# Chemical Data Assimilation at BIRA – IASB

**D. Fonteyn, S. Bonjean, S. Chabrillat, F. Daerden and Q. Errera**

**Belgisch Instituut voor Ruimte – Aëronomie**

***(Belgian Institute for Space Aeronomy)***

**BIRA - IASB**

aeronomie.be

Federal science policy

## >> OUTLINE

- Introduction
- What is chemical data assimilation?
- Why do we need chemical data assimilation?
- 4D –VAR chemical data assimilation system
- Physical consistency, Self consistency, Independent observations
- Added value
- Inverse modelling: emission estimations

## >> OUTLINE

**Belgian Assimilation System of Chemical Observations from Envisat (BASCOE)** http://bascoe.oma.be

**IMAGES**

aeronomie.be

Federal science policy

- **Focus on the Stratosphere:**
  - **Chemical processes are well understood: high level of confidence in modelling results. (?)**
  - **Mature remote sensing technology (UARS, ENVISAT, SAGE, CRISTA, POAM …)**
- **If models are perfect, no data assimilation is needed**

Gas phase chemistry

Chapman Cycle

$$O_2 + h\nu \rightarrow 2O$$
$$O_2 + O + M \rightarrow O_3 + M$$
$$O_3 + O \rightarrow 2O_2$$
$$O_3 + h\nu \rightarrow O_2 + O$$

Catalytic cycles

Hydrogen radicals ($HO_x$)

$$OH + O \rightarrow H + O_2$$
$$H + O_3 \rightarrow OH + O_2$$
Net: $O + O_3 \rightarrow 2\,O_2$

$$OH + O \rightarrow H + O_2$$
$$H + O_2 + M \rightarrow HO_2 + M$$
$$HO_2 + O \rightarrow OH + O_2$$
Net: $O + O_3 \rightarrow O_2$

$$HO_2 + O \rightarrow OH + O_2$$
$$OH + O_3 \rightarrow HO_2 + O_2$$
Net: $O + O_3 \rightarrow 2\,O_2$

Hydrogen Source Gases: $H_2O$, $CH_4$

- Long term trends
- $HO_x$ chemistry in the upper stratosphere and mesosphere

aeronomie.be

Federal science policy

2. Nitrogen radicals (member of $NO_y$)

$$NO_2 + O \rightarrow NO + O_2$$
$$NO + O_3 \rightarrow NO_2 + O_2$$
$$\text{Net:} \quad O + O_3 \rightarrow 2\,O_2$$

Nitrogen Source Gas: $N_2O$ (and …)

- Long term trends
- $NO_y$ partitioning (in the lower stratosphere: aerosols )

3. Chlorine radicals (member of $Cl_y$)

$$ClO + O \rightarrow Cl + O_2$$
$$Cl + O_3 \rightarrow ClO + O_2$$
$$\text{Net:} \quad O + O_3 \rightarrow 2\,O_2$$

Chlorine Source Gases: Organic Chlorine

- Long term trends
- $Cl_y$ partitioning (in the lower stratosphere: aerosols )

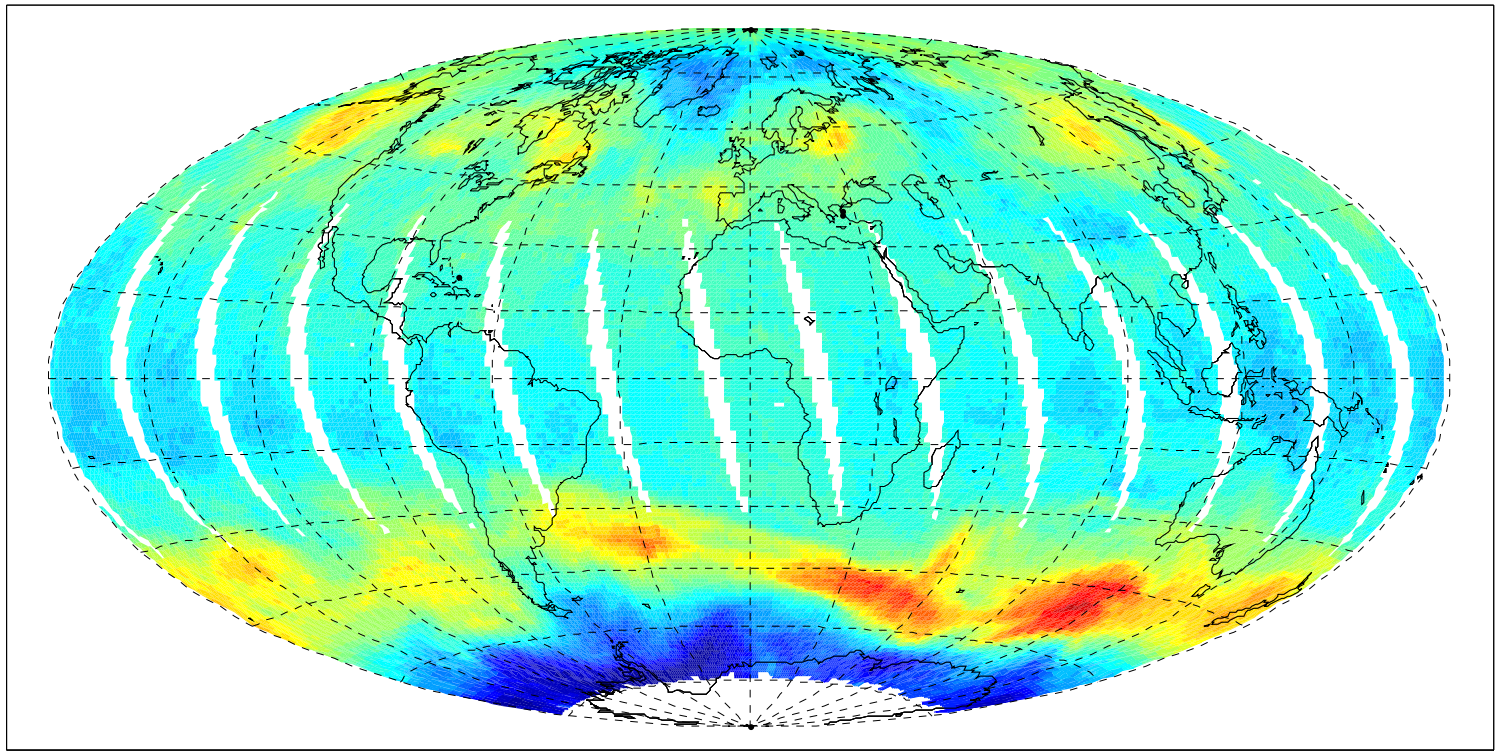
## Chemical data assimilation

- Inert tracer assimilation
- Tracer with parameterized chemistry assimilation
- Multiple species with chemical interactions

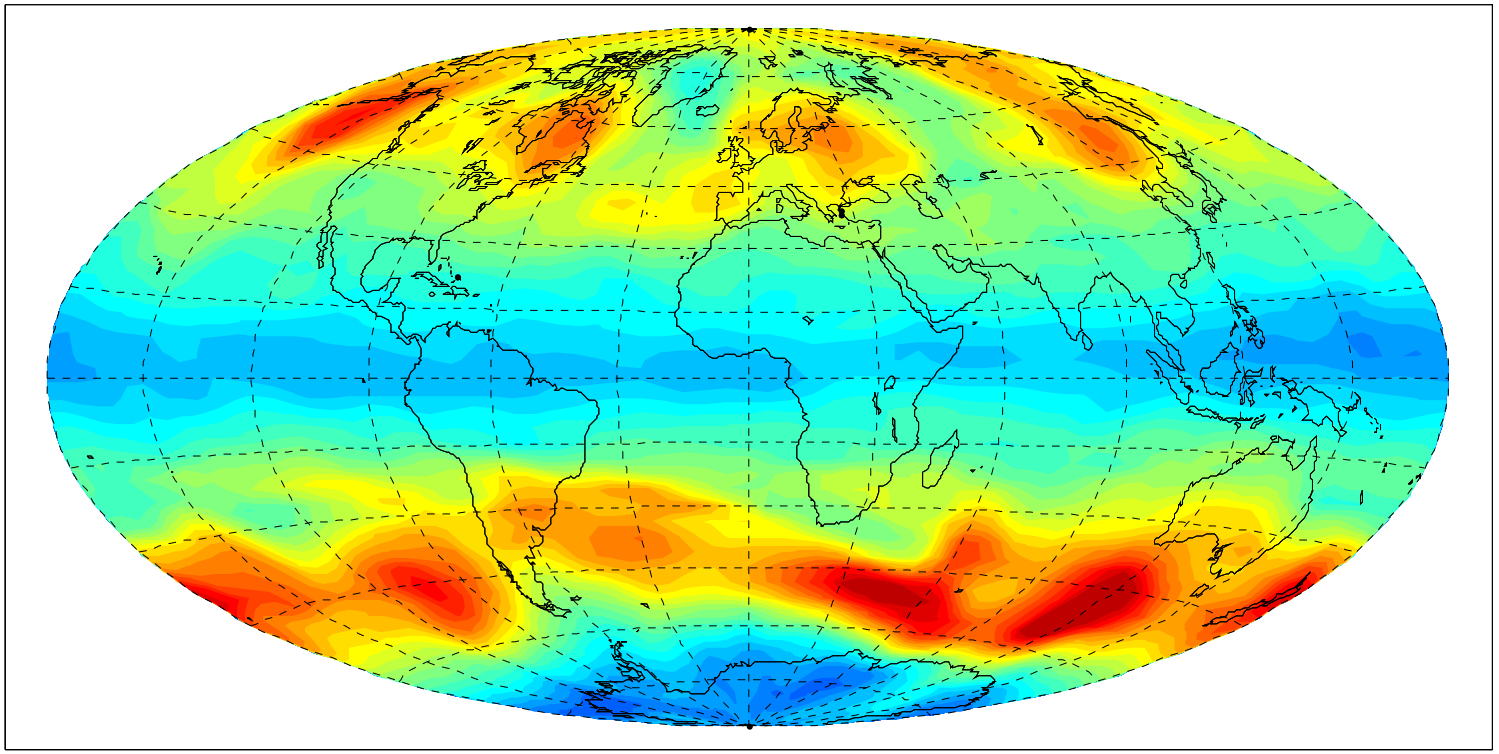
⇓

**Necessity**

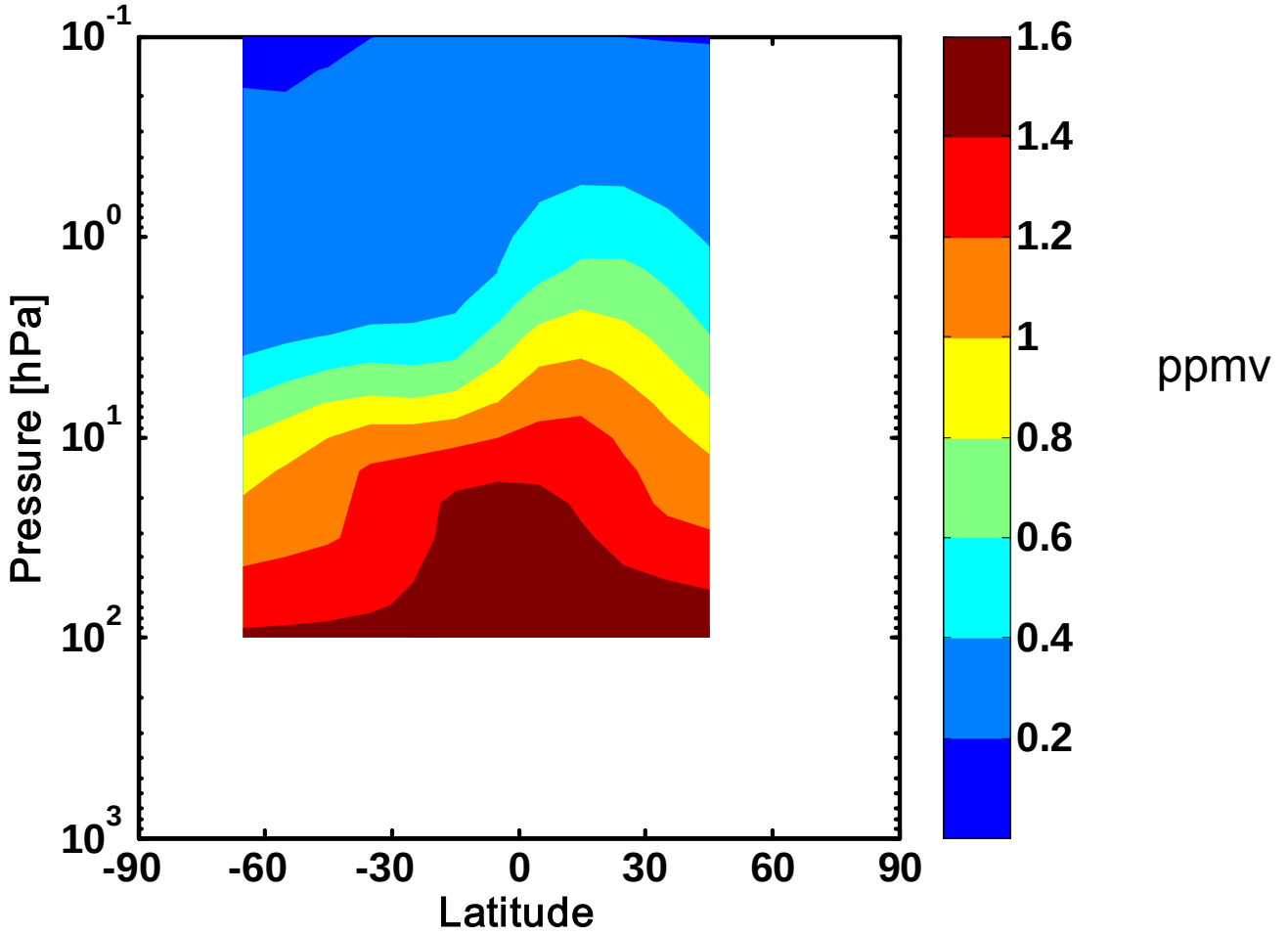
TOMS total ozone 28 August 2003



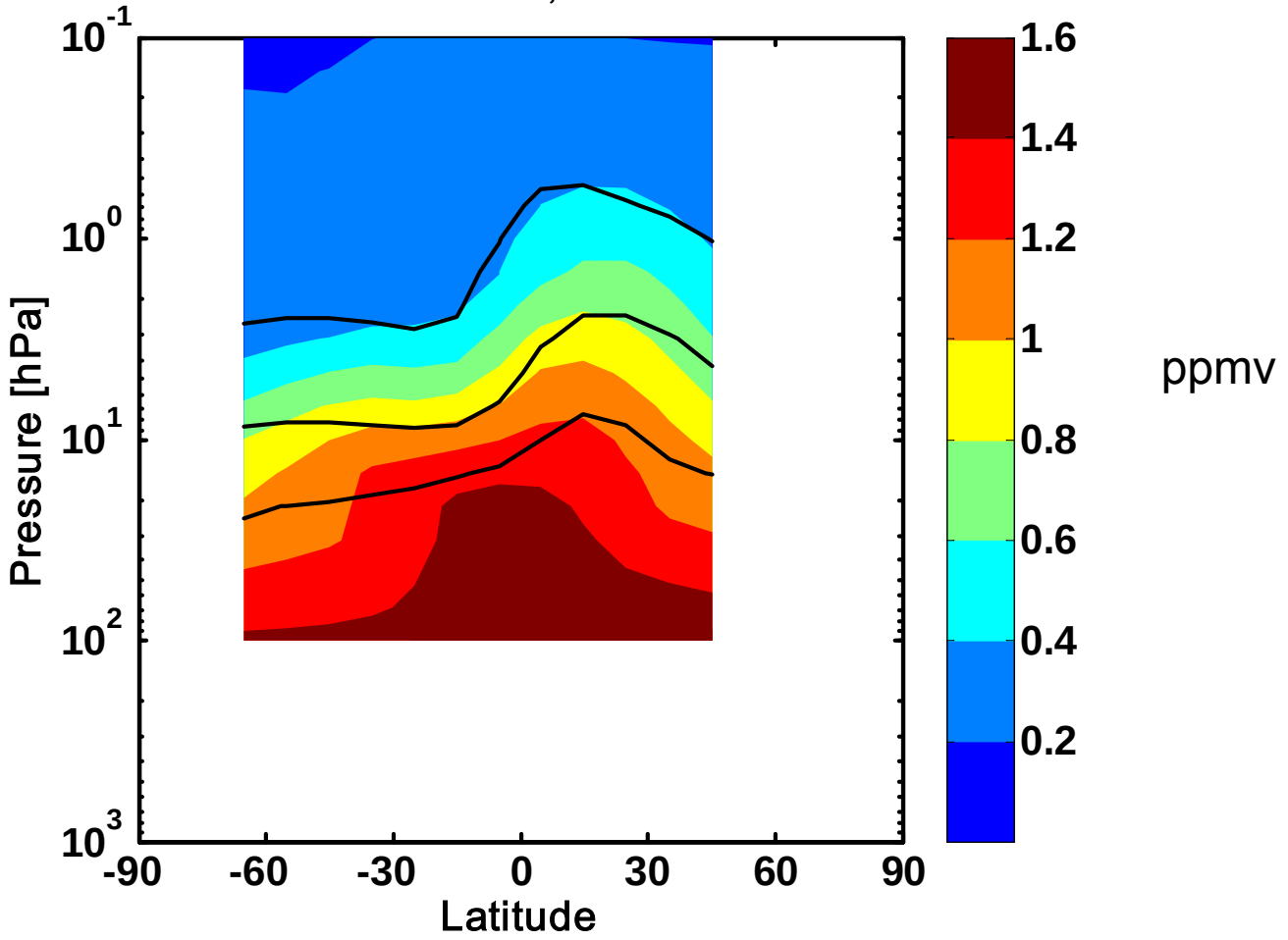
Free model total ozone 28 August 2003, 12 UTC



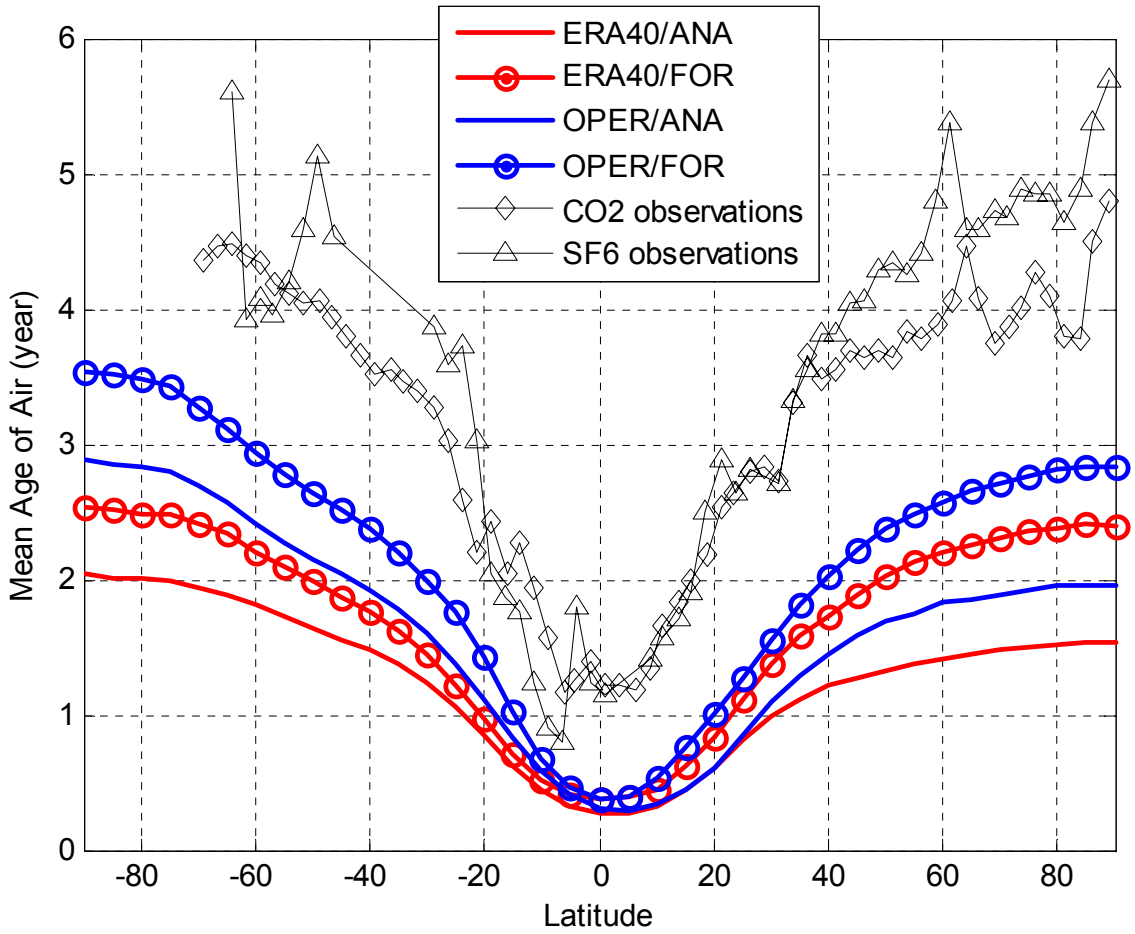
HALOE $CH_4$ monthly gridded zonal mean, August 2003



HALOE $CH_4$ monthly gridded zonal mean, August 2003
Free Model Run co-located, isolines



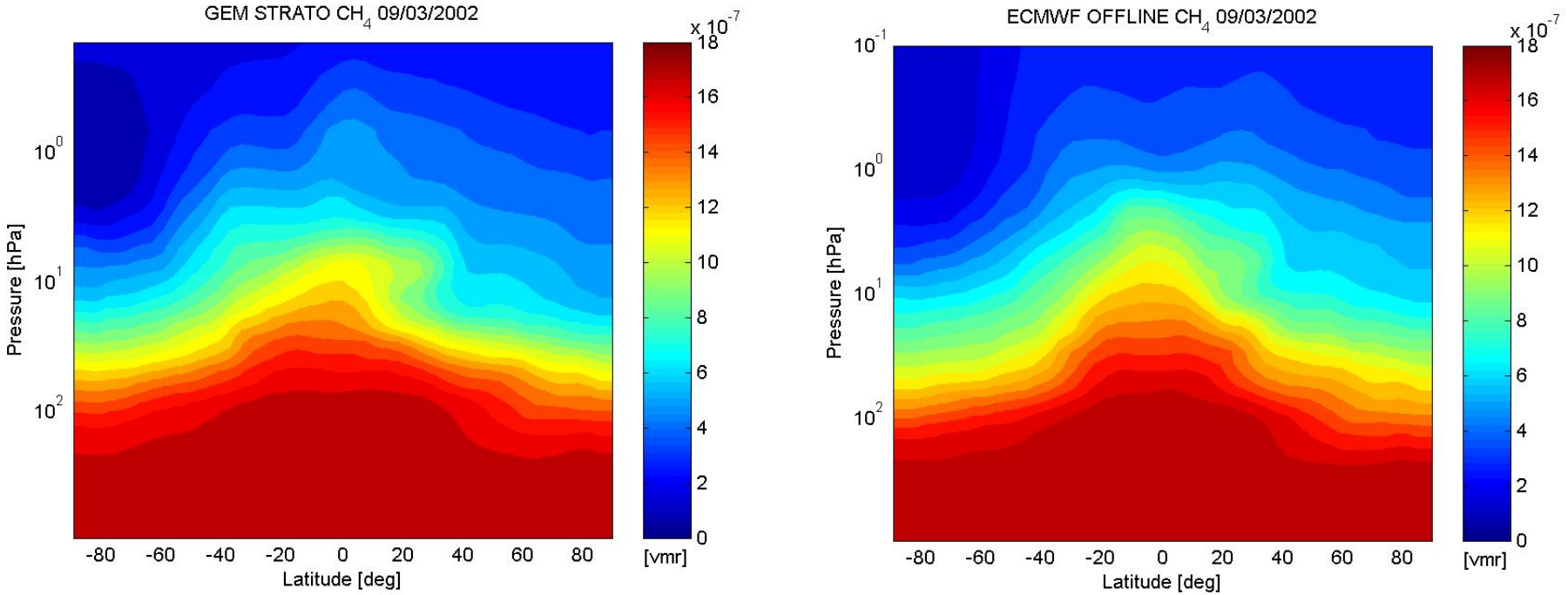
Problem: input dynamics, confirmed by mean age of air experiment



GEM STRATO (MSC) with BASCOE chemistry vs. BASCOE driven by ECMWF

- 3 month free model run
- Same initial conditions
- Matching resolution
- Identical chemistry
- No Feedback

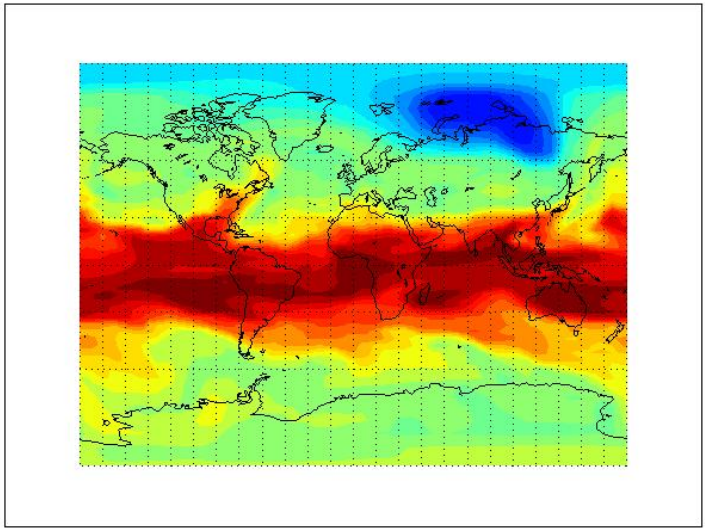
**$CH_4$**

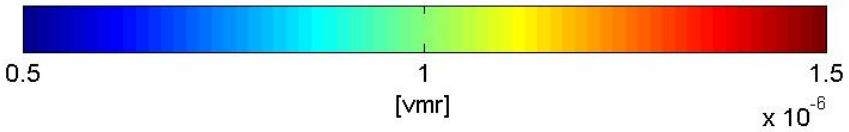


BASCOE driven by GEM-STRATO vs BASCOE driven by ECMWF

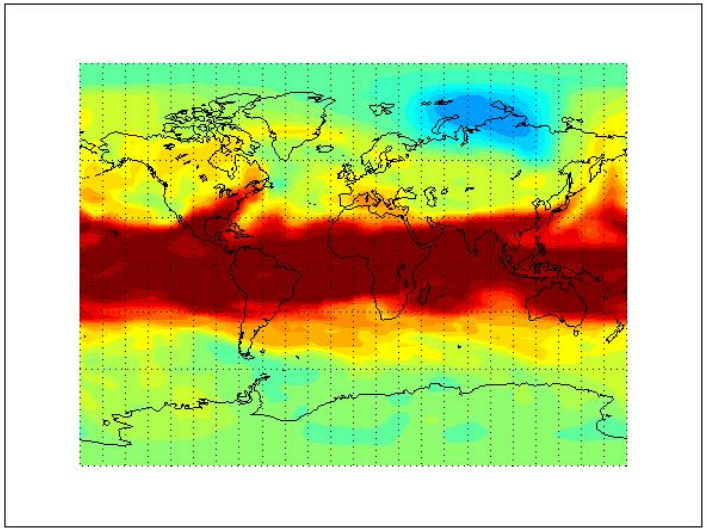
**$CH_4$**

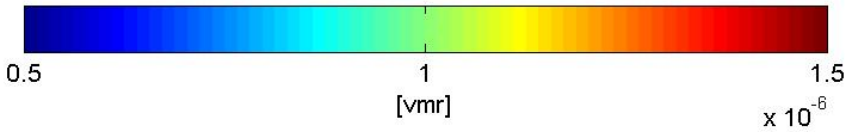
GEM STRATO $CH_4$ @ 600 K 09/03/2002





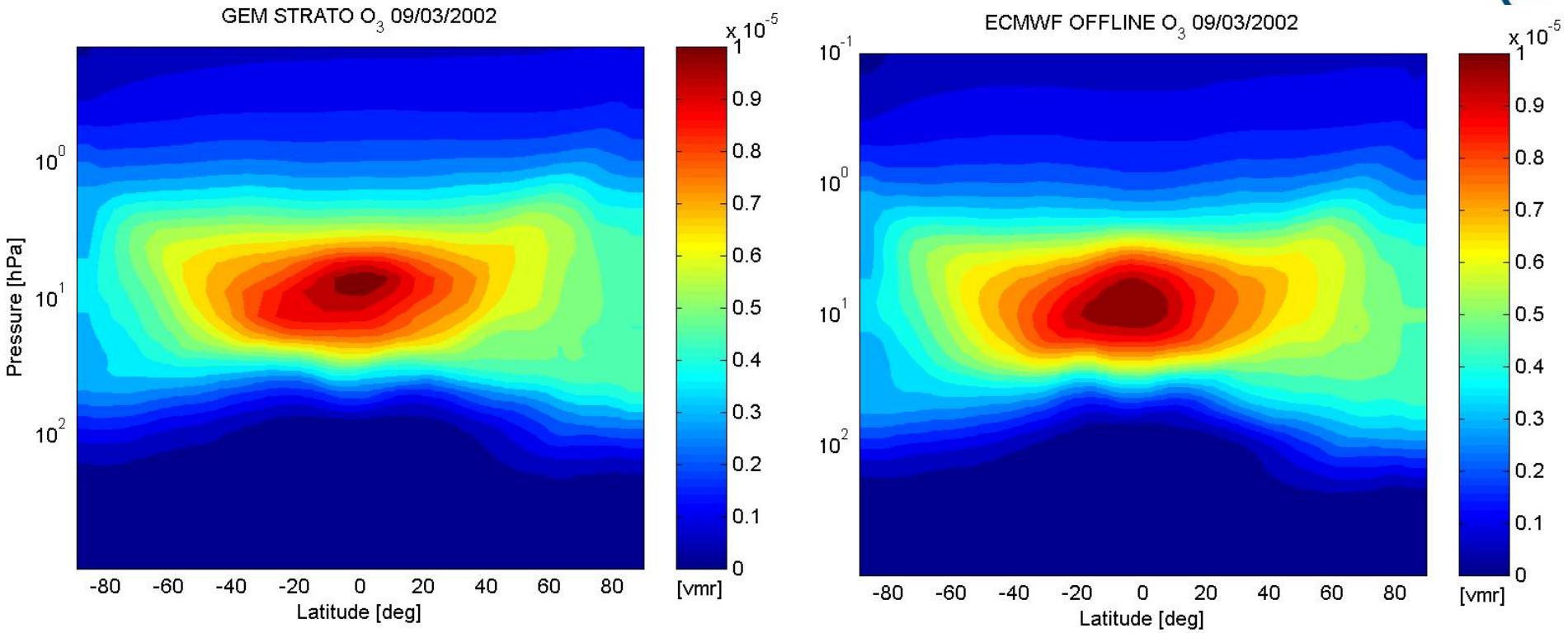

ECMWF $CH_4$ @ 600 K 09/03/2002





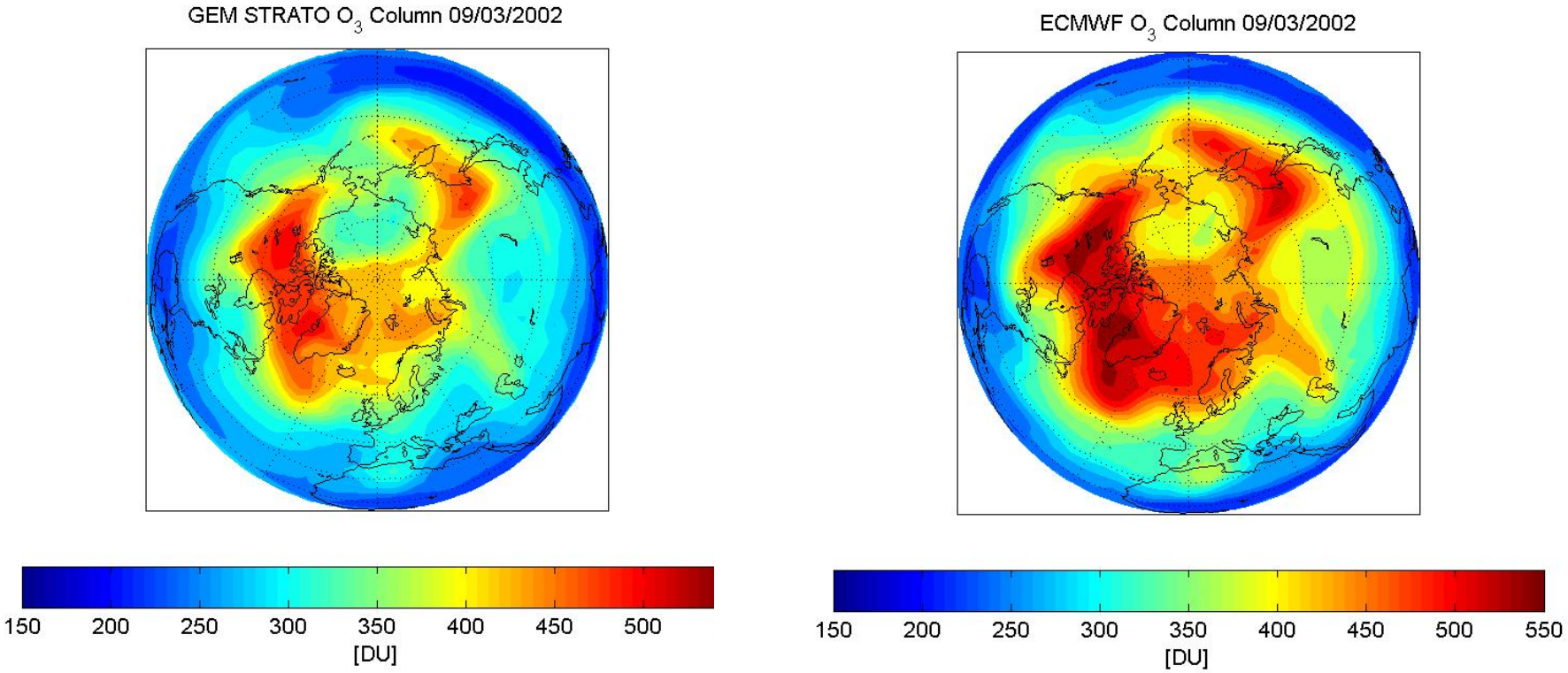
BASCOE driven by GEM-STRATO vs BASCOE driven by ECMWF

**Ozone**



BASCOE driven by GEM-STRATO vs BASCOE driven by ECMWF

**Total ozone**



## Model Shortcomings:

- Effect of dynamical assimilation
- Effect of different dynamical assimilation systems

- Dynamics driven shortcomings

- Chemical modelling shortcomings (not shown)

4D-var assimilation : find $\mathbf{x}(t_0)$ minimizing $J$

$$J = \frac{1}{2}\left[\mathrm{x}(t_0) - \mathrm{x}^b(t_0)\right]^T \mathrm{B}_0^{-1}\left[\mathrm{x}(t_0) - \mathrm{x}^b(t_0)\right] + \frac{1}{2}\sum_{i=1}^{N}\left(\mathrm{y}^o(t_i) - H[\mathrm{x}(t_i)]\right)^T \mathrm{R}_i^{-1}\left(\mathrm{y}^o(t_i) - H[\mathrm{x}(t_i)]\right)$$

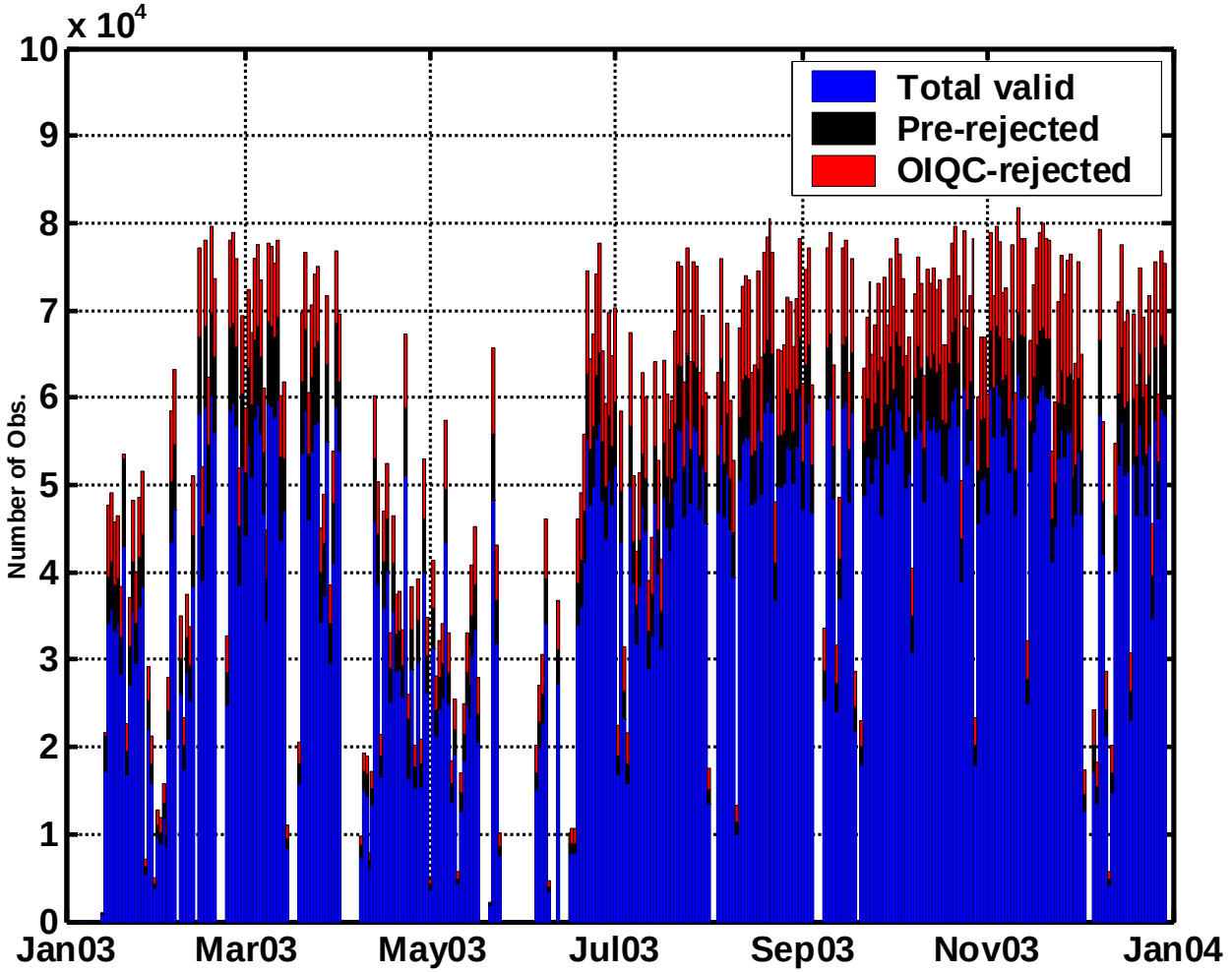
With the constraint

$$\frac{d\mathbf{x}(t)}{dt} = M[\mathbf{x}(t)]$$

$\mathbf{x}(t_0)$: control variable $n \approx 5.6\ 10^6$
$\mathbf{x}^b$: *a priori* state of the atmosphere ( *background*)
$\mathbf{y}^o(t_i)$: observations, de dimension $p \approx 5\ 10^4$ (-7 $10^5$)
$\mathbf{x}(t_i)$: model state
$H$: observational operator
$M$: model operator
$\mathbf{B}$: background error covariance matrix
$\mathbf{R}$: observational error covariance matrix

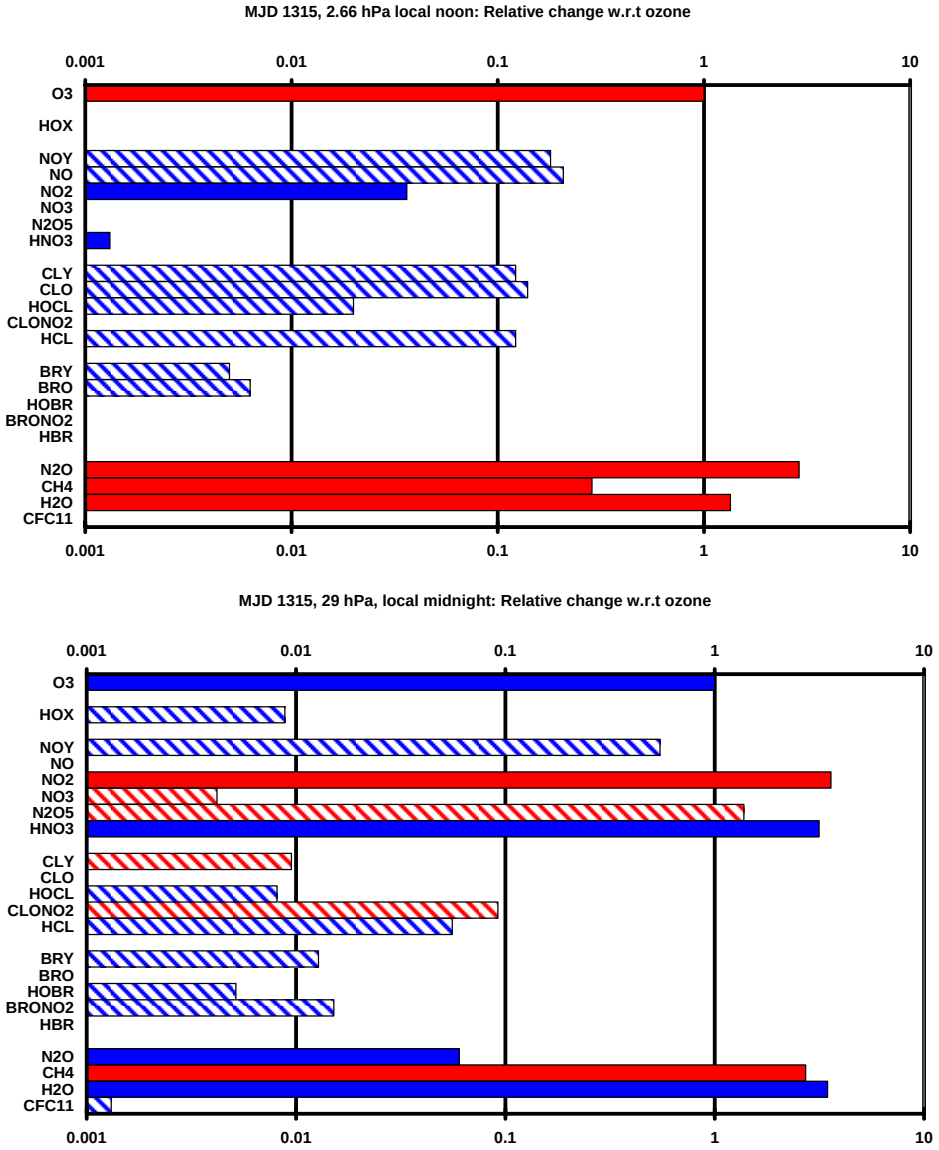
- **Model (3D - Chemical Transport Model)**
  - horizontal: 3°.75 *x* 3°.75 (96 *x* 49 pts); vertical: 37 pressure levels, surface → 0.1 hPa (subset of ECMWF hybrid levels, keeping stratospheric levs)
  - 57 chemical species (control variables), 200 reactions
  - 4 types of PSC particles (36 size bins): NOT assimilated
  - Eulerian, driven by ECMWF 6h analyses/forecast
  - advection by Lin & Rood (1996) with 30' time step
- **Assimilation set-up**
  - Adjoint of chemistry and transport
  - Assimilation time window: 24 hours
  - B diagonal; 20 % of first guess distribution (= univariate)
  - Quality check: 1st climatoligical behaviour; 2 nd first guess based QC
- **Observations**
  - ESA Envisat MIPAS L2 products, Near Real Time (NRT) and Offline (OFL)
  - $O_3$, $H_2O$, $N_2O$, $CH_4$, $HNO_3$, $NO_2$
  - Representativeness error: 8.5 %

# 4D – VAR >> BASCOE >> OFL number of observations




aeronomie.be

# 4D – VAR >> BASCOE >> Multi-variate nature

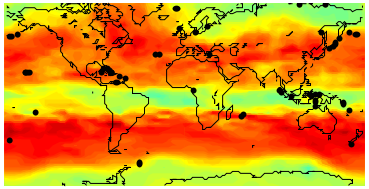



## Multi variate nature

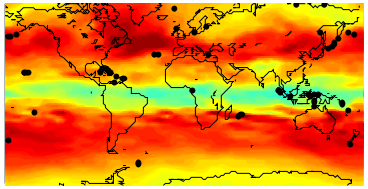
- Diagonal B
- $(x^a(t_0)-x^b(t_0))$
- Local noon and local midnight
- August, 7, 2003
- Full: observed species
- Striped: unobserved species

# 4D – VAR >> BASCOE >> Physical consistency

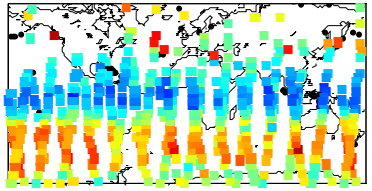
O3 / ANA



O3 / FMR

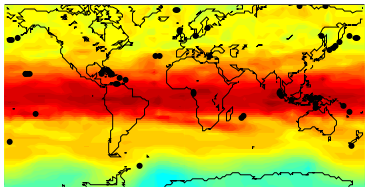


O3 / MIPAS / OFL

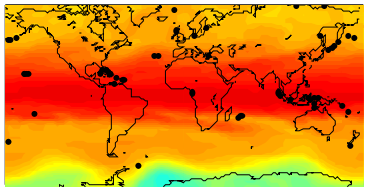


August 5, 2003

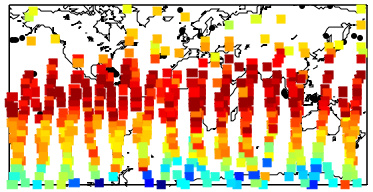
CH4 / ANA



CH4 / FMR

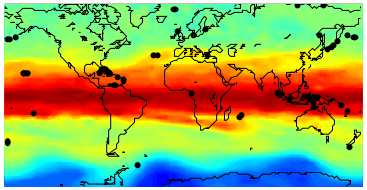


CH4 / MIPAS / OFL

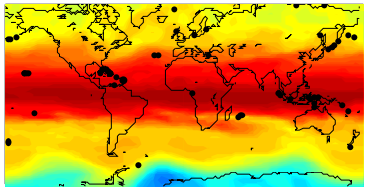


35.8 hPa & obs within 1 km

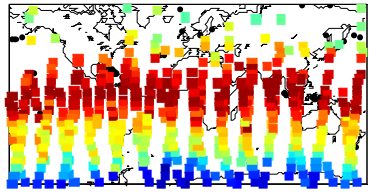
N2O / ANA



N2O / FMR



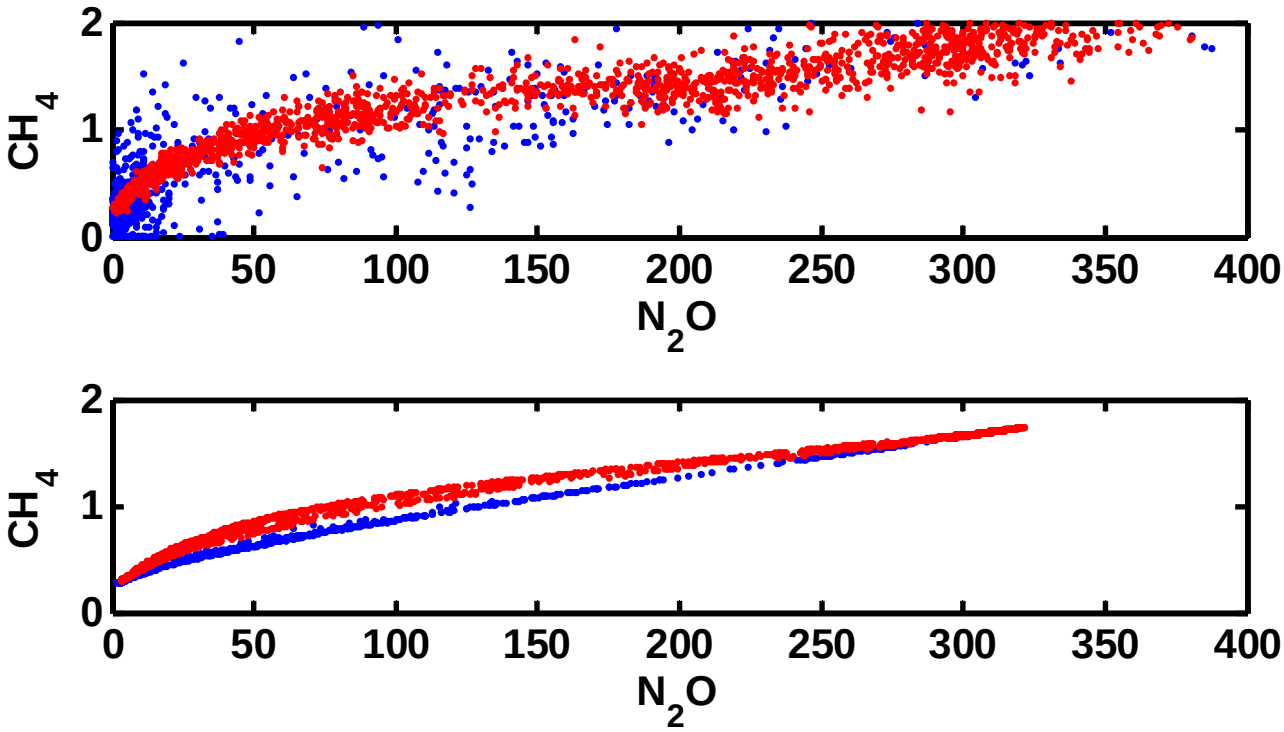
N2O / MIPAS / OFL



aeronomie.be

Federal science policy

# 4D – VAR >> BASCOE >> Physical consistency




**Tracer correlations:**

**$CH_4$ vs $N_2O$ (Aug 5)**

**Tropical**

**South polar**

**MIPAS DATA**

**Co-located FMR**

**Co-located analysis**

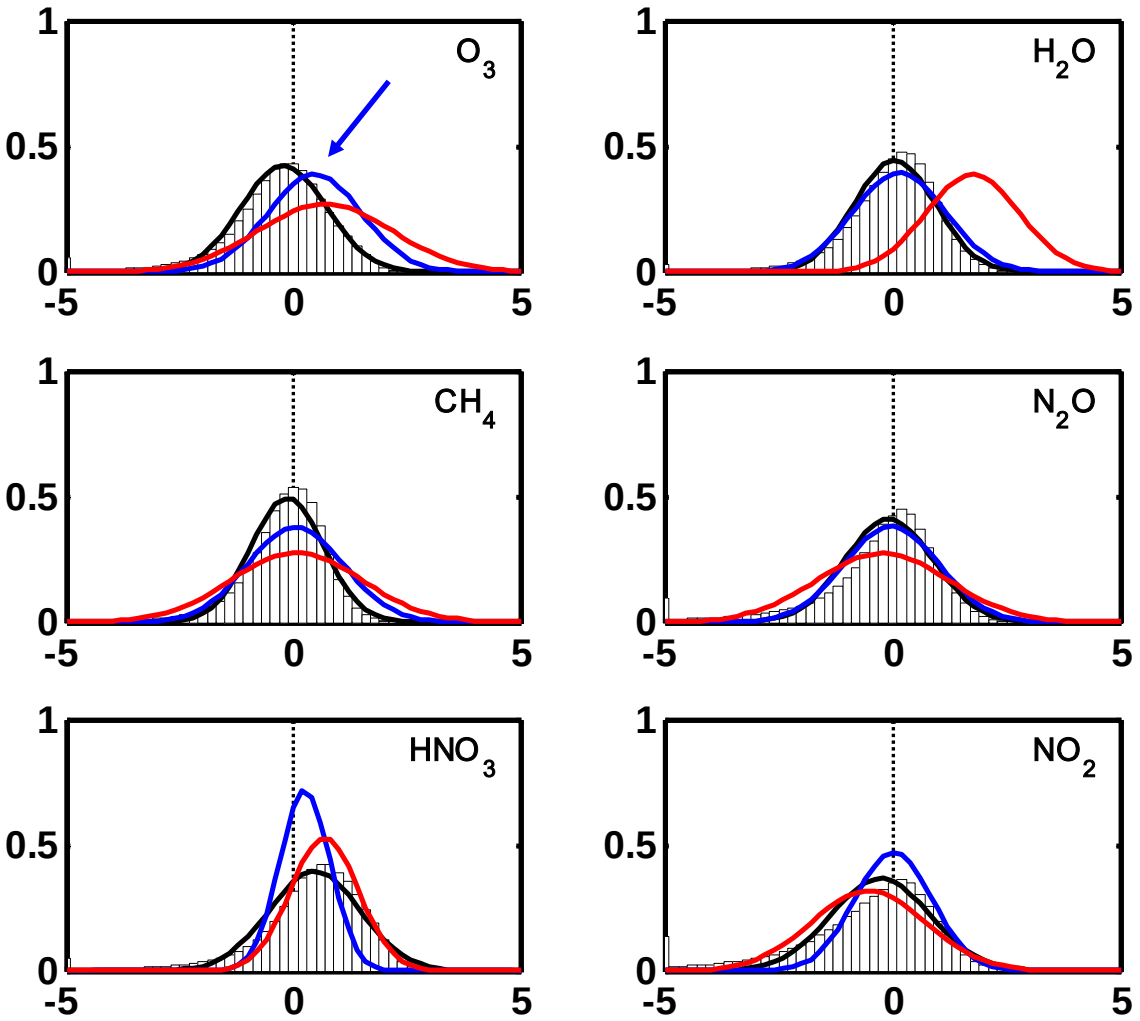
**= correlation**

***Needs validation***

aeronomie.be

# 4D – VAR >> BASCOE >> Self – consistency

- **OmF:**
  - Observation – first guess
  - Normalized by **R**
  - = Gaussian distribution
  - **OFL**
  - **NRT**
  - **FMR**
  - OFL vs NRT
  - Consistency
  - Added value w.r.p FMR



**NRT results:**

Ozone @ 1 hPa underestimated

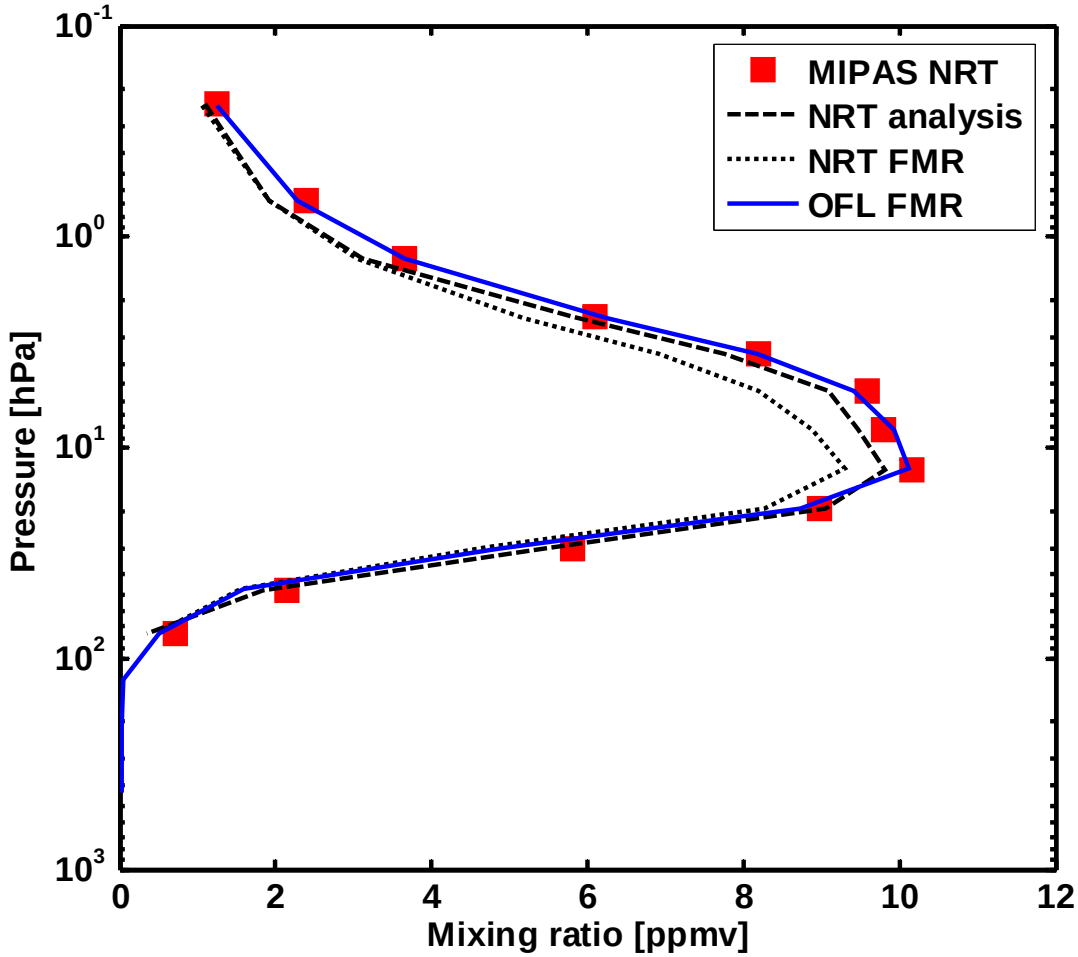
- Analysis = free model
- Model not constrained
- $O_2$ main source of $O_3$
- $O_2$ not a control variable

↓

- $J_{O_2}$ increased by 25 %
- New free model

↓

- Better agreement



**Self – consistency 4D – VAR:**

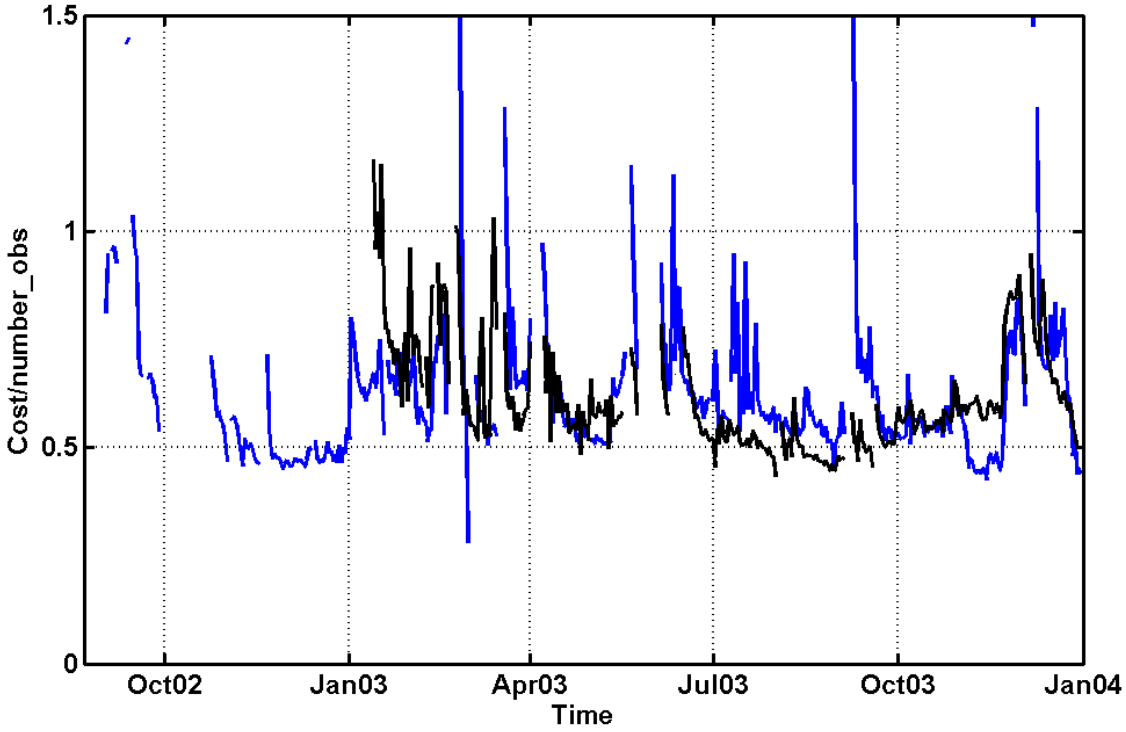
**$E[J_{analysis}] = p/2$**

Time series $J_{analysis}/p$

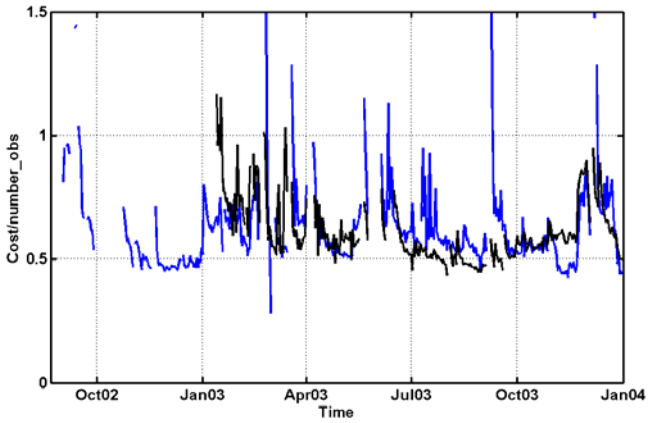
**NRT**

**OFL**

Monitoring capability



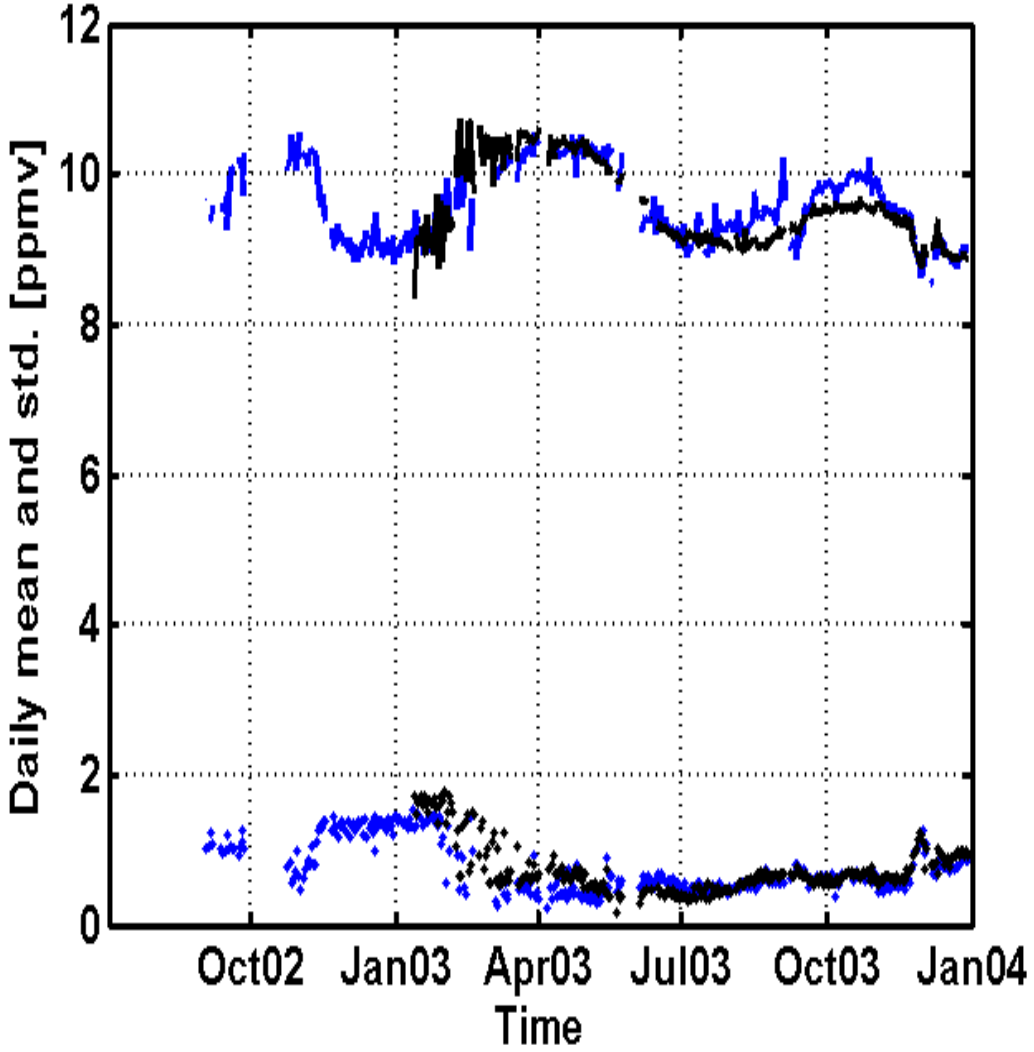
# 4D – VAR >> BASCOE >> Self – consistency >> monitoring




Monitoring capability

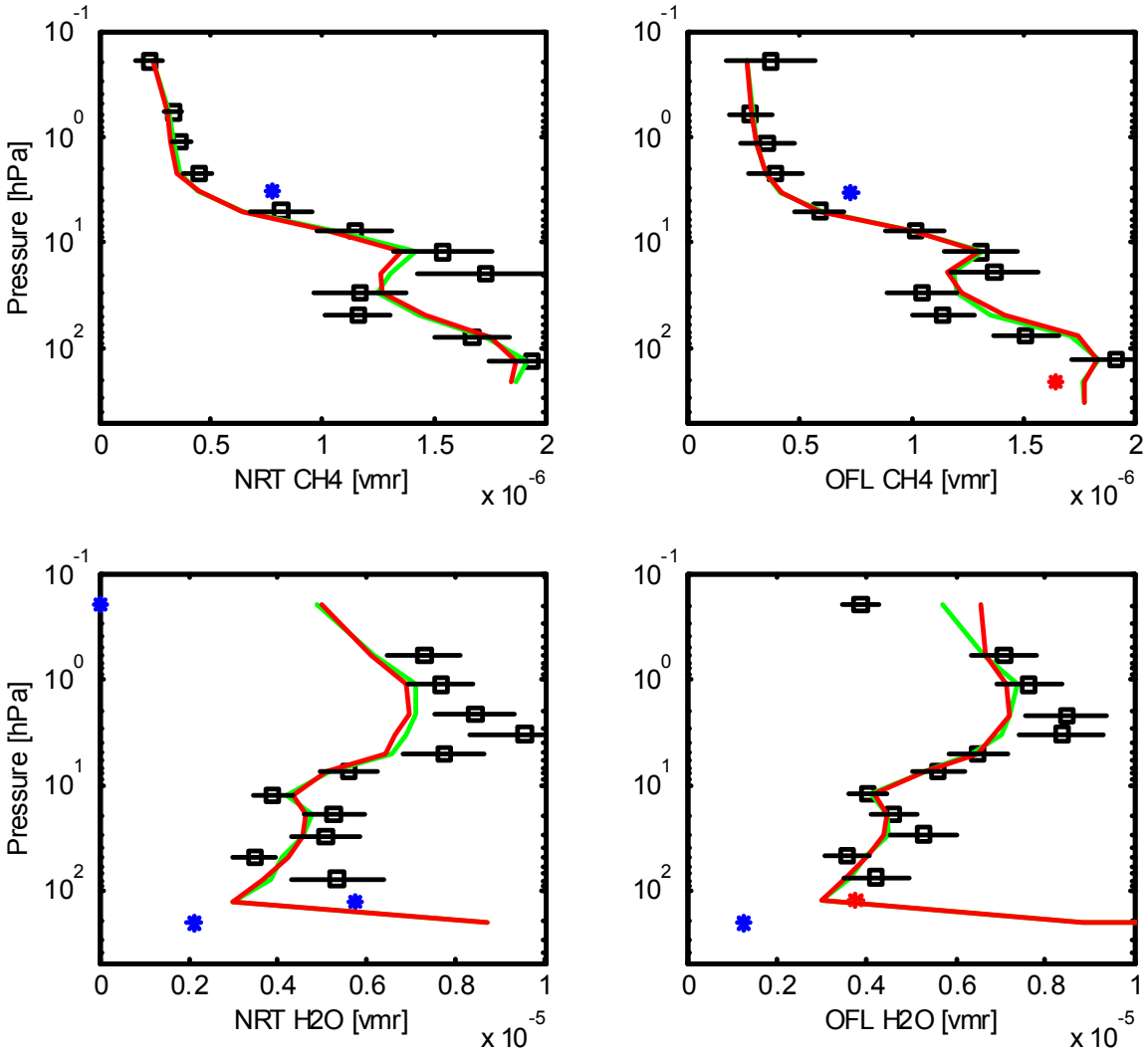
Daily mean MIPAS ozone, [-10,10] at 14 hPa

$J_{analysis}$ transients correlate with ozone daily mean transients




aeronomie.be

# 4D – VAR >> BASCOE >> Example



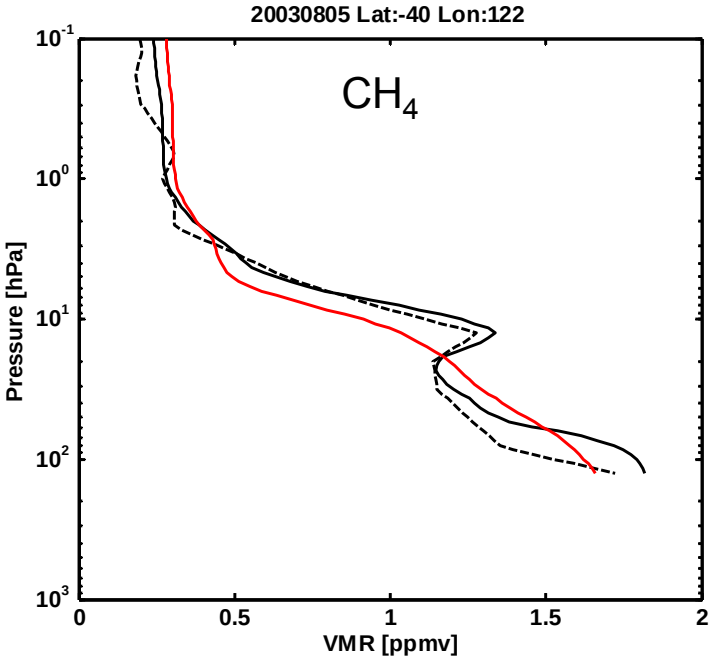

Illustrative example:
August 5, 2003
Lat: -38.6° Lon: 83.3°

- NRT vs OFL data
- Quality check
  - Pre-check
  - OI qc
- First guess
- Analysis

- At 1 hPa: methane rich tropical air, and tropical dry air

aeronomie.be

# 4D – VAR >> BASCOE >> Independent observations




Individual profile

OFL analysis

HALOE

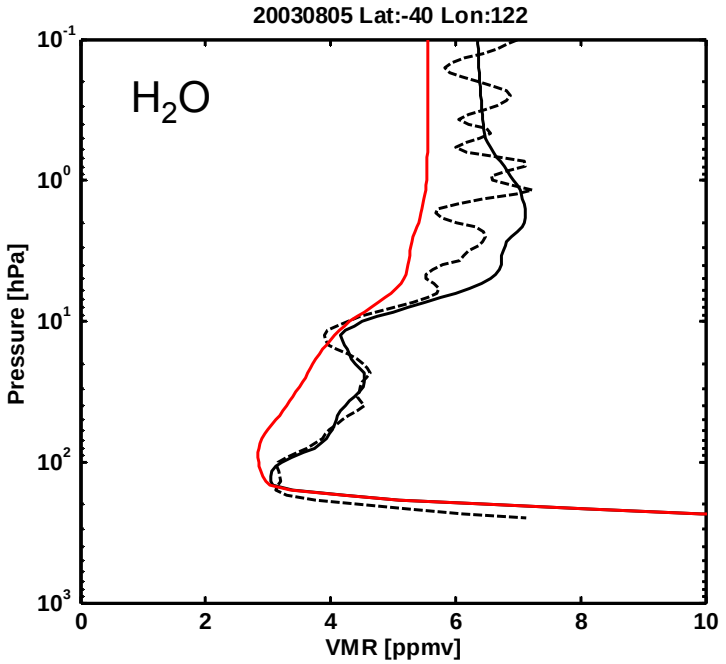
Free Model run

Independent observations:

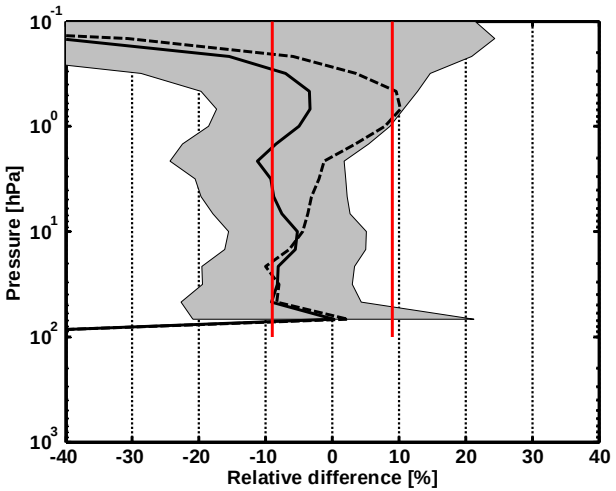
HALOE v19

Periode: August 2003

1. Individual profiles
2. Statistics



# 4D – VAR >> BASCOE >> HALOE August 2003



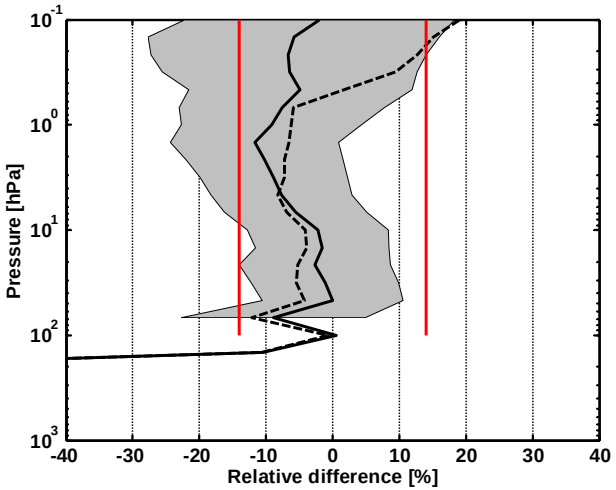

$O_3$

(HALOE-BASCOE)/HALOE

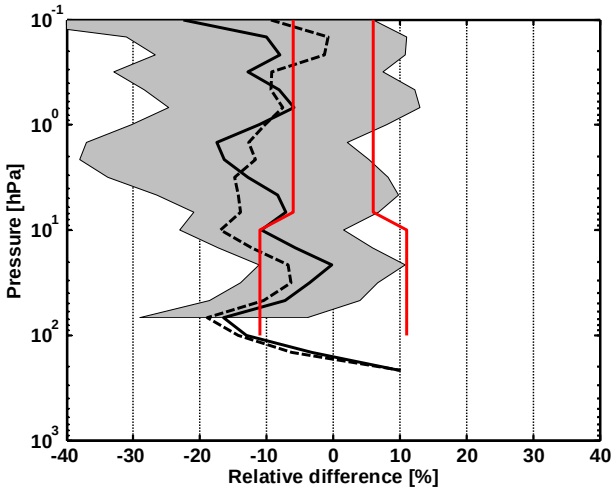
OFL analysis

NRT analysis

HALOE error



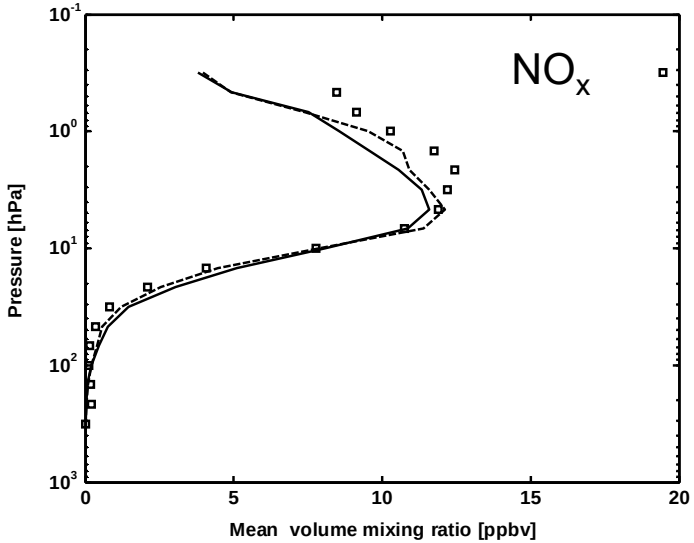

$H_2O$

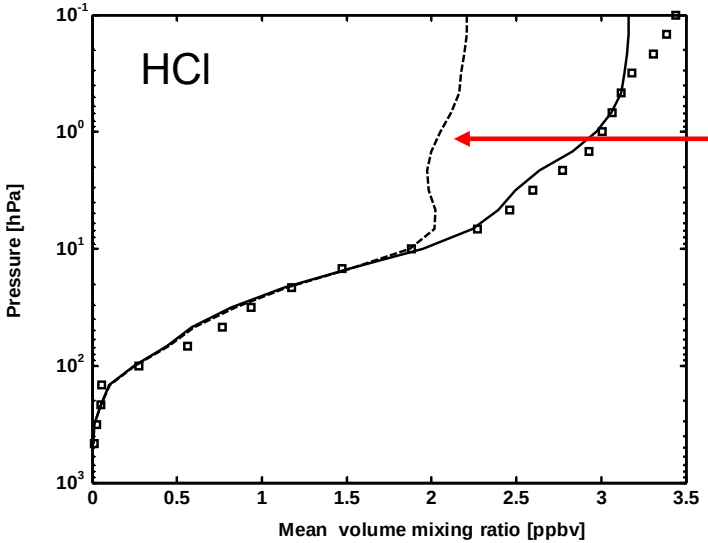



$CH_4$

aeronomie.be

# 4D – VAR >> BASCOE >> HALOE August 2003




Mean HALOE and BASCOE co-located profiles:

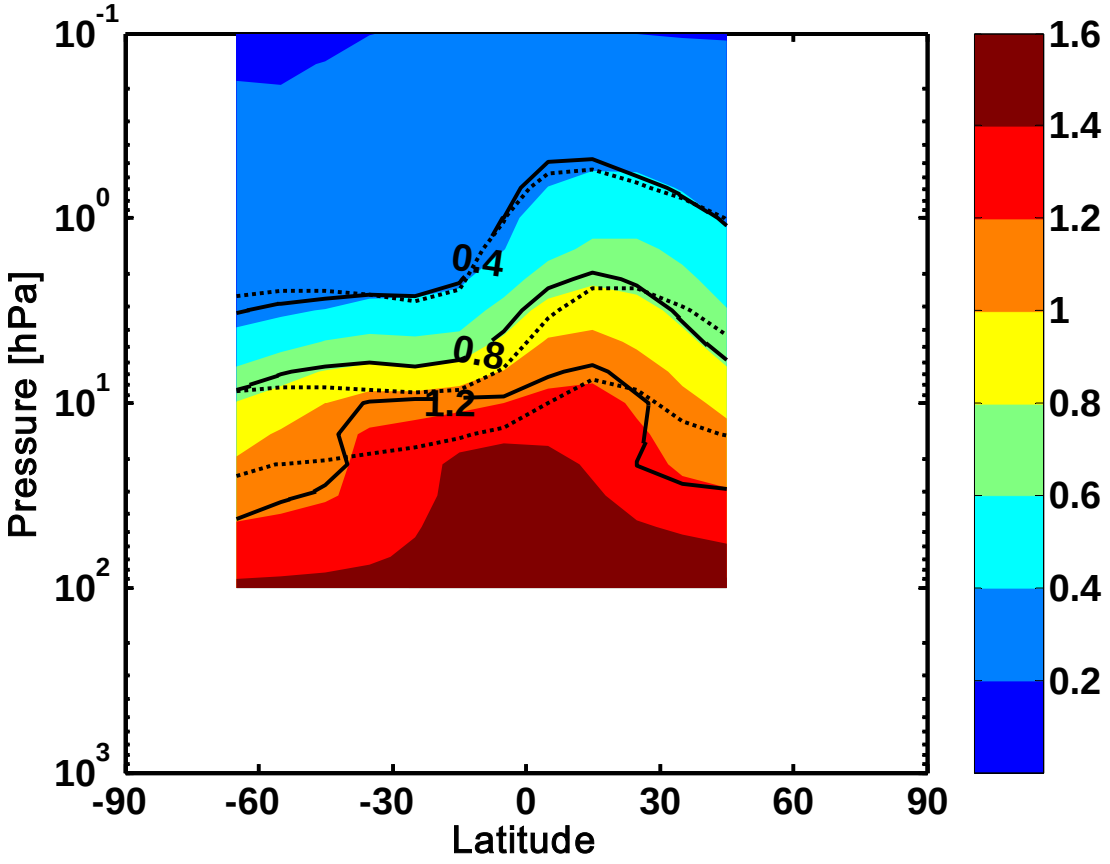
OFL analysis

NRT analysis

HALOE

Ozone model bias & 4D – VAR chemical coupling reduces $Cl_y$

# 4D – VAR >> BASCOE >> Added value




HALOE and BASCOE co-located gridded zonal monthly mean

OFL analysis

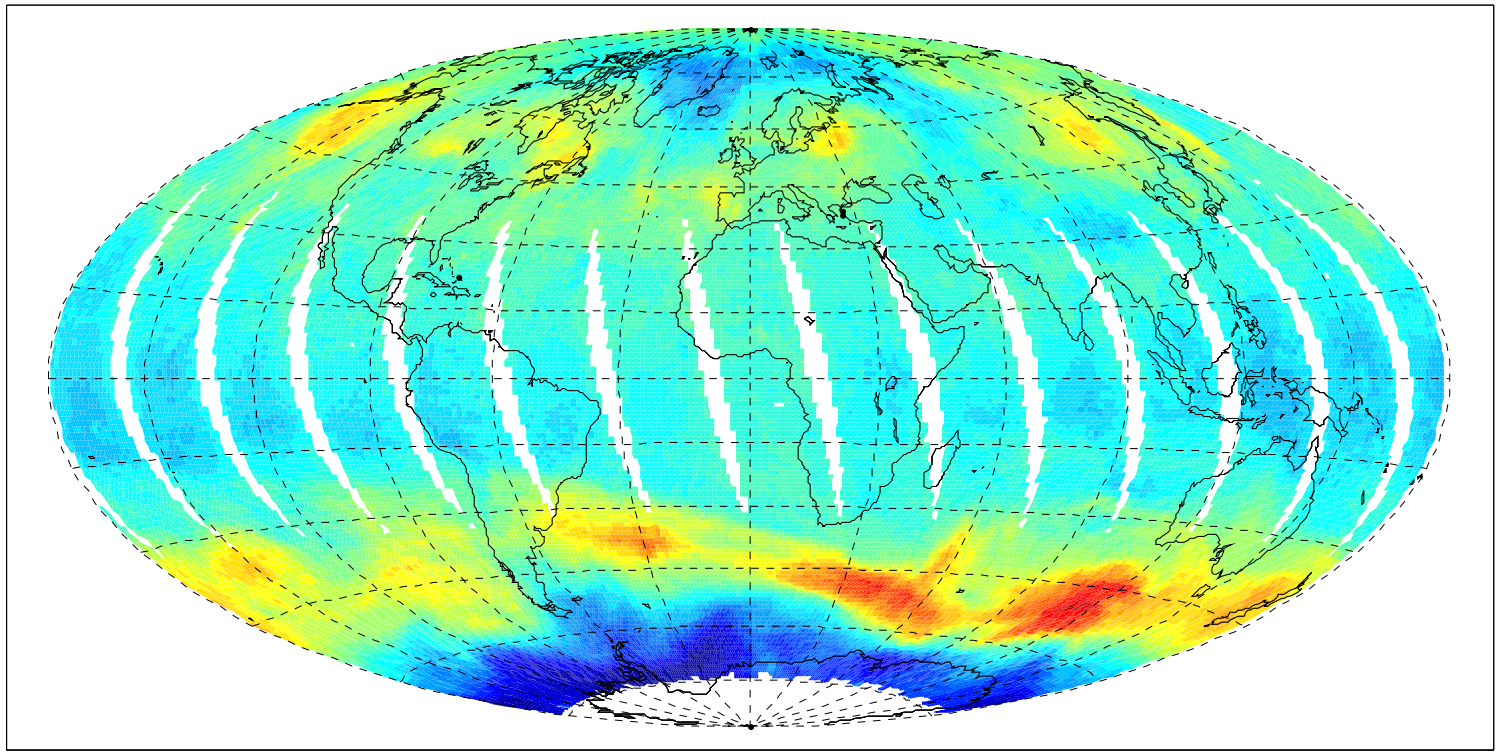
FMR

HALOE

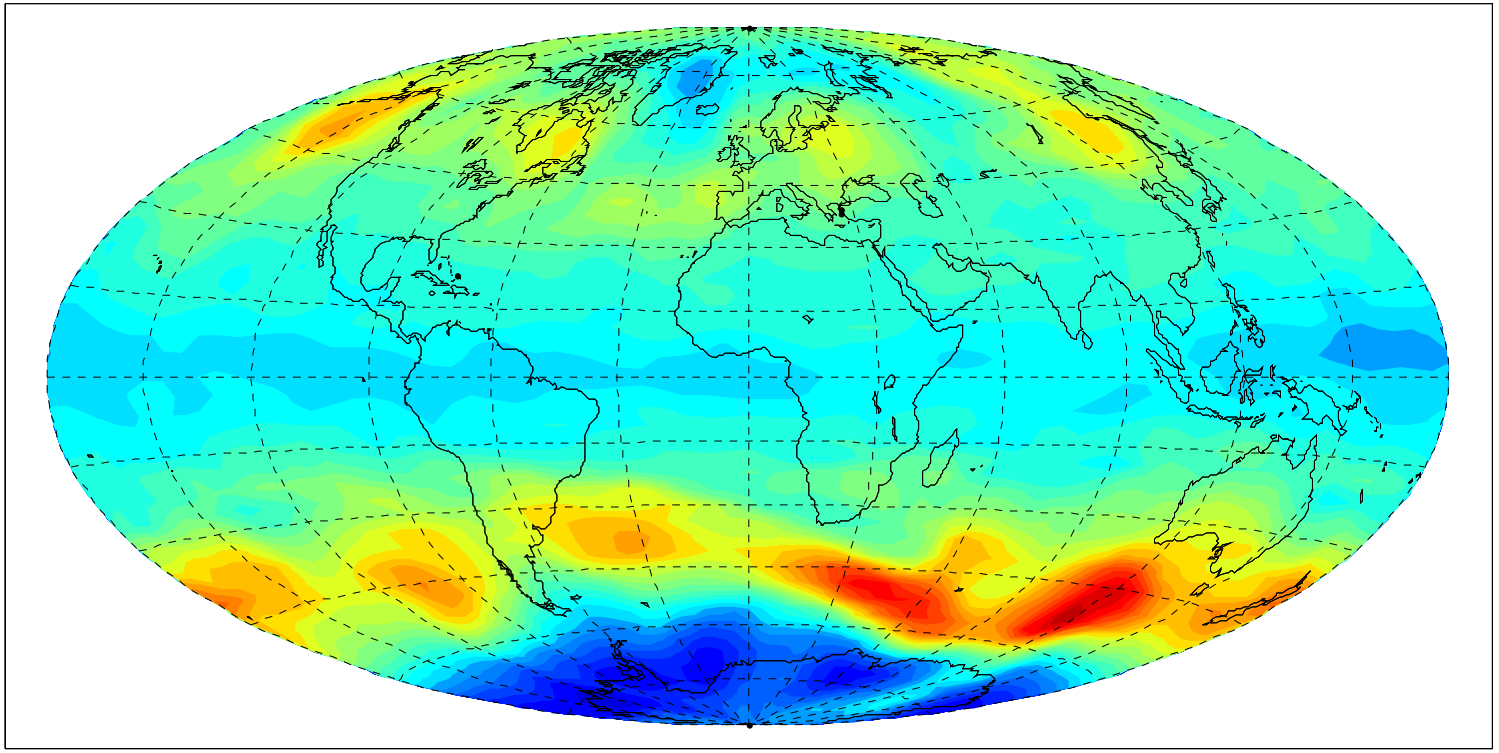
OFL analyis vs Free Model

(Schoeberl et al., JGR 2003)

TOMS total ozone 28 August 2003

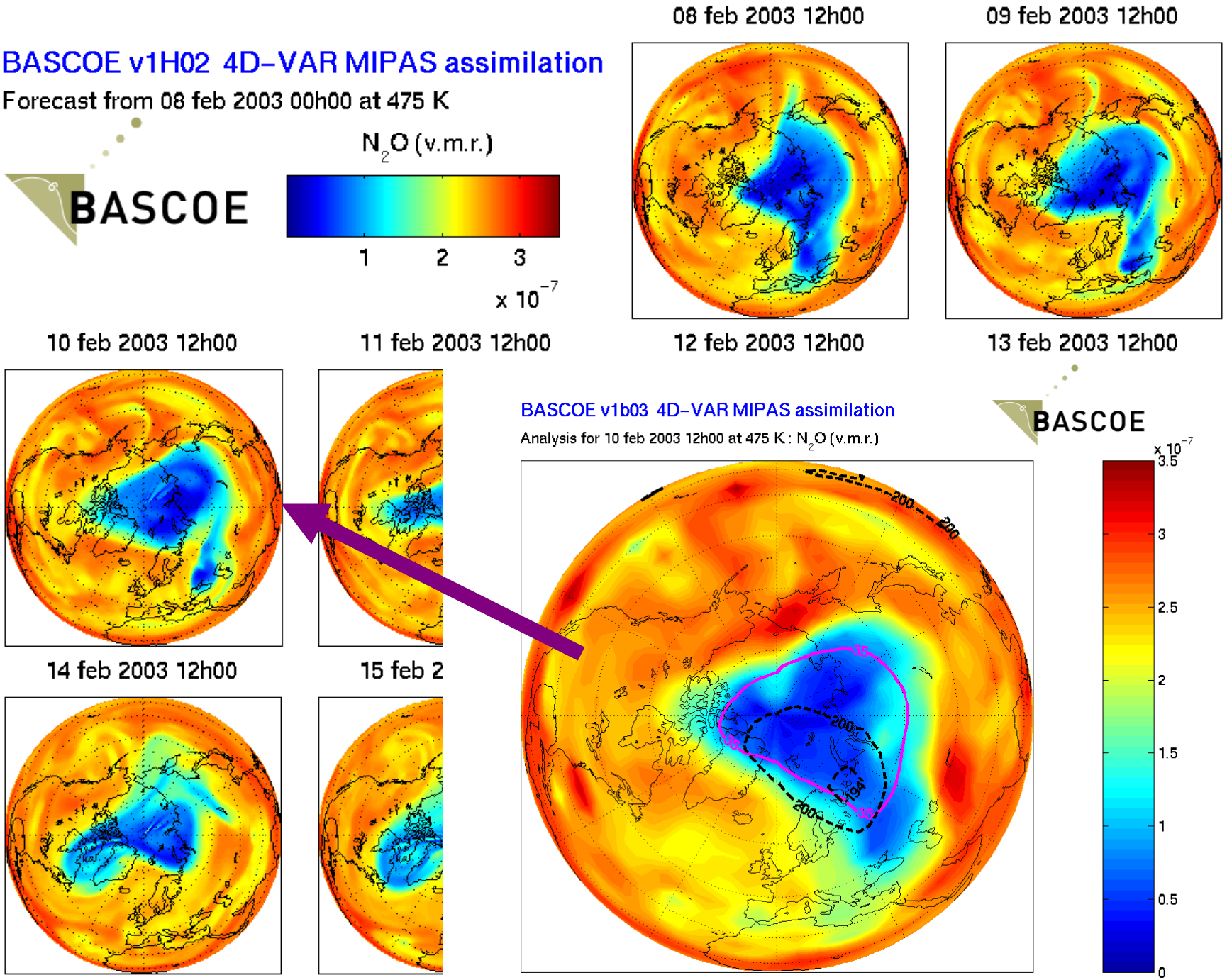


Analysis total ozone 28 August 2003, 12 UTC



The operational implementation with NRT MIPAS allows to produce chemical forecasts

**Examples with verification**


BASCOE v1H02 4D-VAR MIPAS assimilation
Forecast from 08 feb 2003 00h00 at 475 K
BASCOE
N2O (v.m.r.)
1
2
3
x 10-7
08 feb 2003 12h00
09 feb 2003 12h00
10 feb 2003 12h00
11 feb 2003 12h00
12 feb 2003 12h00
13 feb 2003 12h00
14 feb 2003 12h00
15 feb 2
BASCOE v1b03 4D-VAR MIPAS assimilation
Analysis for 10 feb 2003 12h00 at 475 K : N2O (v.m.r.)
BASCOE
x 10-7
3.5
3
2.5
2
1.5
1
0.5
0
200
194
35

# BASCOE v1H02 4D-VAR MIPAS assimilation

Forecast from 10 feb 2003 00h00 at 475 K

BASCOE

$O_3$ column (D.U.)

200 300 400 500

10 feb 2003 12h00

11 feb 2003 12h00

Assimilated GOME total ozone

15- 2-03 12h

KNMI/ESA

14 feb 2003 12h00

15 feb 2003 12h00

18 feb 2003 12h00

19 feb 2003 12h00

no data

<150 175 200 225 250 275 300 325 350 375 400 425 450 475 >500 DU

**4D –VAR chemical data assimilation system**

- Multi-variate nature of 4D – VAR
- Benefit
- Model bias sensitivity

- **Overall Consistency**
- **Independent observations**
- **Added value (non-exhaustive)**
  - Monitoring
  - Bias detection
  - Correction for dispersive dynamics
  - Chemical forecasts
- **Potential related to efforts**

# Inverse modelling at BIRA – IASB

**J. – F. Muller & J. Stavrakou**

**Belgisch Instituut voor Ruimte – Aëronomie**

***(Belgian Institute for Space Aeronomy)***

**BIRA - IASB**

aeronomie.be

**Focus:**

**Tropospheric reactive gases (ozone precursors CO, NOx, non-methane VOCs)**

*Matrix of errors on the observations*

*Matrix of errors on the emission parameters*

$$J(\mathbf{f}) = \tfrac{1}{2}\Sigma_i \, (H_i(\mathbf{f}) - y_i)^T \, \mathbf{E}^{-1} (H_i(\mathbf{f}) - y_i) + \tfrac{1}{2} \, (\mathbf{f} - \mathbf{f}_B)^T \mathbf{B}^{-1} (\mathbf{f} - \mathbf{f}_B)$$

*Model operator acting on the control variables*

*observations*

*first guess value for the control parameters*

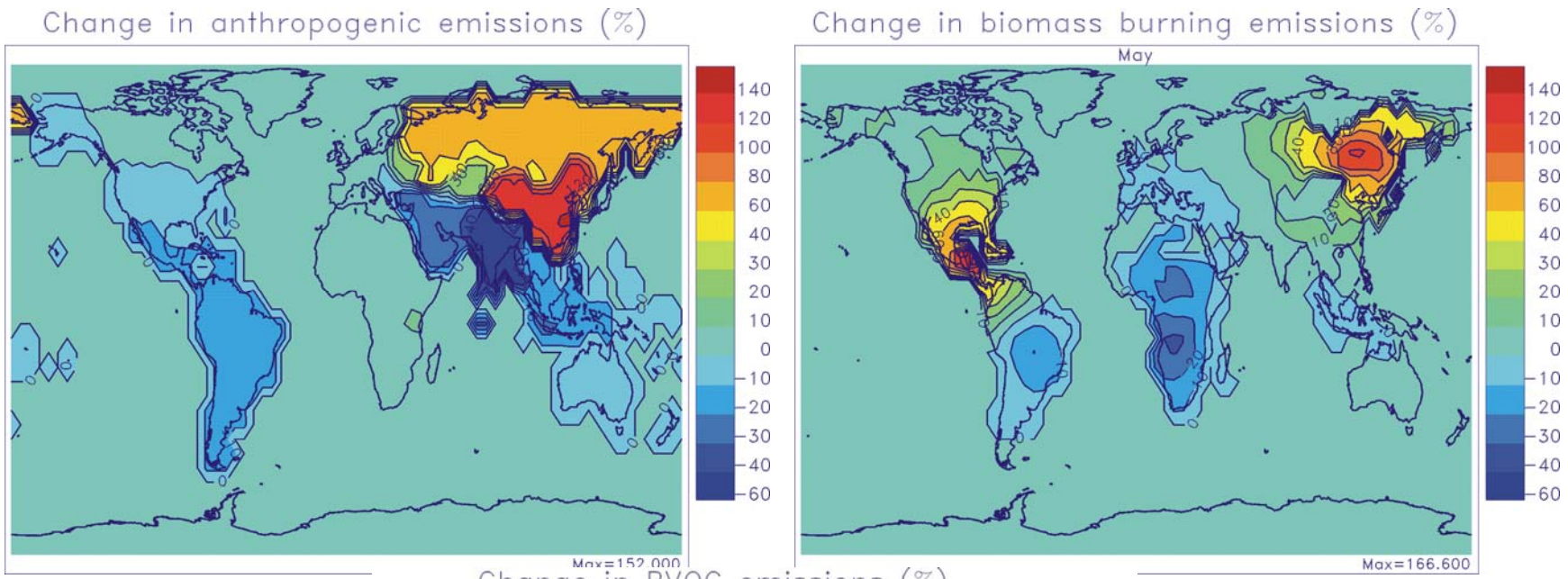
- Find best values of emission parameters, i.e. minimize the cost function
- Previous studies for reactive gases (CO, NOx, CH2O) inverted for a small number of emission parameters (big-region approach)
- Most previous studies used a linearized CTM, (i.e. OH unchanged by emission updates) ⇒ straightforward minimization of the cost (matrix inversion)
- Non-linearity is best handled using the adjoint model technique (Muller & Stavrakou 2005) also used in 4D-Var assimilation
- This technique allows also to perform grid-based inversions

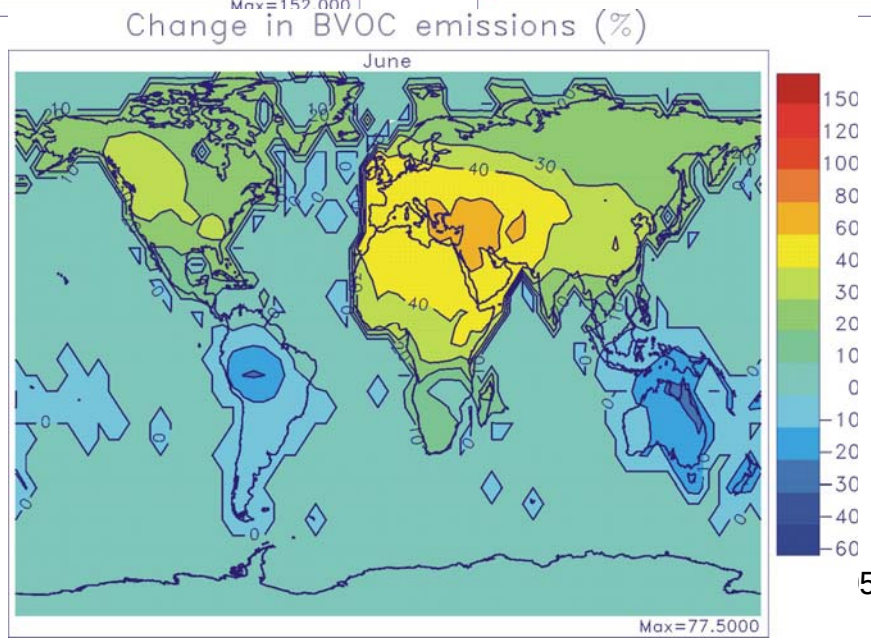
## Grid – based inversion

- Observations used: CO columns from MOPITT (05/2000 – 04/2001)
- Model used: IMAGES, 5°x5° (Müller and Stavrakou 2005)
- Number of control parameters >> number of independent observations

⇒ need additional information : correlations between errors on a priori emissions, estimated based on country boundaries, ecosystem distribution, geographical distance

# >> Inverse modelling




aeronomie.be

Federal science policy