Chemical data assimilation at BIRA – IASB

Belgisch Instituut voor Ruimte – Aëronomie
(Belgian Institute for Space Aeronomy)
BIRA – IASB

>> 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

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>> OUTLINE

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

IMAGES

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>> Introduction

- **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**

>> Introduction >> Overview chemistry

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

>> Introduction >> Overview chemistry

2. Nitrogen radicals (member of NO_y)

$$NO_2 + O \rightarrow NO + O_2$$
$$NO + O_3 \rightarrow NO_2 + O_2$$
Net: $$O + O_3 \rightarrow 2\,O_2$$

Nitrogen Source Gas: N_2O (and …)

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

3. Chlorine radicals (member of Cl_y)

$$ClO + O \rightarrow Cl + O_2$$
$$Cl + O_3 \rightarrow ClO + O_2$$
Net: $$O + O_3 \rightarrow 2\,O_2$$

Chlorine Source Gases: Organic Chlorine

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

>> Chemical data assimilation

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Chemical data assimilation

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

⇓

Necessity

>> Why chemical data assimilation >> Model shortcomings

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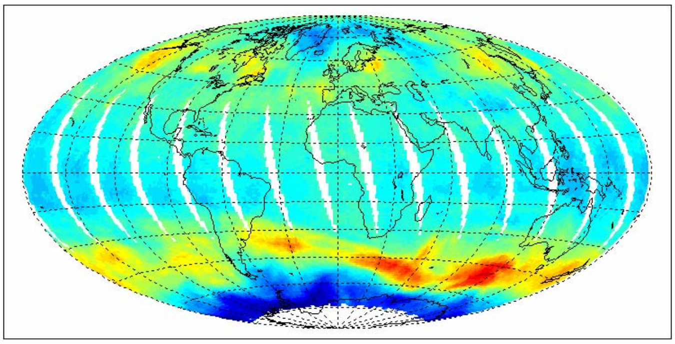
TOMS total ozone 28 August 2003



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>> Why chemical data assimilation >> Model shortcomings

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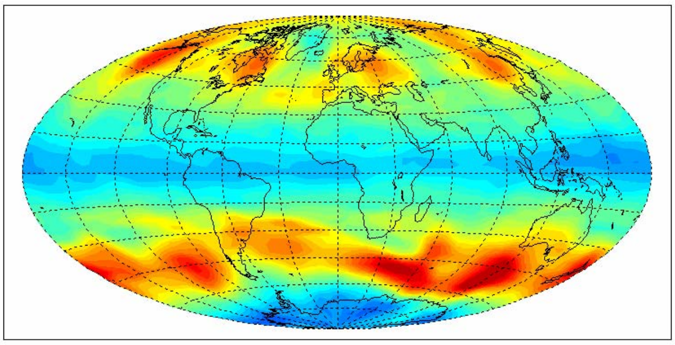
Free model total ozone 28 August 2003, 12 UTC



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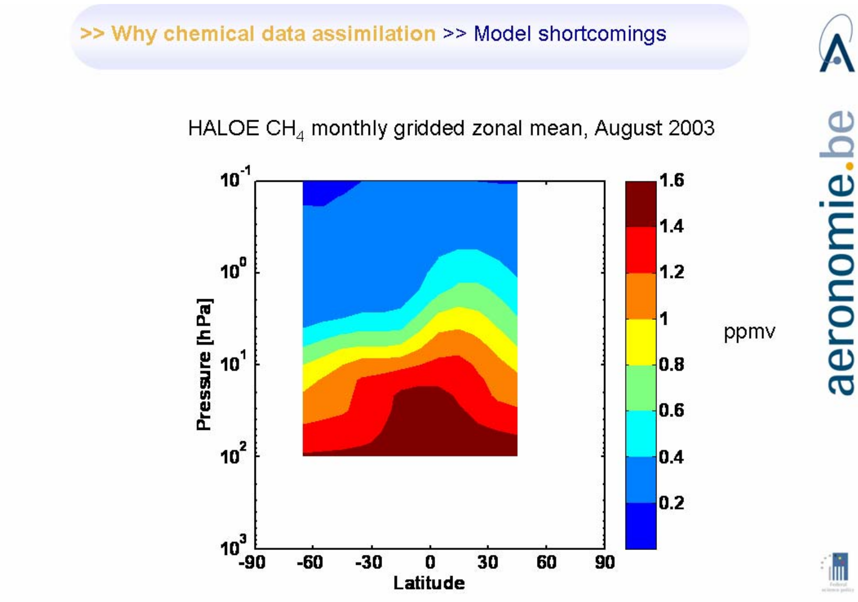
>> Why chemical data assimilation >> Model shortcomings
HALOE CH4 monthly gridded zonal mean, August 2003
Pressure [hPa]
Latitude
ppmv
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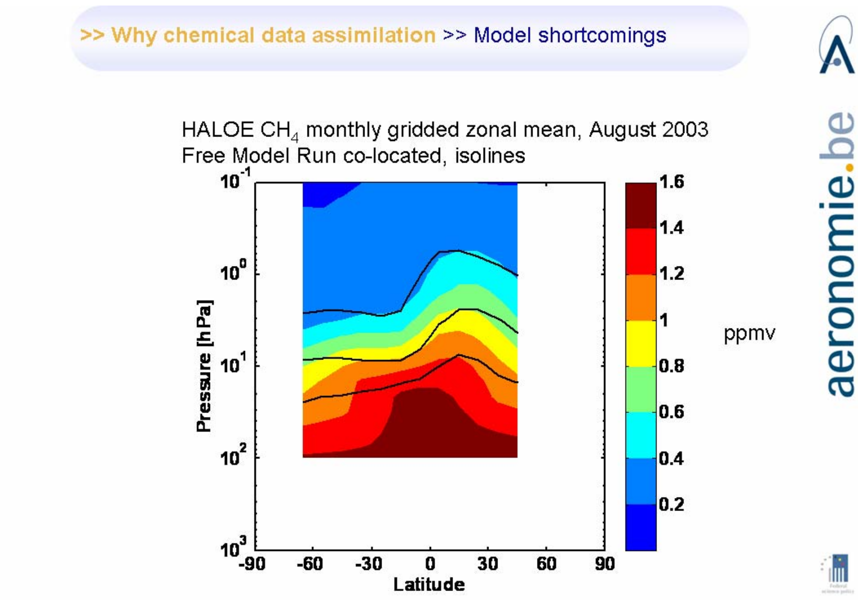
>> Why chemical data assimilation >> Model shortcomings
HALOE CH4 monthly gridded zonal mean, August 2003
Free Model Run co-located, isolines
Pressure [hPa]
Latitude
ppmv
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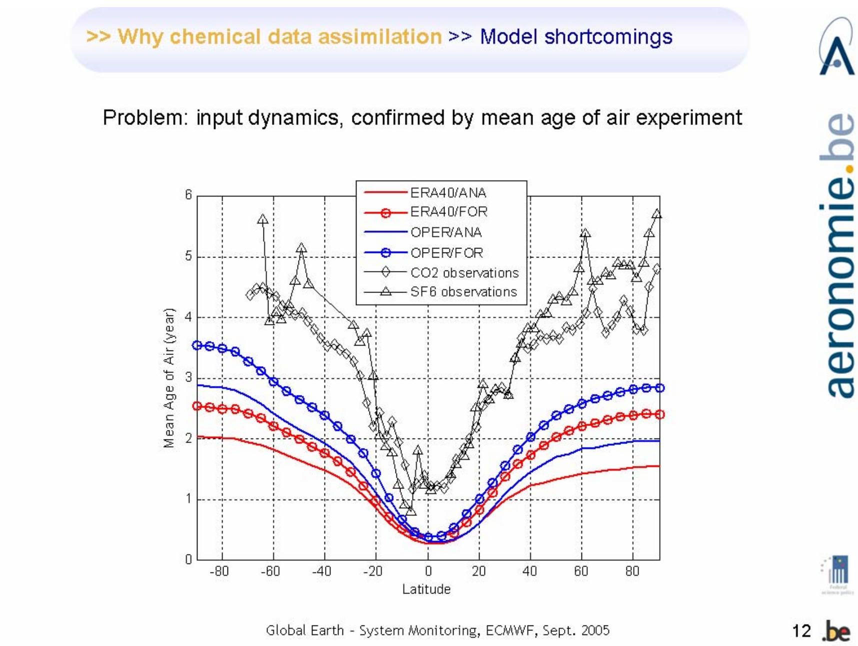
>> Why chemical data assimilation >> Model shortcomings
Problem: input dynamics, confirmed by mean age of air experiment
ERA40/ANA
ERA40/FOR
OPER/ANA
OPER/FOR
CO2 observations
SF6 observations
Mean Age of Air (year)
Latitude
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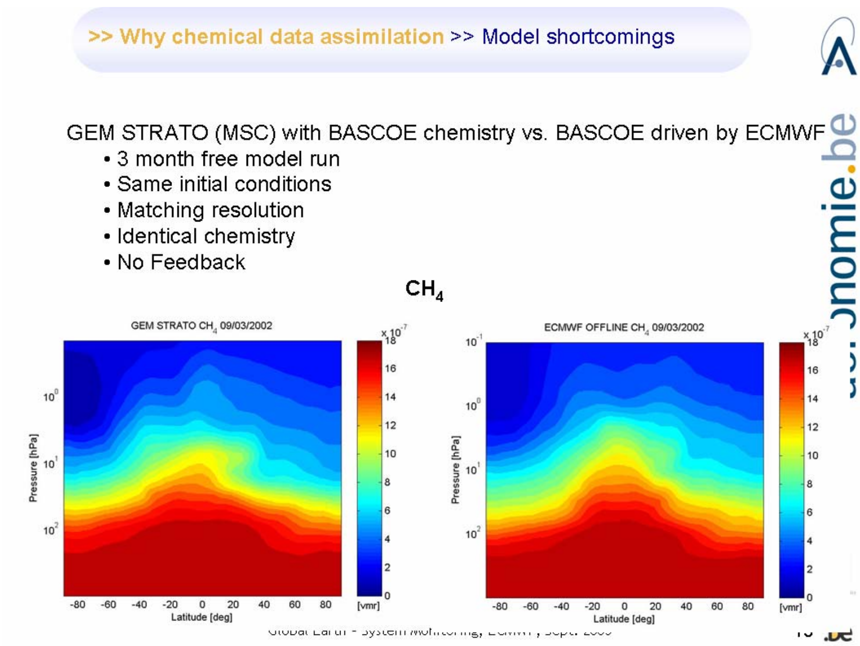
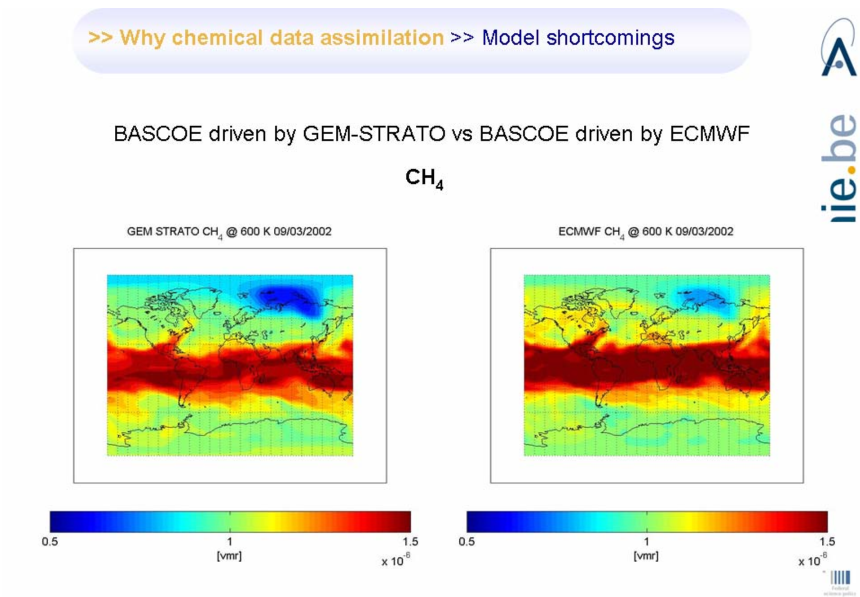
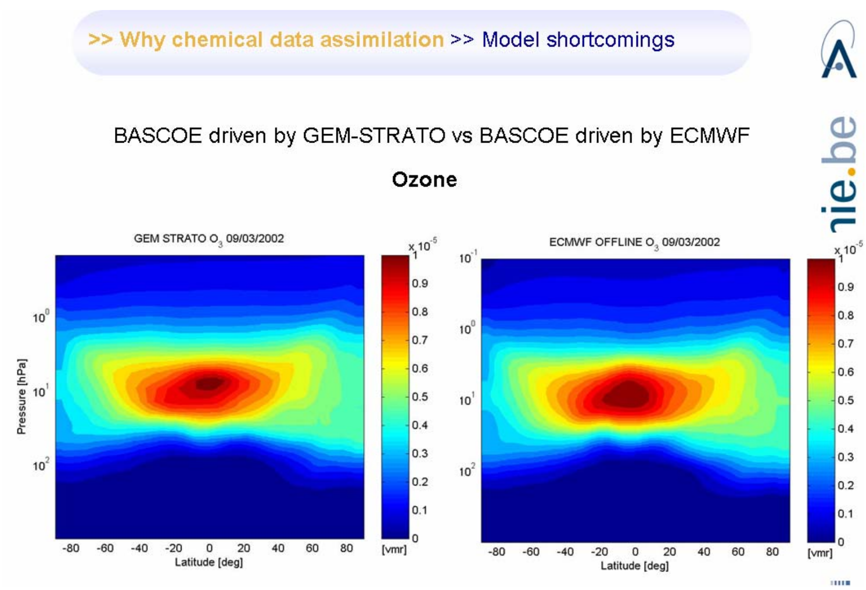

>> Why chemical data assimilation >> Model shortcomings
GEM STRATO (MSC) with BASCOE chemistry vs. BASCOE driven by ECMWF
• 3 month free model run
• Same initial conditions
• Matching resolution
• Identical chemistry
• No Feedback
CH4
GEM STRATO CH4 09/03/2002
ECMWF OFFLINE CH4 09/03/2002
Pressure [hPa]
Latitude [deg]
[vmr]

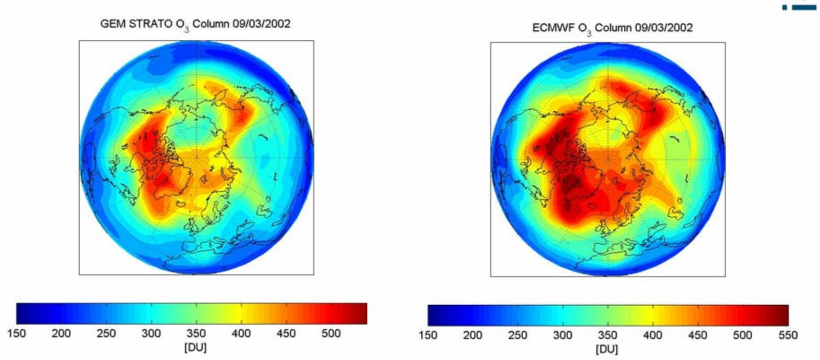

>> Why chemical data assimilation >> Model shortcomings
BASCOE driven by GEM-STRATO vs BASCOE driven by ECMWF
CH4
GEM STRATO CH4 @ 600 K 09/03/2002
ECMWF CH4 @ 600 K 09/03/2002
[vmr]


>> Why chemical data assimilation >> Model shortcomings
BASCOE driven by GEM-STRATO vs BASCOE driven by ECMWF
Ozone
GEM STRATO O3 09/03/2002
ECMWF OFFLINE O3 09/03/2002
Pressure [hPa]
Latitude [deg]
[vmr]

>> Why chemical data assimilation >> Model shortcomings

BASCOE driven by GEM-STRATO vs BASCOE driven by ECMWF

Total ozone



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>> Why chemical data assimilation >> Model shortcomings

Model Shortcomings:

- **Effect of dynamical assimilation**
- **Effect of different dynamical assimilation systems**
- **Dynamics driven shortcomings**
- **Chemical modelling shortcomings (not shown)**

>> 4D – VAR

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
B:	background error covariance matrix
R:	observational error covariance matrix

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>> 4D – VAR >> BASCOE

- **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: 1[st] 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 %

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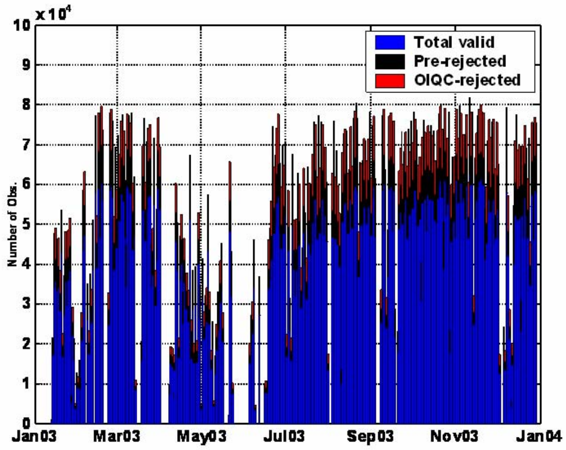
4D – VAR >> BASCOE >> OFL number of observations



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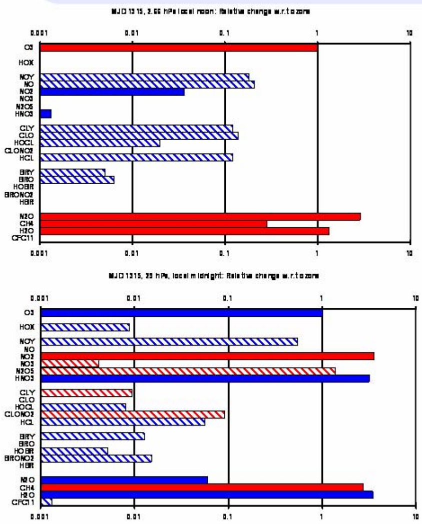
4D – VAR >> BASCOE >> Multi-variate nature



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

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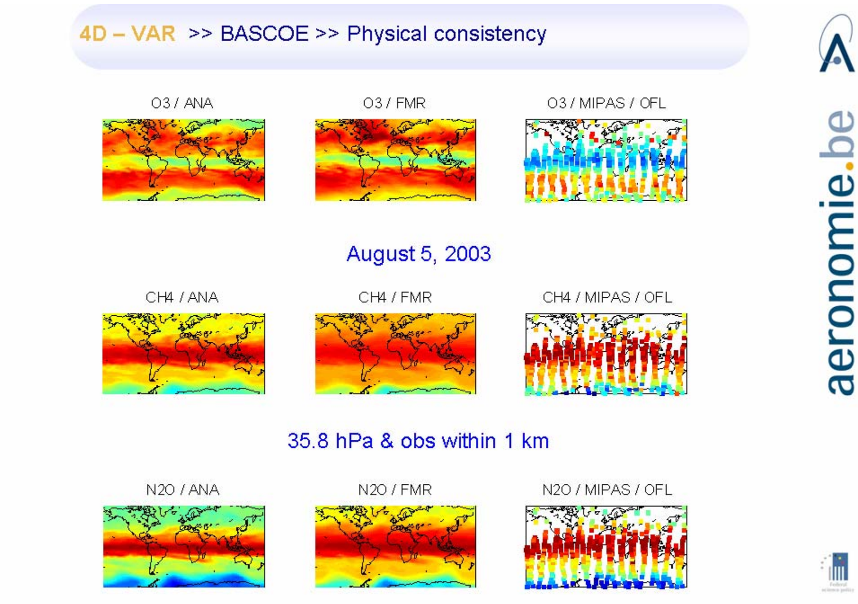
4D – VAR >> BASCOE >> Physical consistency
O3 / ANA
O3 / FMR
O3 / MIPAS / OFL
August 5, 2003
CH4 / ANA
CH4 / FMR
CH4 / MIPAS / OFL
35.8 hPa & obs within 1 km
N2O / ANA
N2O / FMR
N2O / MIPAS / OFL
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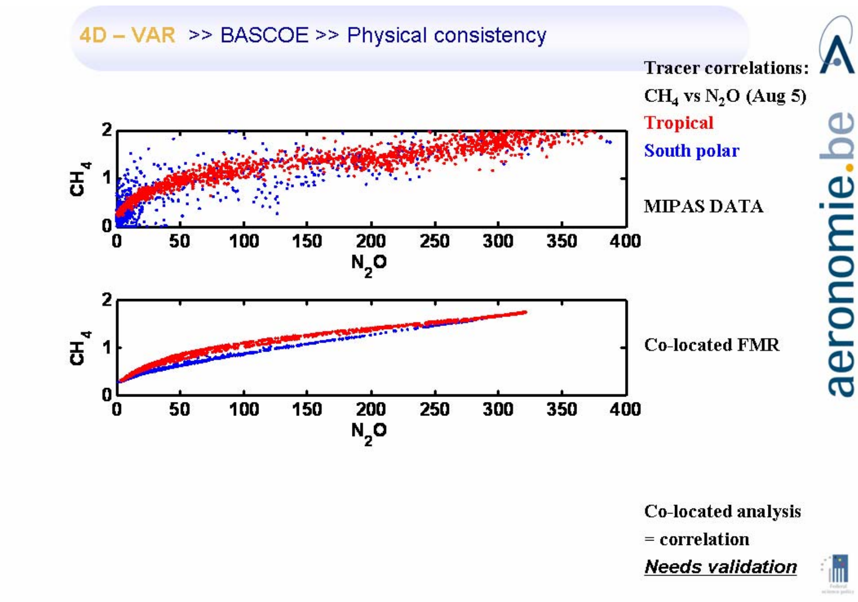
4D – VAR >> BASCOE >> Physical consistency
Tracer correlations:
CH_4 vs N_2O (Aug 5)
Tropical
South polar
MIPAS DATA
CH_4
N_2O
0
50
100
150
200
250
300
350
400
Co-located FMR
Co-located analysis
= correlation
Needs validation
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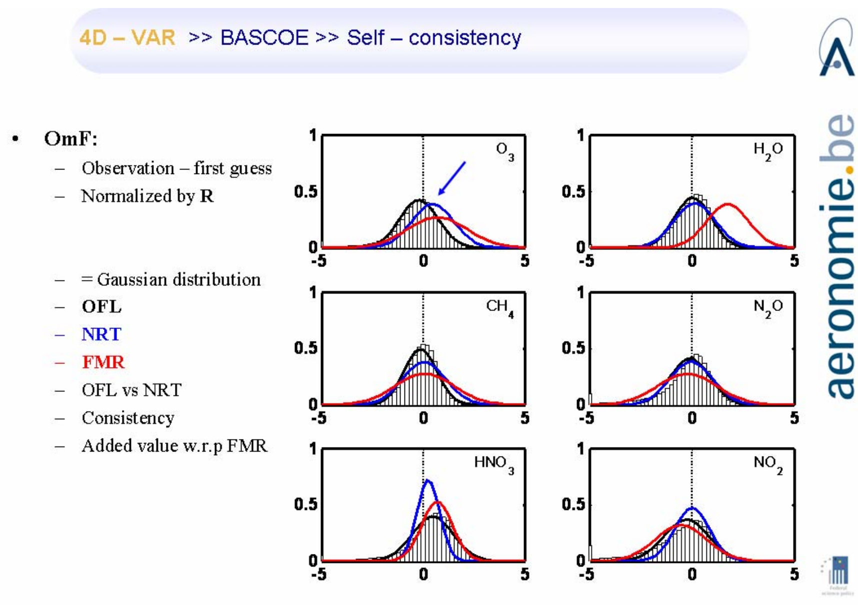
4D – VAR >> BASCOE >> Self – consistency
• OmF:
– Observation – first guess
– Normalized by R
– = Gaussian distribution
– OFL
– NRT
– FMR
– OFL vs NRT
– Consistency
– Added value w.r.p FMR
O_3
H_2O
CH_4
N_2O
HNO_3
NO_2
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4D – VAR >> BASCOE >> Self – consistency >> model improvement

NRT results:

Ozone @ 1 hPa underestimated

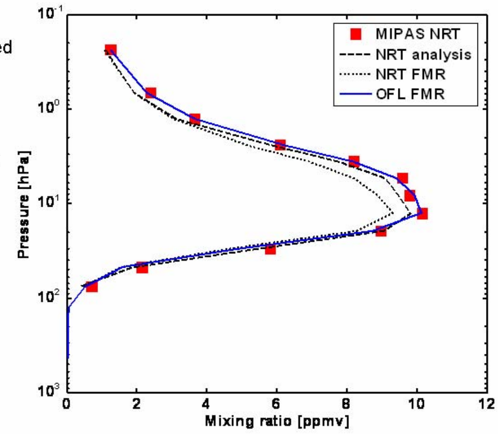
- Analysis = free model
- Model not constrained
- O_2 main source of O_3
- O_2 not a control variable

↓

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

↓

- Better agreement



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

Self – consistency 4D – VAR:

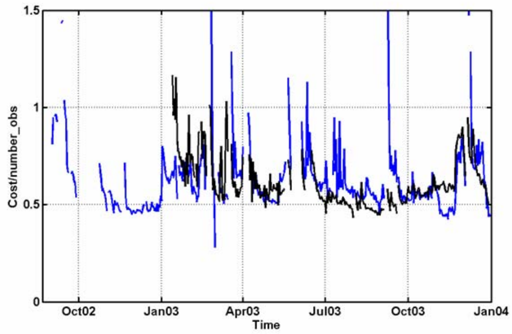
$E[J_{analysis}] = p/2$

Time series $J_{analysis}/p$

NRT

OFL

Monitoring capability



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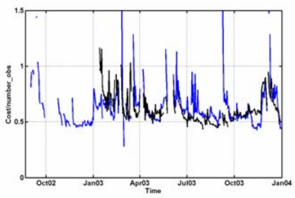
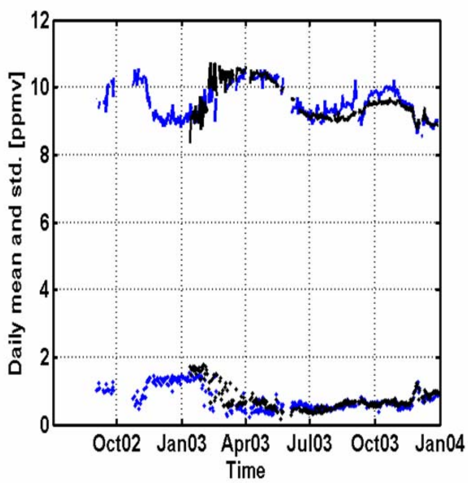
4D – VAR >> BASCOE >> Self – consistency >> monitoring



Monitoring capability

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

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



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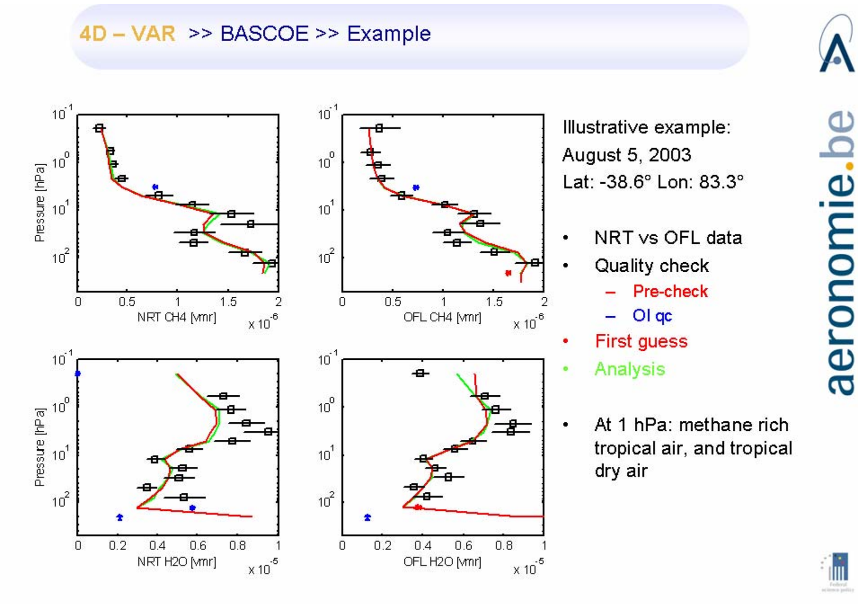
4D – VAR >> BASCOE >> Example
Pressure [hPa]
NRT CH4 [vmr]
OFL CH4 [vmr]
NRT H2O [vmr]
OFL H2O [vmr]
Illustrative example:
August 5, 2003
Lat: -38.6° Lon: 83.3°
NRT vs OFL data
Quality check
– Pre-check
– OI qc
First guess
Analysis
At 1 hPa: methane rich tropical air, and tropical dry air
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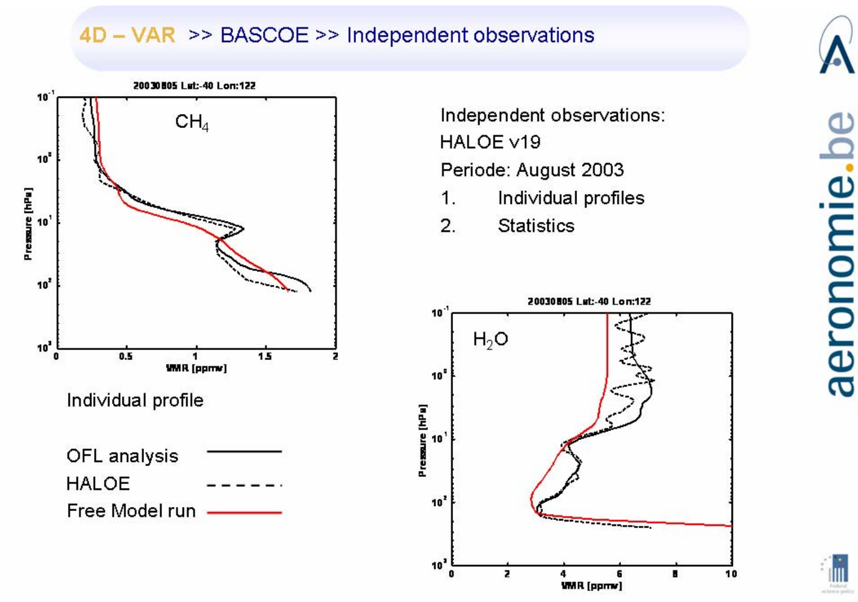
4D – VAR >> BASCOE >> Independent observations
20030805 Lat:-40 Lon:122
CH4
Pressure [hPa]
VMR [ppmv]
Independent observations:
HALOE v19
Periode: August 2003
1. Individual profiles
2. Statistics
Individual profile
OFL analysis
HALOE
Free Model run
H2O
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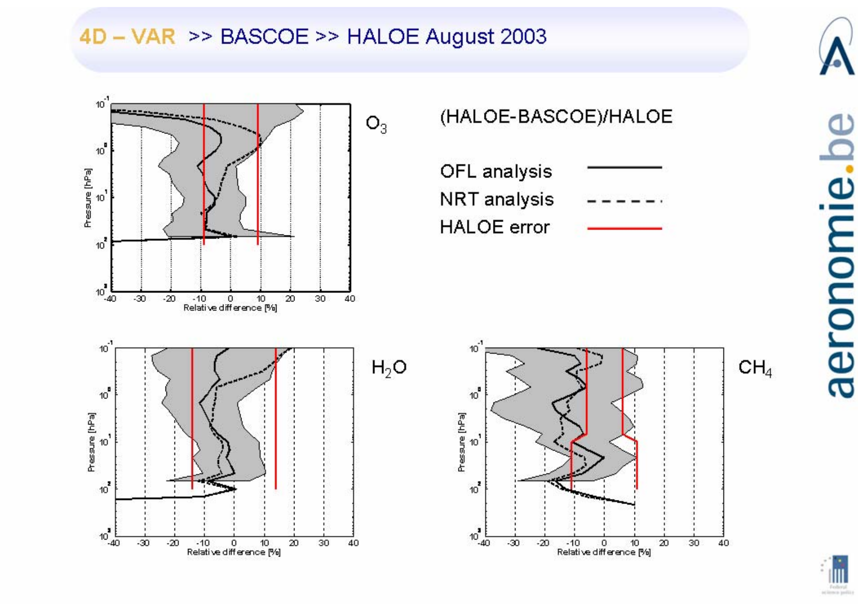
4D – VAR >> BASCOE >> HALOE August 2003
O3
(HALOE-BASCOE)/HALOE
OFL analysis
NRT analysis
HALOE error
H2O
CH4
Pressure [hPa]
Relative difference [%]
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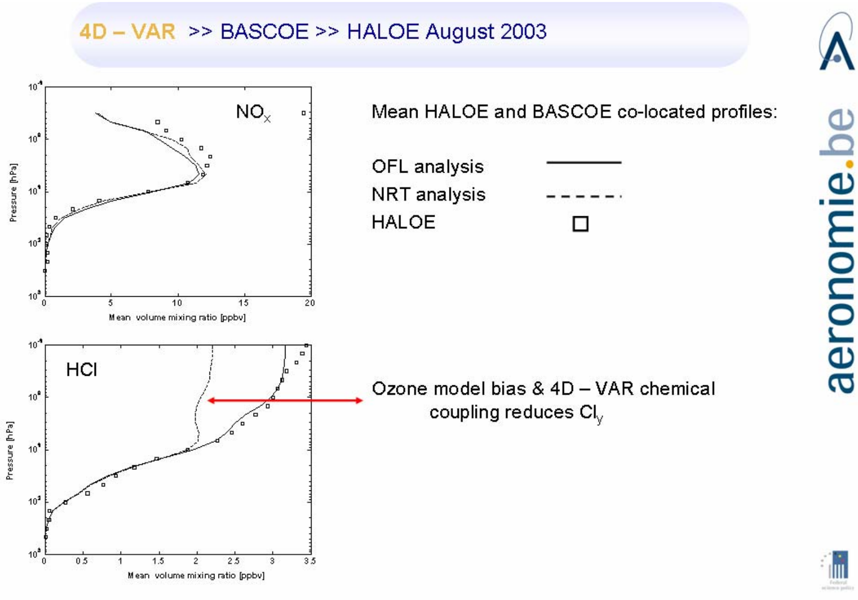
4D – VAR >> BASCOE >> HALOE August 2003
NOx
Mean volume mixing ratio [ppbv]
Pressure [hPa]
Mean HALOE and BASCOE co-located profiles:
OFL analysis
NRT analysis
HALOE
HCl
Ozone model bias & 4D – VAR chemical coupling reduces Cly
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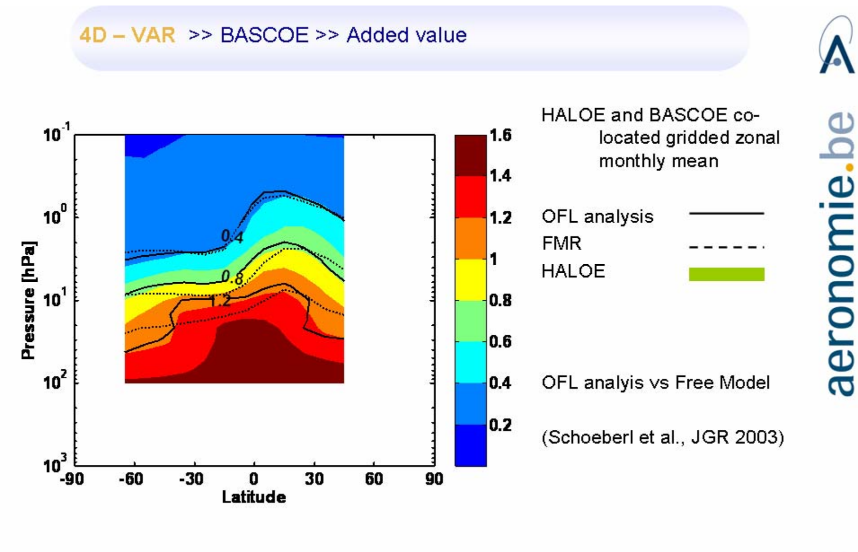
4D – VAR >> BASCOE >> Added value
Pressure [hPa]
Latitude
HALOE and BASCOE co-located gridded zonal monthly mean
OFL analysis
FMR
HALOE
OFL analyis vs Free Model
(Schoeberl et al., JGR 2003)
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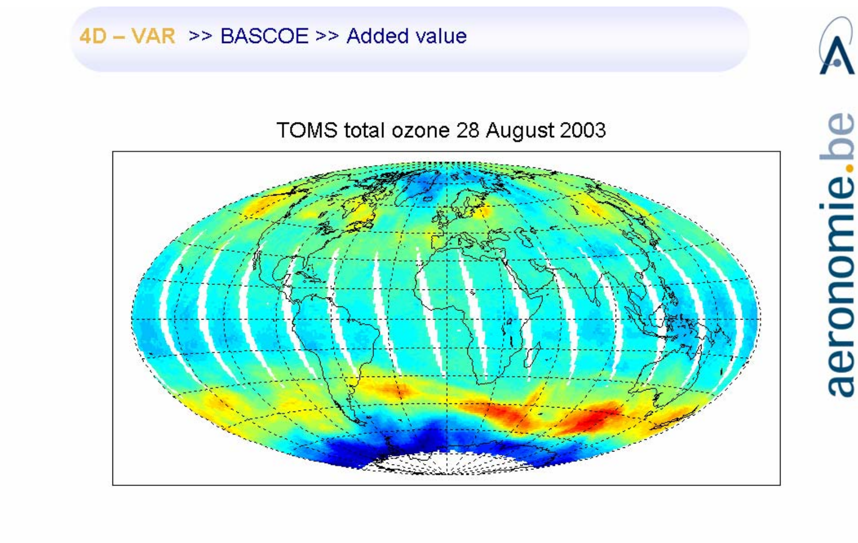
4D – VAR >> BASCOE >> Added value
TOMS total ozone 28 August 2003
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4D – VAR >> BASCOE >> Added value

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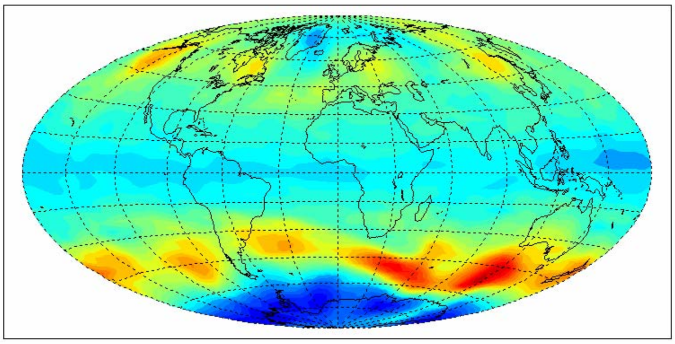
Analysis total ozone 28 August 2003, 12 UTC



4D – VAR >> BASCOE >> Added value >> Chemical forecasts

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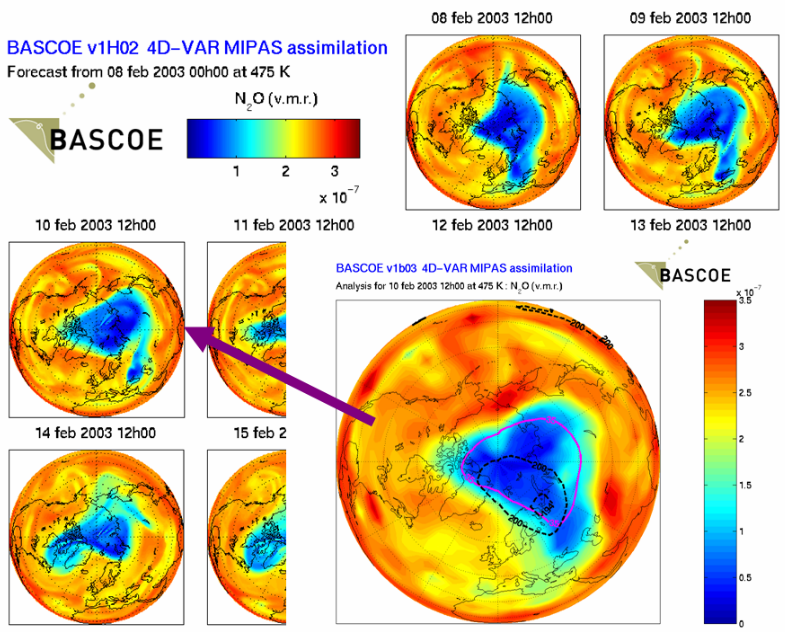
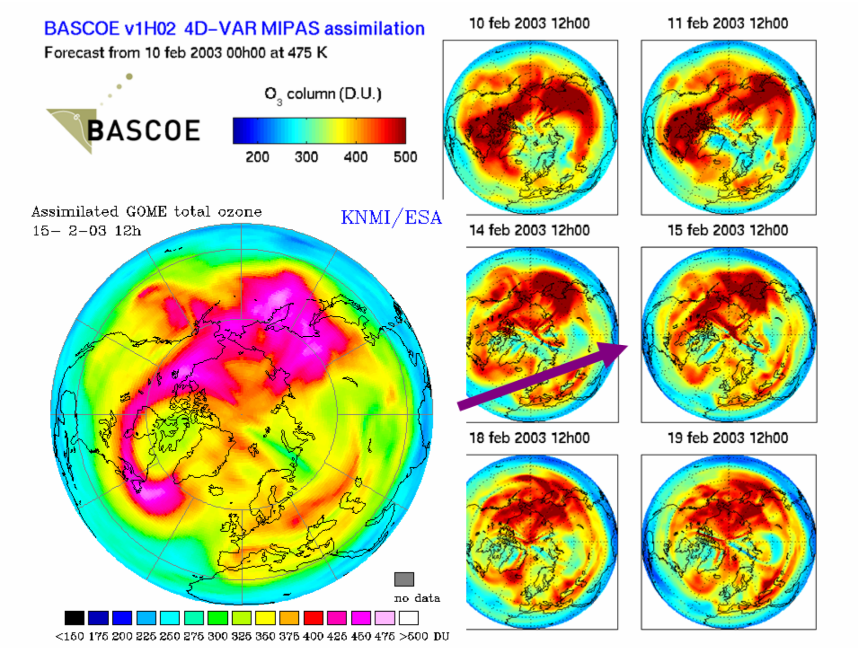
The operational implementation with NRT MIPAS allows to produce chemical forecasts

Examples with verification





4D – VAR >> BASCOE >> Conclusions

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**

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>> Inverse modelling

Inverse modelling at BIRA – IASB

J. – F. Muller & J. Stavrakou

Belgisch Instituut voor Ruimte – Aëronomie

(Belgian Institute for Space Aeronomy)

BIRA - IASB

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>> Inverse modelling

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Focus:

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

>> Inverse modelling

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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

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>> Inverse modelling

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- **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**

>> Inverse modelling

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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

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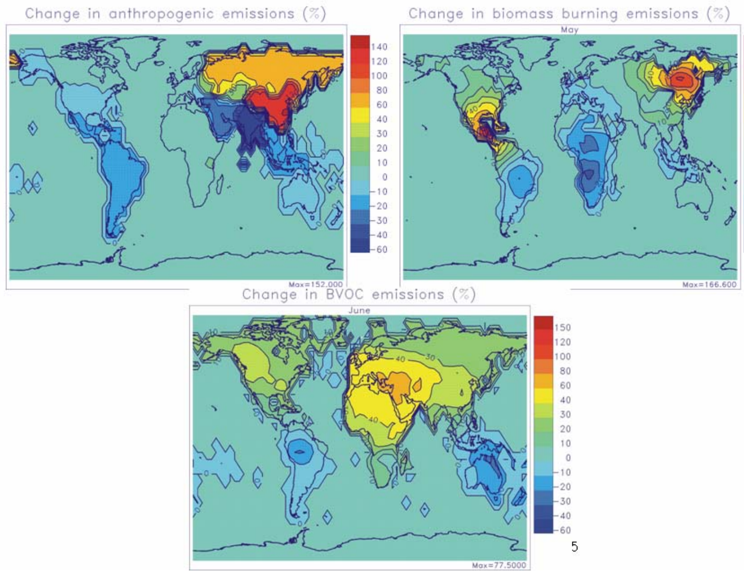

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