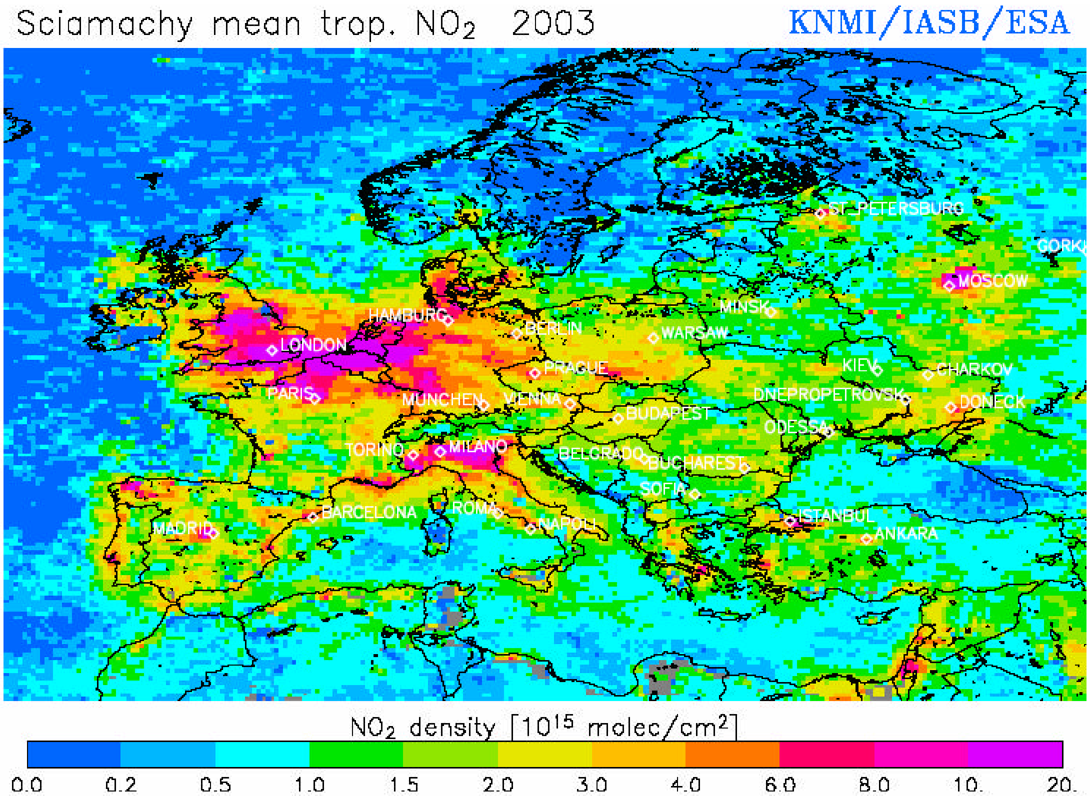


SCIAMACHY mean tropospheric NO_2 2003 **KNMI / IASB / ESA**



Henk Eskes, ESA Summer School 2004

Sciamachy NO_2 : Europa



1) From sequential sets of data points to synoptic global fields

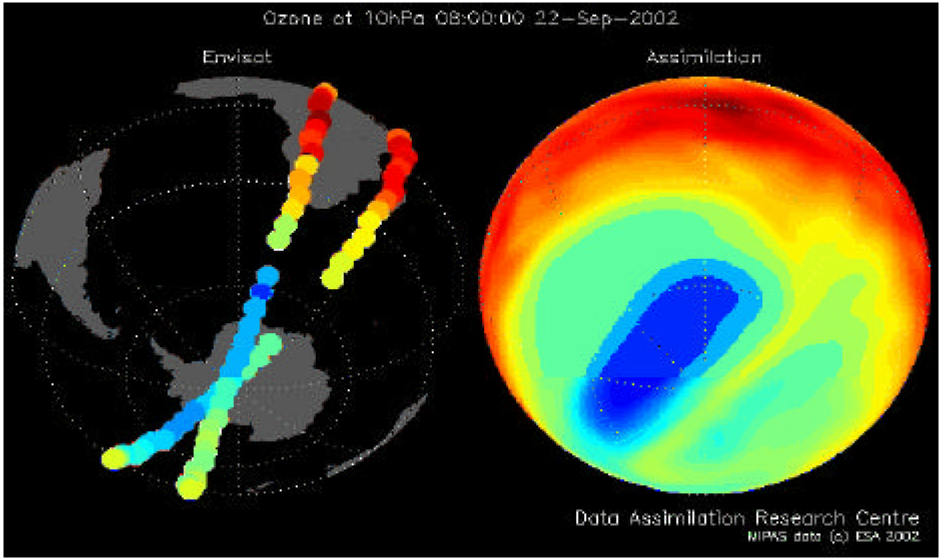
Complementarity:
Measurements - Snapshots of the atmospheric state
Model - Describes the evolution (time dependence) of the atmosphere

Time scales:
Data assimilation works best for long-lived tracers
(or slowly-varying emissions)

Value adding:
Easy to use synoptic 3D fields ("from gaps to maps")

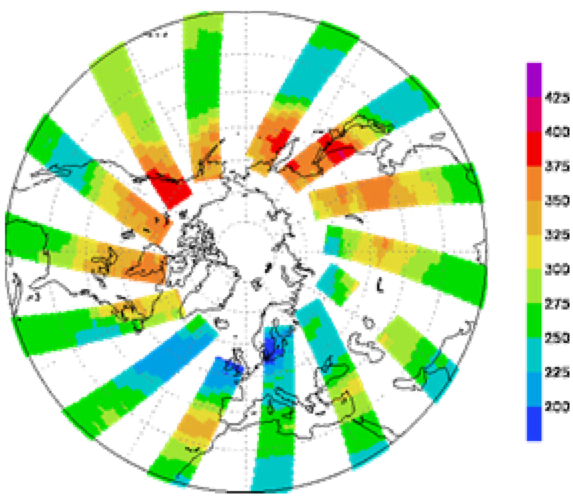
"from gaps to maps"

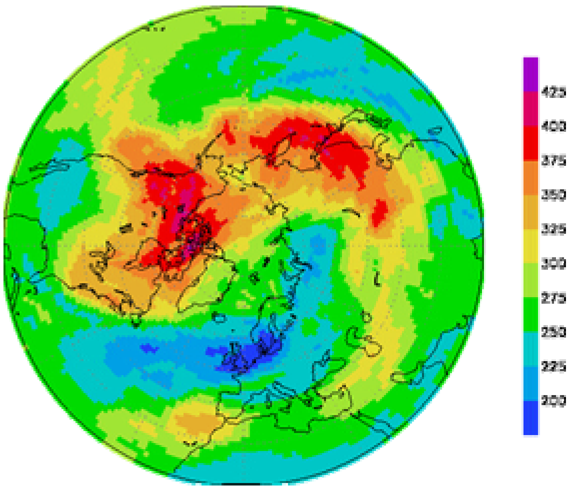
MIPAS
ozone analysis
10 hPa
22 Sep 2002



Courtesy:
Alan Geer, DARC

"from gaps to maps": low-ozone event





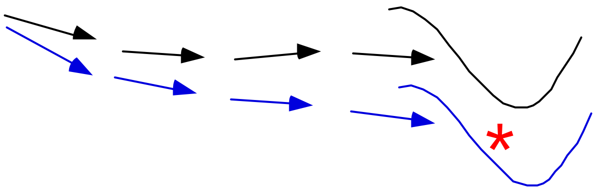
Ozone mini hole as observed by GOME, 30 November 1999

2) Propagation of information to data-poor regions and unobserved variables, unobserved chemical species

Examples:

- Atmospheric chemistry: effective number of degrees of freedom smaller than number of species. Measurement information transferred to unobserved species
- Tracer transport: the wind will carry information from observed to unobserved regions, e.g. the dark winter pole
- NWP and ozone: ozone observations contain information on the wind field

Depends critically on the quality of the model, observations and assimilation



Unobserved species

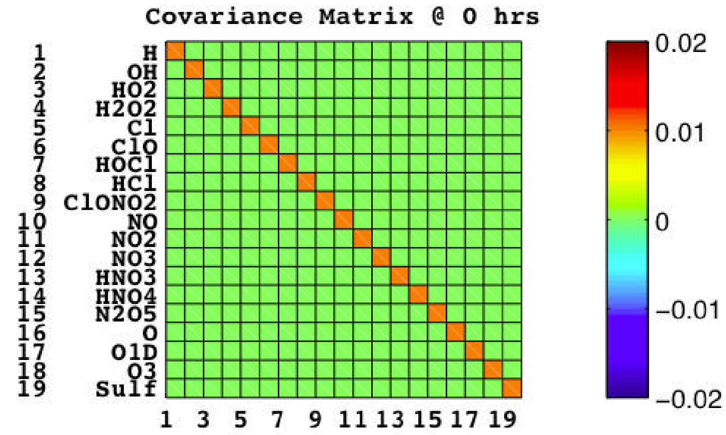
- Atmospheric chemistry characterised by small number of
  effective degrees of freedom
- Information efficiently transferred from observed to
  unobserved species
- Not all observations have same impact in assimilation:
  Use assimilation to optimise choice of species to be
  measured (by future satellite missions)

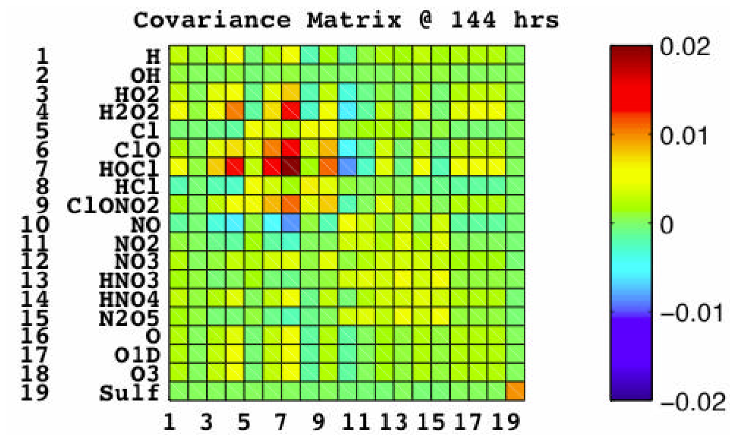
Refs on chemical 4D-Var, Kalman filter:

Fisher, Lary, QJRMS 121, 1681 (1995)
Elbern, Schmidt, JGR 104, 18583 (1999)
Khattatov, JGR 104, 18715 (1999)
Errera, Fonteyn, JGR 106, 12253 (2001)

Unobserved species

Chemical covariance matrix (Kalman filter) becomes singular

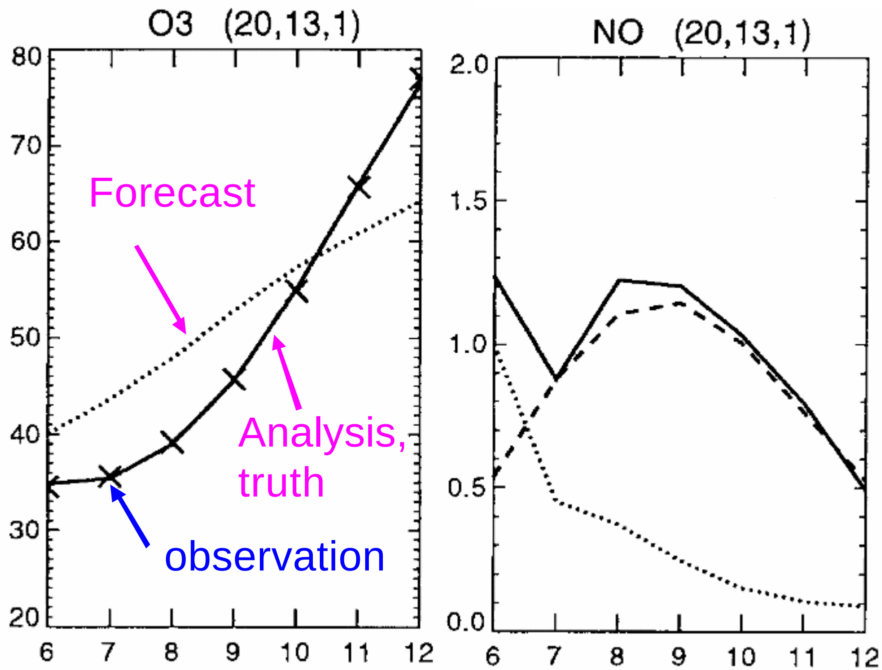




Khattatov, JGR 104, 18715 (1999)

Unobserved species

Impact of ozone observations on NO, NO_2 in 4D-Var



Elbern, Schmidt
JGR 104, 18583 (1999)

3) Confronting models with data, data with analyses

Detailed feedback on:

- quality of the model - understanding
- quality of the observations

Central quantity: Observation minus forecast statistics (OmF)

Validation with data assimilation

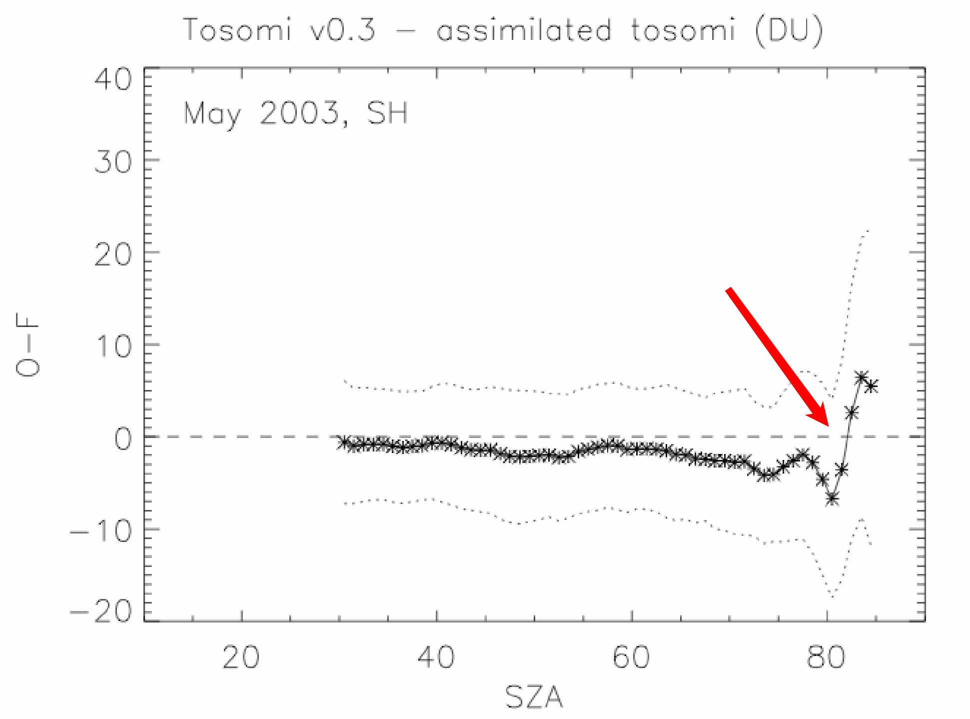
Complementary to validation with ground based observations:

1. Very good statistics: results normally significant
2. Look at relative biases, dependency of bias wrt to parameters in the retrieval, dependence with time, rms
3. Overall bias: only from comparison with other instruments
4. Difficulty of separating model from observation errors

Feedback on retrieval

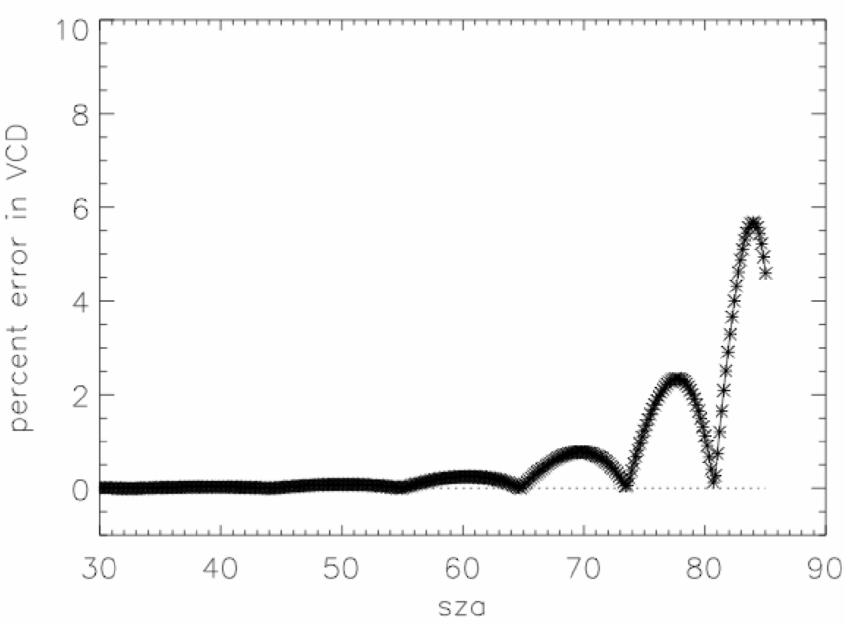
Sciamachy
ozone column
retrieval
at KNMI

Observation
minus
forecast
vs.
Solar zenith angle



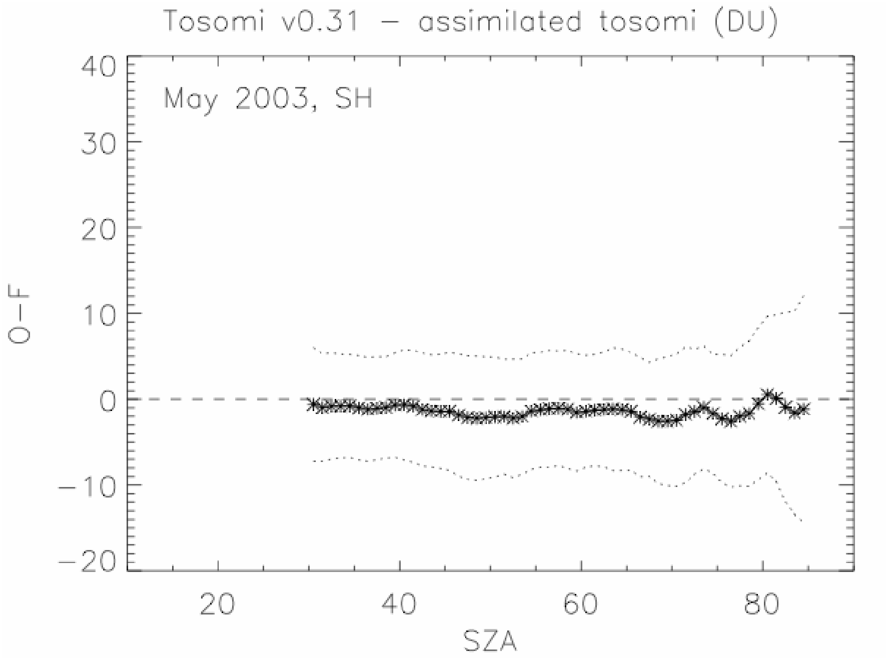
Feedback on retrieval

Theoretical curve: Estimated error in total ozone due to inaccuracies in the lookup table ...



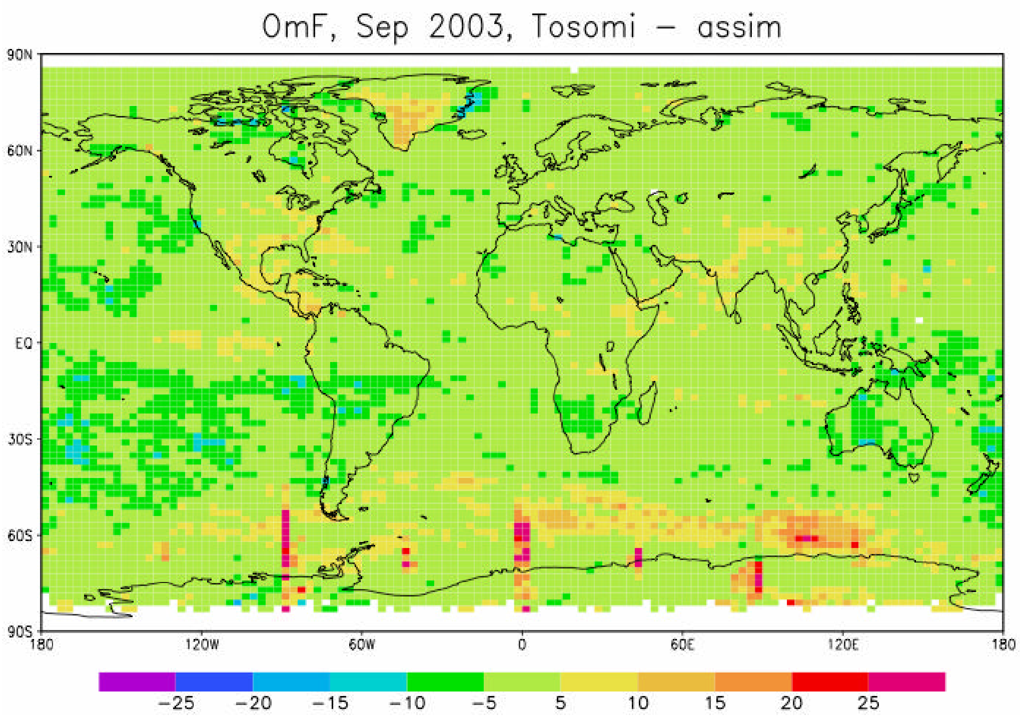
Feedback on retrieval

After improving the definition of the radiative transfer lookup table in the retrieval ...



Feedback on retrieval

A mistake in calculating the centre (lon,lat) of the Sciamachy pixels at the date line



4) Use of complex observations and heterogeneous data sets

Complex observations:

Satellite (remote sensing) observations have complicated relation with atmospheric composition

Described by averaging kernels, which complicates interpretation

$$x^r = \mathbf{x}^a + \mathbf{A}(\mathbf{x}^t - \mathbf{x}^a)$$

Use of averaging kernel in data assimilation straightforward (in principle): Observation operator = averaging kernel

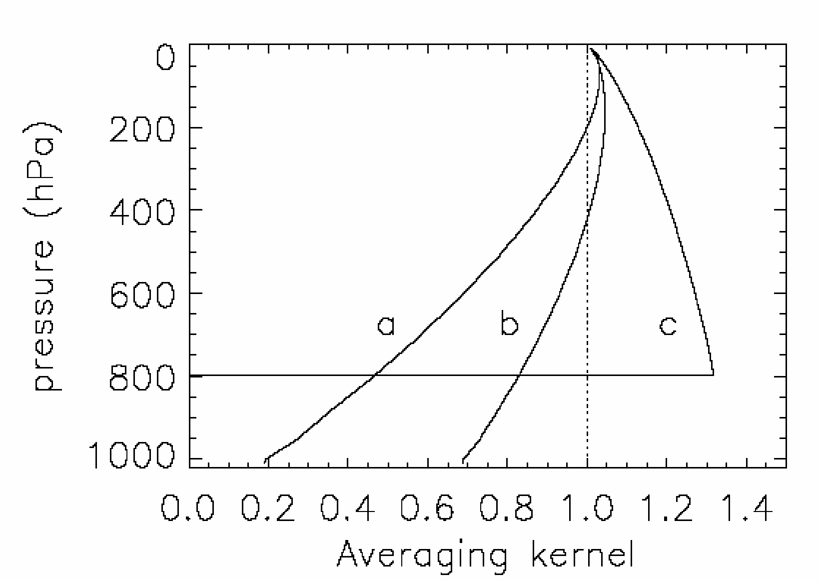
Heterogeneous data sets:

Combine satellite observations (different geometries, techniques) and routine surface observations, e.g. NWP

Kernels for total column observations

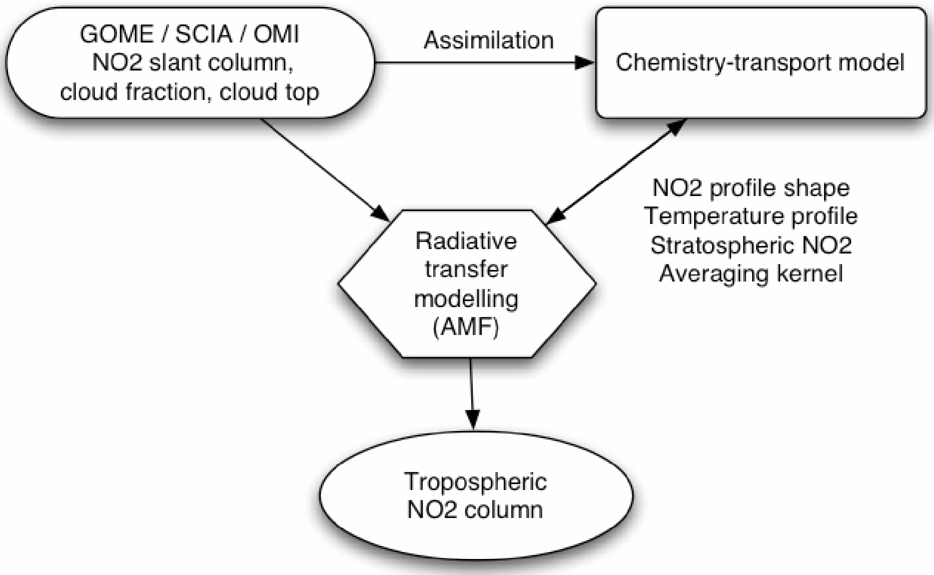
Examples:
- TOMS O_3
- GOME NO_2, H_2CO
- MOPITT CO

Rodgers,
Inverse methods for atmospheric sounding,
2000

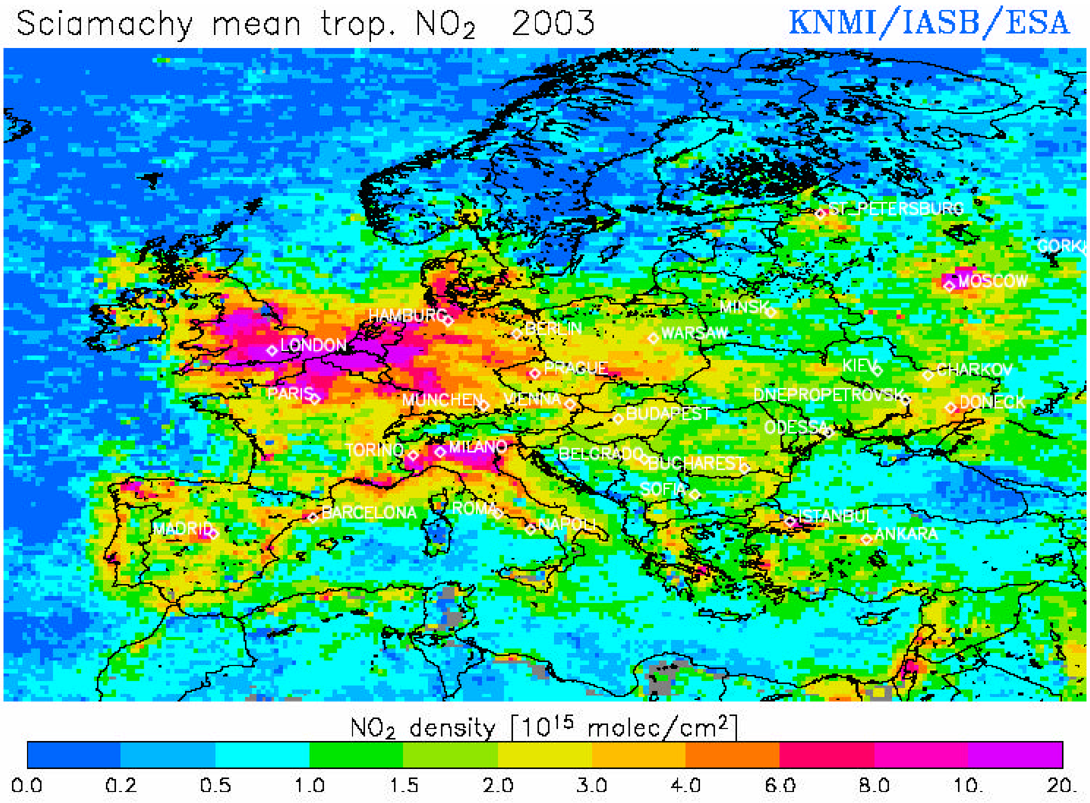


Sciamachy NO_2 retrieval

Combined retrieval-modelling-assimilation approach



Sciamachy NO_2 : Europa



Henk Eskes, ESA Summer School 2004

Assimilation of radiances

to avoid mixing the information content of the measurement with *a-priori* assumptions needed in the retrieval method that may be inconsistent with the model field

Success story:

assimilation of TOVS radiances in NWP (as opposed to the assimilation of retrieved temperature profiles) has significantly improved the forecast skill of NWP models

5) Emission estimates based on satellite observations

Data assimilation and inverse modelling based on the same principles

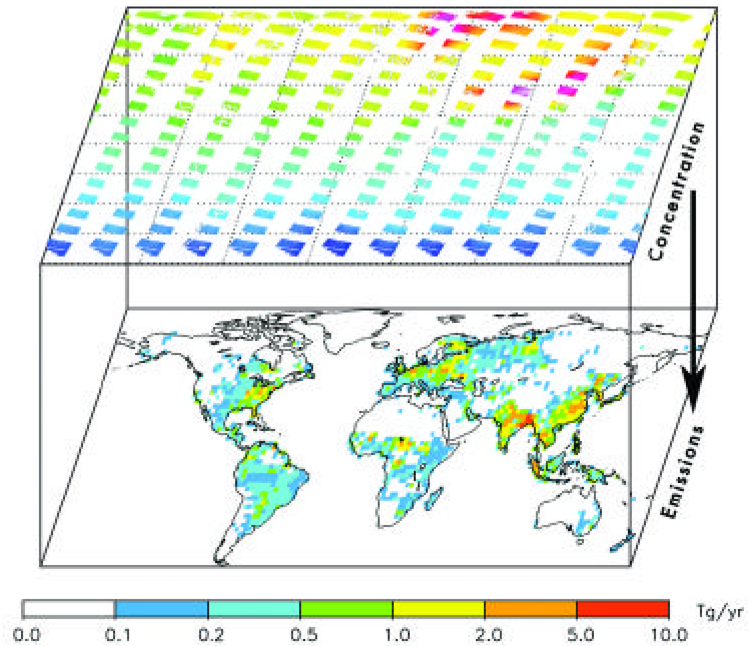
Assimilation: state analysis
Inverse modelling: source/sink estimates

Assimilation is more general and combined 3D field and source/sink analysis logical extension of state analysis

Example:
4D-Var source/state approach, applied to CH_4 from Sciamachy

Reference:
Ian Enting, *Inverse problems in atmospheric constituent transport,* Cambridge University Press, 2002

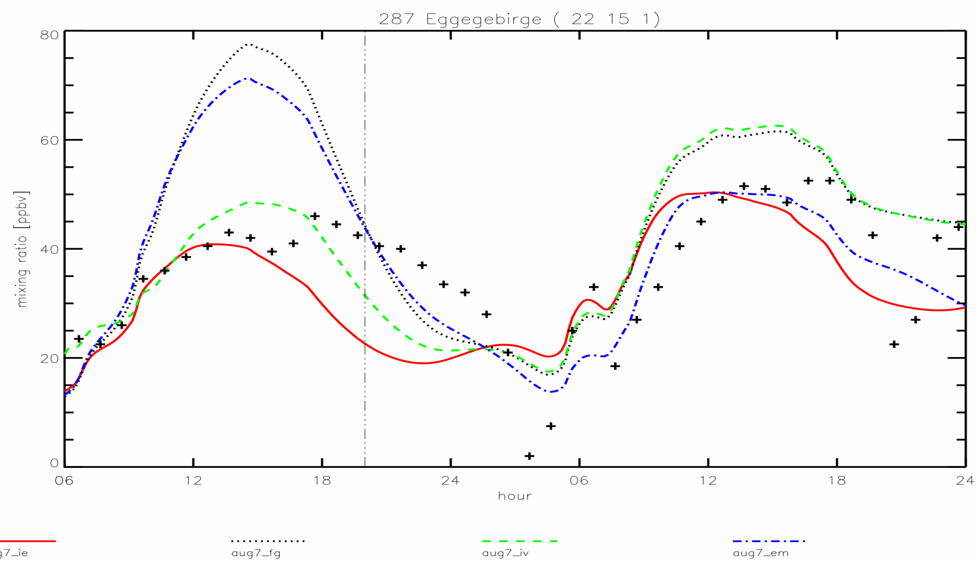
CH_4 emission analyses based on Sciamachy observations



Courtesy:
Jan Fokke Meirink
KNMI

Surface ozone assimilation: time scales

7. August 8. August 1997



+ observations
no optimisation

initial value opt.

emis. rate opt.

joint emis +
ini val opt.

assimilation interval

forecast

Courtesy: Hendrik Elbern, Köln

6) Monitoring of the environment, trends

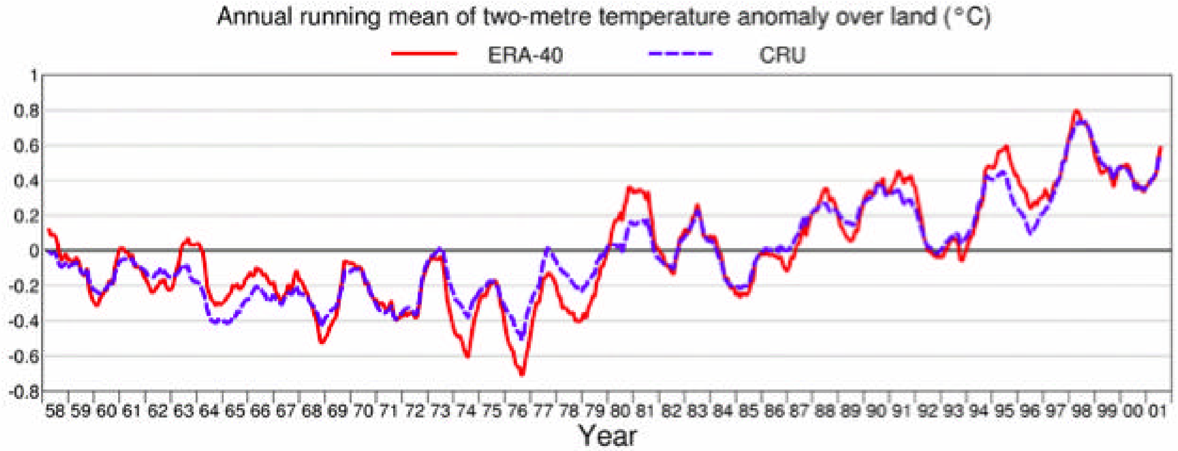
Re-analysis based on available satellite and ground-based observations

Combination of different data sets with a model allows a detailed bias correction to be determined and applied to the various data sets to account for differences between instruments, techniques, drifts.

Trend analysis: Very tricky!

Examples:
- ECMWF temperature data set from ERA-40
- GOME ozone assimilation data set, 1995-2003

ECMWF ERA-40 reanalysis temperature trend



Red: ERA-40 (EU final report, nov 2003)
Blue: Jones & Moberg, J. Climate, 16 (2003)

7) Quantify benefit for future missions: OSSE

Observing system simulation experiment:

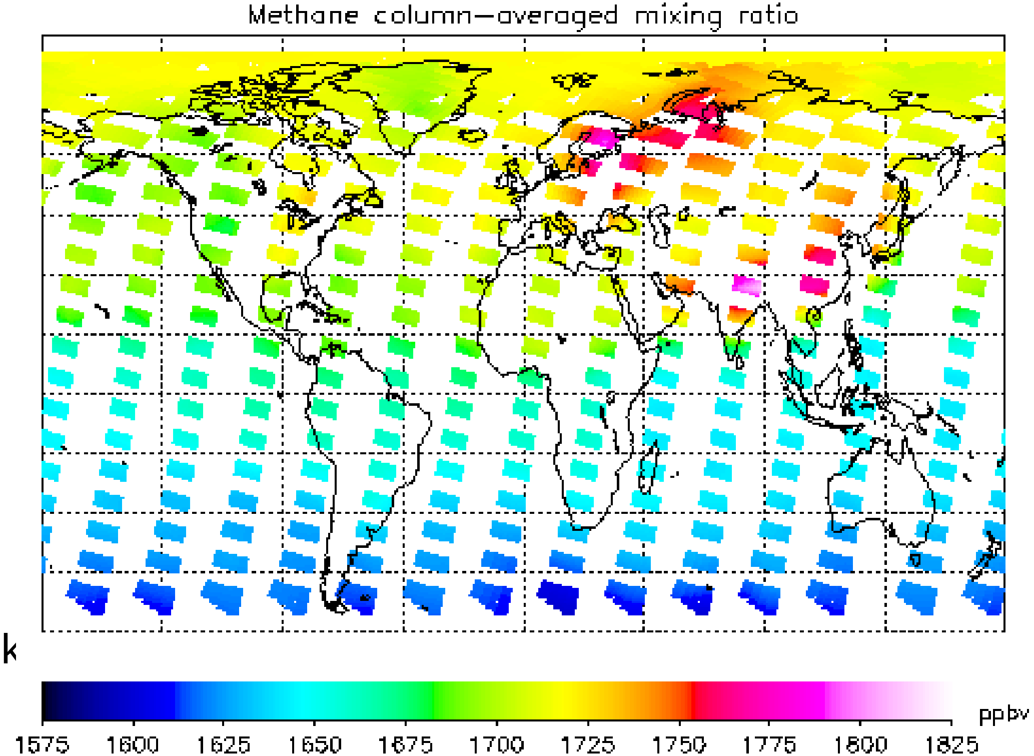
Approach:

- Draw synthetic observations from reference run
- Assimilate these in a model run with
  perturbed initial conditions / emissions / model parameters
- Quantify the impact of these synthetic observations

Examples of OSSE:

- Impact of SWIFT stratospheric winds on NWP
  W. Lahoz et al, QJRMS submitted, 2003
- Impact of ozone observations on wind field
- Impact of Sciamachy CH_4 column observations

OSSE: Impact of Sciamachy CH_4 for emission estimates

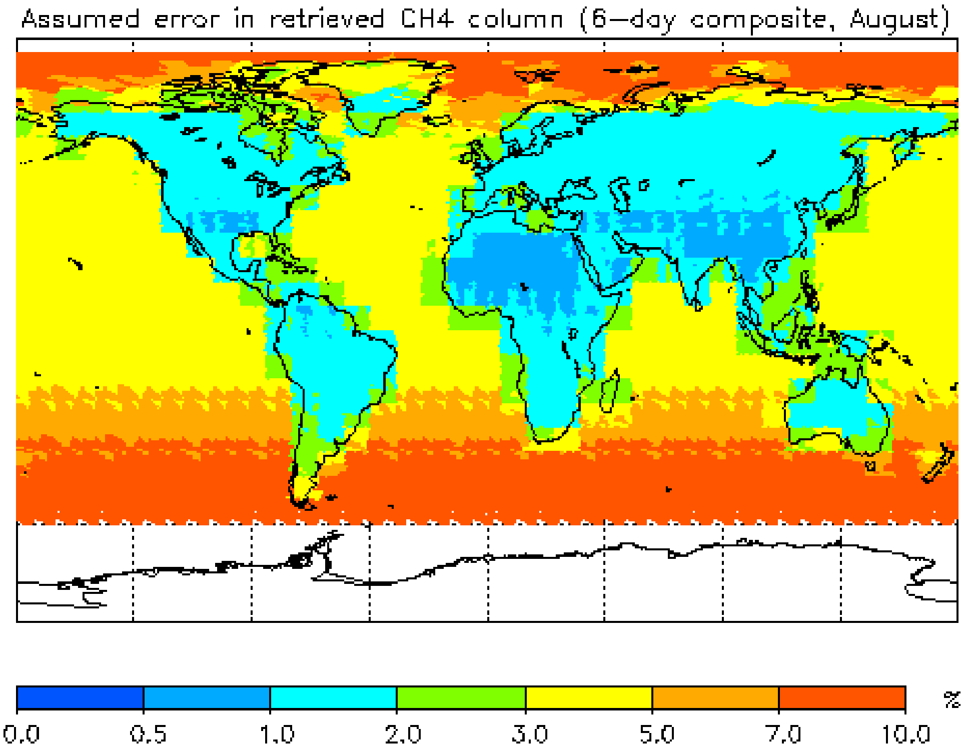


Simulated observations

Courtesy:
Jan Fokke Meirink
KNMI

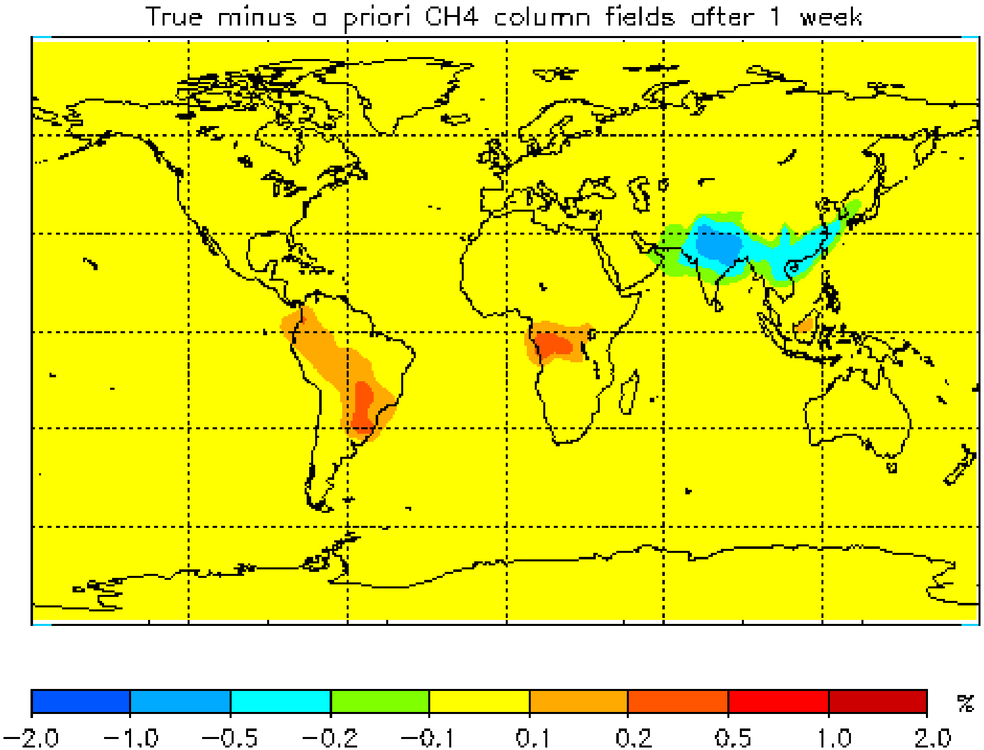
OSSE: Impact of Sciamachy CH_4 for emission estimates

Simulated observation errors



Courtesy:
Jan Fokke Meirink
KNMI

OSSE: Impact of Sciamachy CH_4 for emission estimates

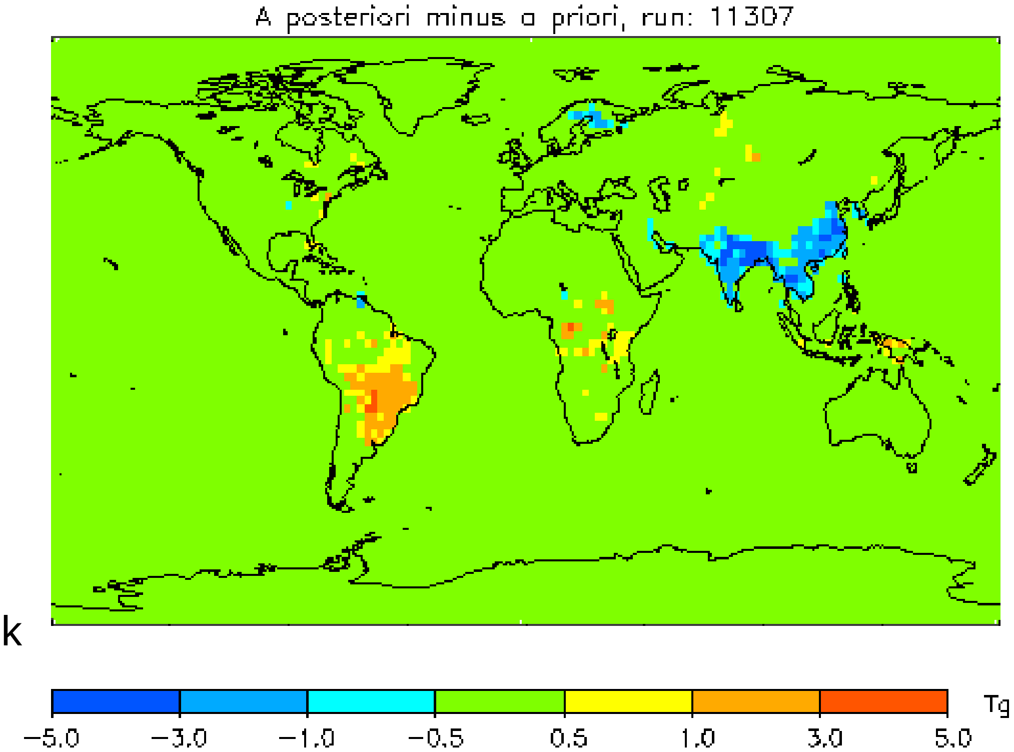


Changes in the methane field:
Rice and biomass emission perturbations

Courtesy:
Jan Fokke Meirink
KNMI

OSSE: Impact of Sciamachy CH_4 for emission estimates

Analysis
minus
forecast
emissions



Courtesy:
Jan Fokke Meirink
KNMI

OSSE: Impact of Sciamachy CH_4 for emission estimates

R = RMS reduction factor

EXPERIMENT	*R*
default	0.21
all pixels cloudfree	0.61
perfect obs.	0.88
correlation between emissions	0.65

Courtesy: Jan Fokke Meirink, KNMI

8) Atmospheric composition forecasts - chemical weather

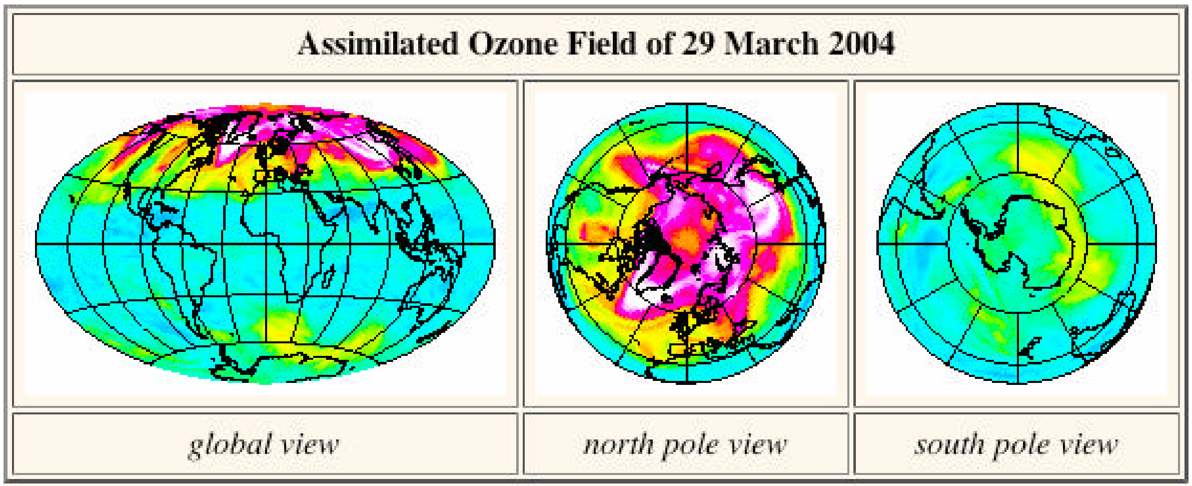
Assimilation analysis to initialise a chemical forecast:

Examples:

- Stratospheric ozone forecast
- BASCOE
- ECMWF ozone forecasts
- NCEP ozone forecasts

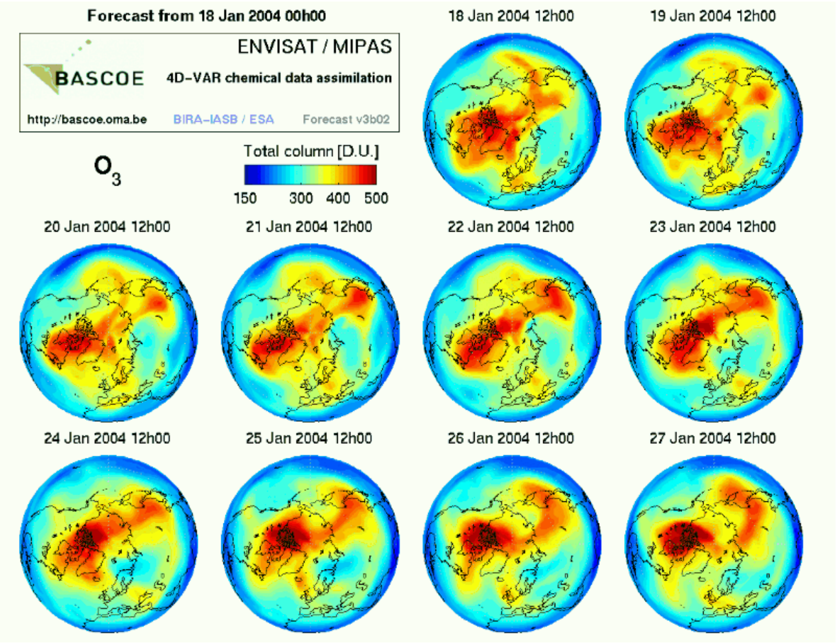
TEMIS (ESA-DUP)

Tropospheric Emission Monitoring Internet Service
http://www.temis.nl/
SCIAMACHY ozone assimilation + forecasts



Stratospheric chemical forecasts from MIPAS observations

www.bascoe.oma.be



Courtesy:
Dominique Fonteyn

Summary

Data assimilation as value-adding instrument:

- Fill gaps in data records
- Propagation of information:
  data-poor regions, unobserved variables and chemicals, emissions
- Confronting models with data (understanding),
  observations with models (validation)
- improvement of retrievals
- Use of complex data: heterogeneous data sets, remote sensing
- Sources and sinks as part of the analysis
- Long-term monitoring, trends, climate change
- Quantify benefit of future missions: OSSE studies
- Forecasts of atmospheric composition: "chemical weather"