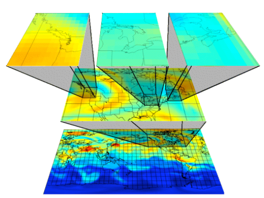
# Coupled Chemical-Dynamical Data Assimilation


Richard Ménard, Cecillien Charette, Martin Charron, Pierre Gauthier, Jean deGrandpre, Alain Robichaud, Yves Rochon, Yan Yang
*Meteorological Service of Canada*

Simon Chabrillat, Dominique Fonteyn
*Belgium Institute for Space Aeronomy*

Jack McConnell, Jacek Kaminski
*York University*


YORK UNIVERSITÉ UNIVERSITY



BIRA-IASB

BASCOE


**Environment Canada**
**Meteorological Service of Canada**

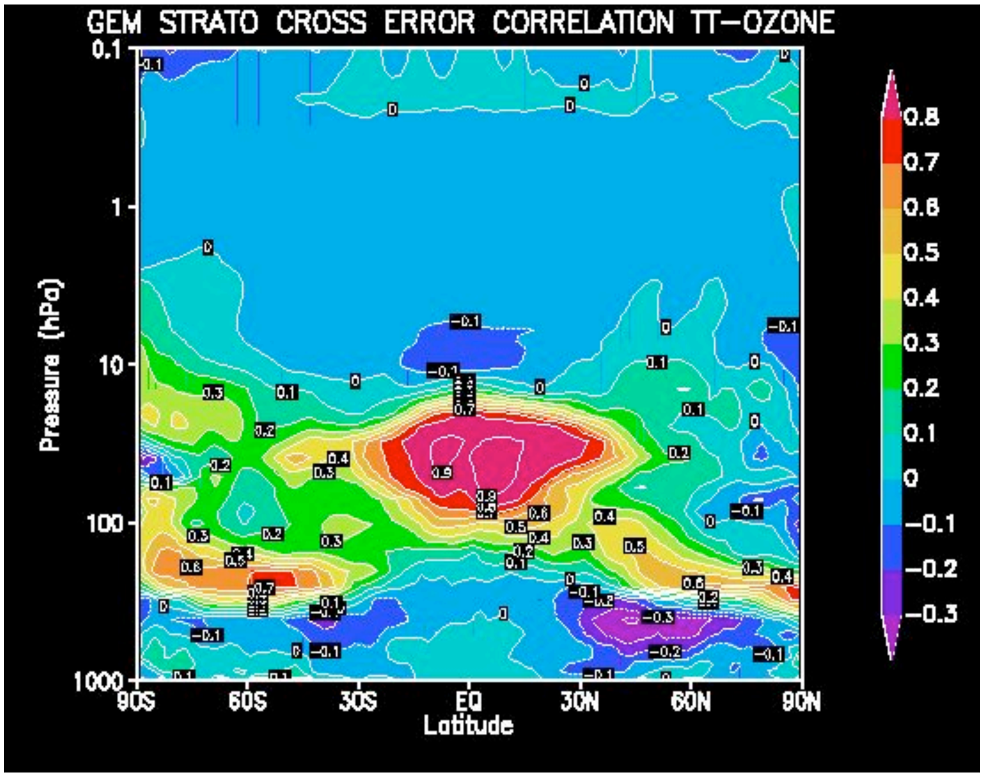
**Environnement Canada**
**Service Météorologique du Canada**

# Outline

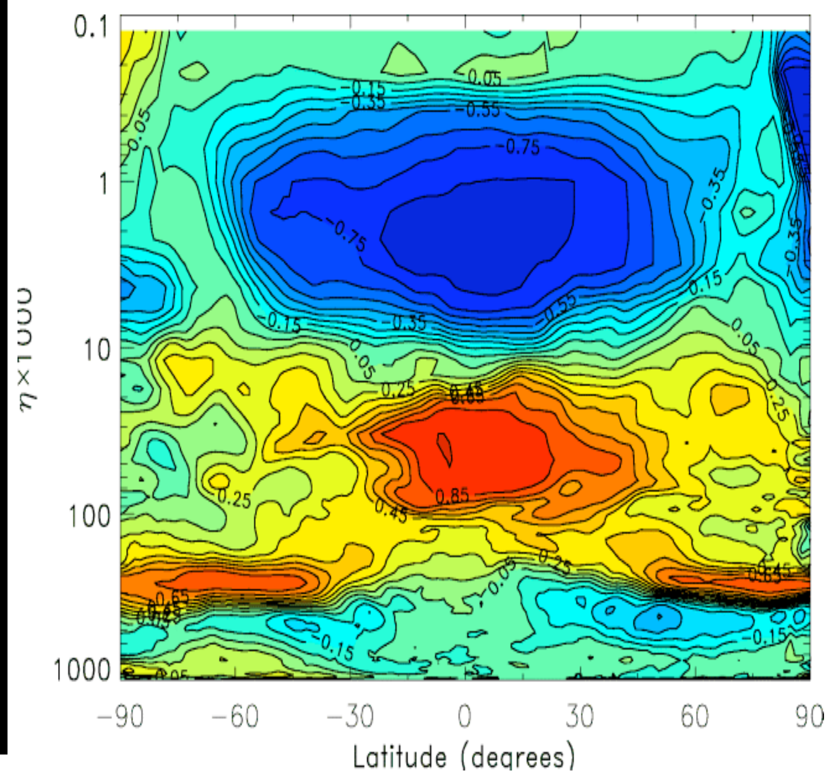
- Why consider the coupling in DA
- GEM-Strato-BIRA model: Description and evaluation
- Changes in the Canadian DAS
- Stratospheric forecast skill
- AMSU-a bias in the stratosphere
- Error statistics for chemical species

## $O_3$–T correlation using forecast difference method (i.e. Canadian Quick Covariance method)

**Without ozone-rad. interaction**




**With ozone-rad. interaction**

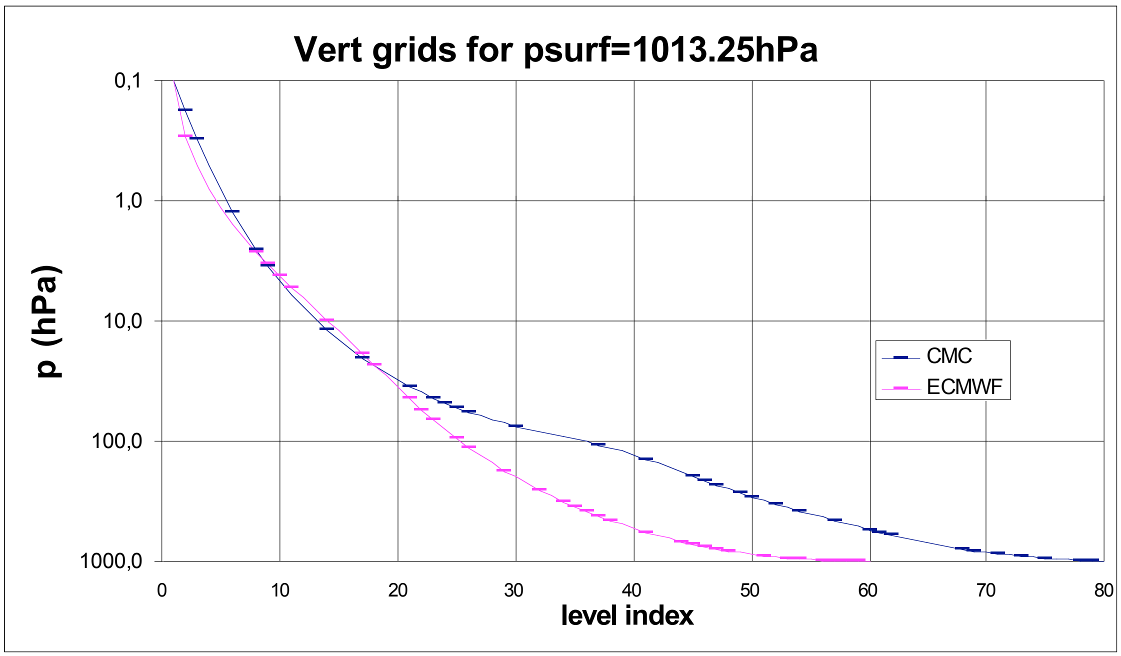


## From the operational NWP model « GEM » to the stratospheric GCCM « GEM-Stato-BIRA »

- Raised upper boundary
  from 10 hPa (27 levels) to 0.1 hPa (80 levels)
- Updated/added physical parameterizations
  to improve strato dyn
    - GEM-Strato
- Implemented strato photochemistry module
  from BASCOE
    - GEM-BIRA, “passive” chemistry
- Allowed new chemical fields ($O_3$, $H_2O$) to interact with radiation,
  hence dynamics
    - GEM-BIRA, “active” chemistry

# Model grid

- Horiz. grid: lat-lon, polar poles, 1.5°×1.5° (≈150×150km)
- Vertical grid: 80 hybrid levels from surface to 0.1 hPa. Comparing with ECMWF operational grid:



## Either hydrostatic with pressure based vertical coordinate or nonhydrostatic with mass-based vertical coordinate

**Euler equations in height coordinate**

Horizontal momentum
$$\frac{d\mathbf{V}}{dt} + f\mathbf{k}\times\mathbf{V} + \alpha\nabla_z p = 0$$

Vertical momentum
$$\gamma\frac{dw}{dt} + g + \alpha\frac{\partial p}{\partial z} = 0$$

$$\gamma = \begin{cases} 0 & \text{hydrostatic} \\ 1 & \text{nonhydrostatic} \end{cases}$$

Thermodynamics
$$\frac{dT}{dt} + \frac{RT}{C_V}D_3 = 0$$

$$D_3 = \nabla_z\cdot\mathbf{V} + \frac{\partial w}{\partial z}$$

Continuity
$$\frac{d\alpha}{dt} - \alpha D_3 = 0$$

*Under normal atmospheric conditions nonhydrostatic effects become perceptible when the scale of interest is < 100 km and necessary when the scale is < 10 km*

## Hydrostatic-pressure coordinate system

Continuity equation in any vertical coordinate, *s*

$$\left[\frac{\partial}{\partial t}\left(\rho\frac{\partial z}{\partial s}\right)\right]_s + \nabla_s\cdot\left(\rho\mathbf{V}\frac{\partial z}{\partial s}\right)+\frac{\partial}{\partial s}\left(\rho\dot{s}\frac{\partial z}{\partial s}\right)=0 \qquad \text{where } \dot{s}=\frac{ds}{dt}$$

taking *s* such that $\boxed{\rho\frac{\partial z}{\partial s}=C^{te}}$ leads to the simplification

$$\nabla_s\cdot\left(\rho\mathbf{V}\frac{\partial z}{\partial s}\right)+\frac{\partial}{\partial s}\left(\rho\dot{s}\frac{\partial z}{\partial s}\right)=0$$

*A diagnostic equation !*

Setting $C^{te}=g^{-1}$ and let this new coordinate $s=\pi$

$$\boxed{\nabla_\pi\cdot\mathbf{V}+\frac{\partial\dot{\pi}}{\partial\pi}=0}$$

and with this choice of constant it can be shown that $\frac{\partial\pi}{\partial z}=-\rho g$

So that $\pi$ is an hydrostatic-pressure coordinate (or mass coordinate) system. The continuity equation retains the same form as with the hydrostatic assumption with pressure coordinate.

Conserving a similar set of equations, but changing the definition of the vertical coordinate, GEM can accurately simulate all scales, from the large (planetary) scale to a plume model (few meters).

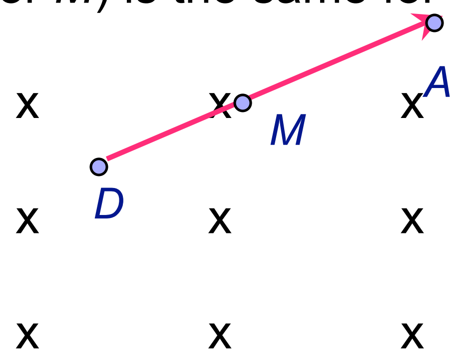
## Semi-Lagrangian Transport

♣ Do not conserve any transport properties (e.g. mass, monotonic, …) except correlation between tracers (for a number interpolation schemes)

♣ Computationally efficient for large number of tracers

*Can save computation in semi-Lagrangian advection transport*

- upstream point (*D* or *M*) is the same for all advected species




- interpolation weights $C_i(x)$ are the same for all advected species

*e.g. cubic Lagrange interpolation*

$$\varphi(x) = \sum_{i=1}^{4} C_i(x)\varphi_i \quad \text{with weights} \quad C_i(x) = \frac{\prod_{k \neq i}^{4} (x - x_k)}{\prod_{k \neq i}^{4} (x_i - x_k)}$$

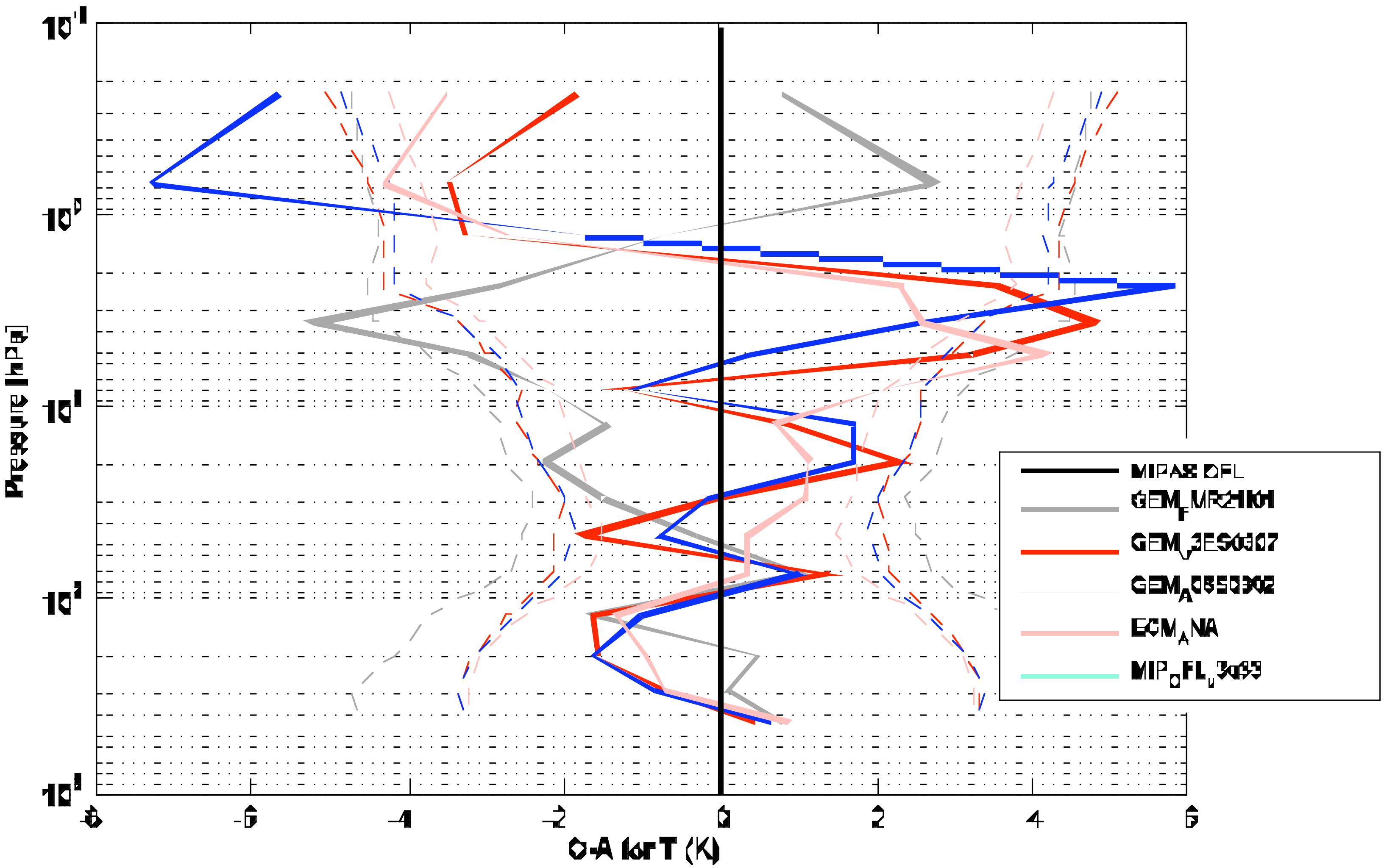
## Chemistry

- Chemical interface (next official release of GEM)

BASCOE chemistry

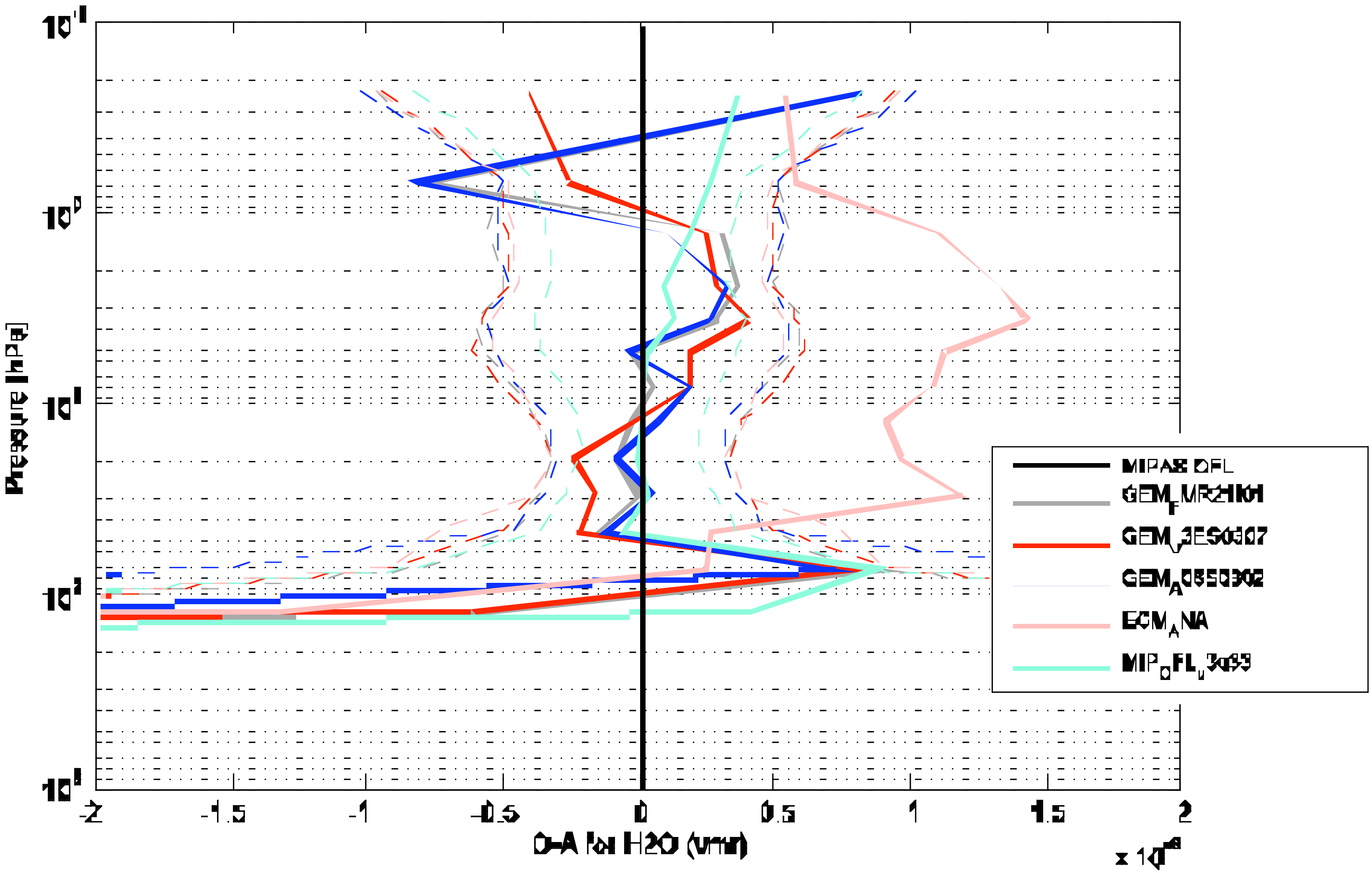
- Look-up tables J values (height, overhead total column $O_3$, SZA)
- 57 chemical species, all advected
- $O_x$, $HO_x$, $NO_x$, $ClO_x$, $BrO_x$ and few hydrocarbons
- Source species: $N_2O$, $CH_4$, $H_2O$, CFCs, HCFCs and Halons
- 142 gas-phase, 7 heterogeneous and 52 photodissociation reactions
- Photochemical rates are taken from JPL-2002
- Rosenbrock solver 3$^{rd}$ order
- Heterogeneous chemistry is fully resolved, with simplified parameterizations for surface area densities

# Temperature comparison with MIPAS observations
# Tropics (30S, 30N)



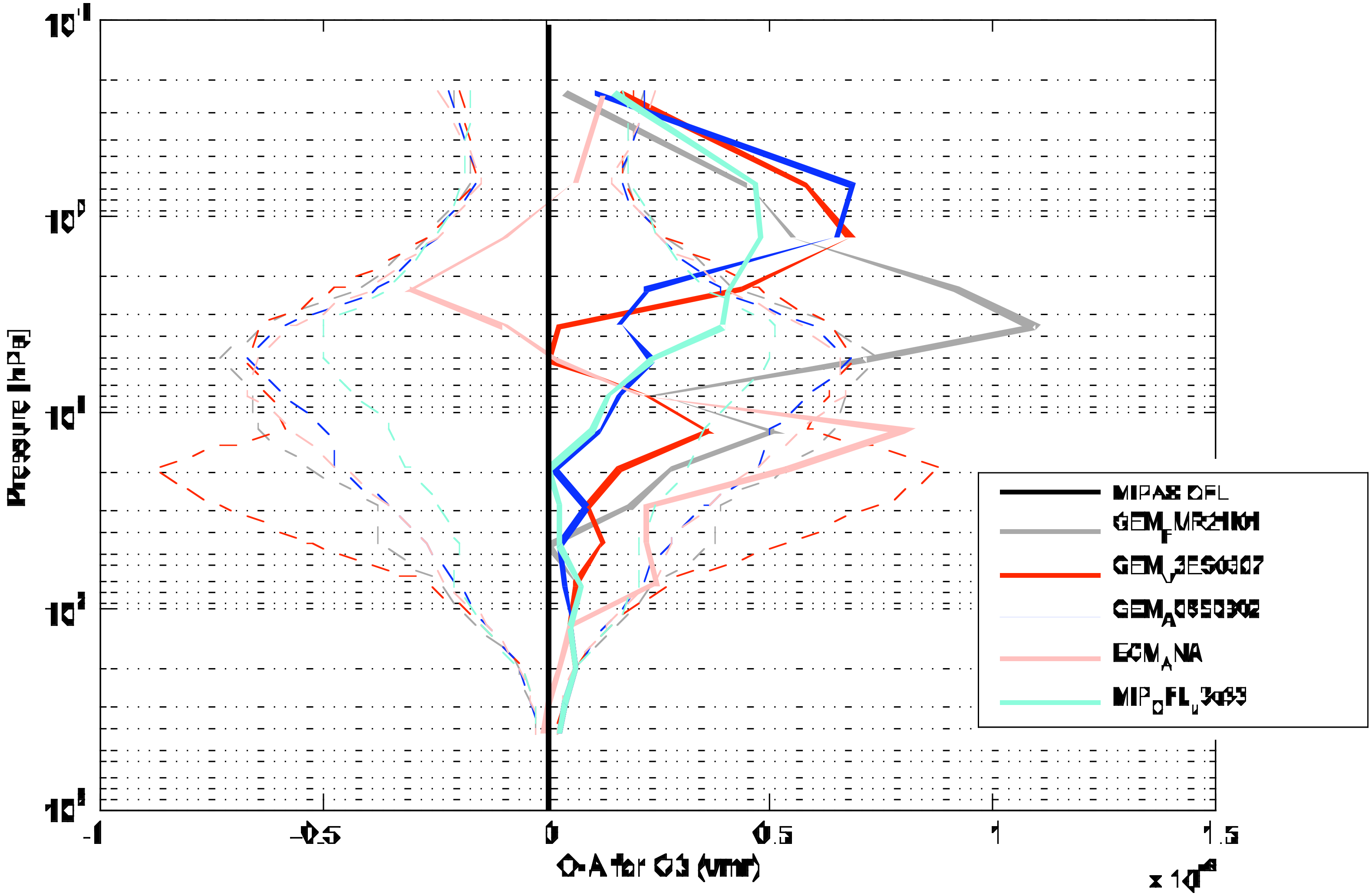

see S. Chabrillat's poster

# Water vapor comparison with MIPAS observations
# Tropics (30S, 30N)




see S. Chabrillat's poster

# Ozone comparison with MIPAS observations Tropics (30S, 30N)




see S. Chabrillat's poster

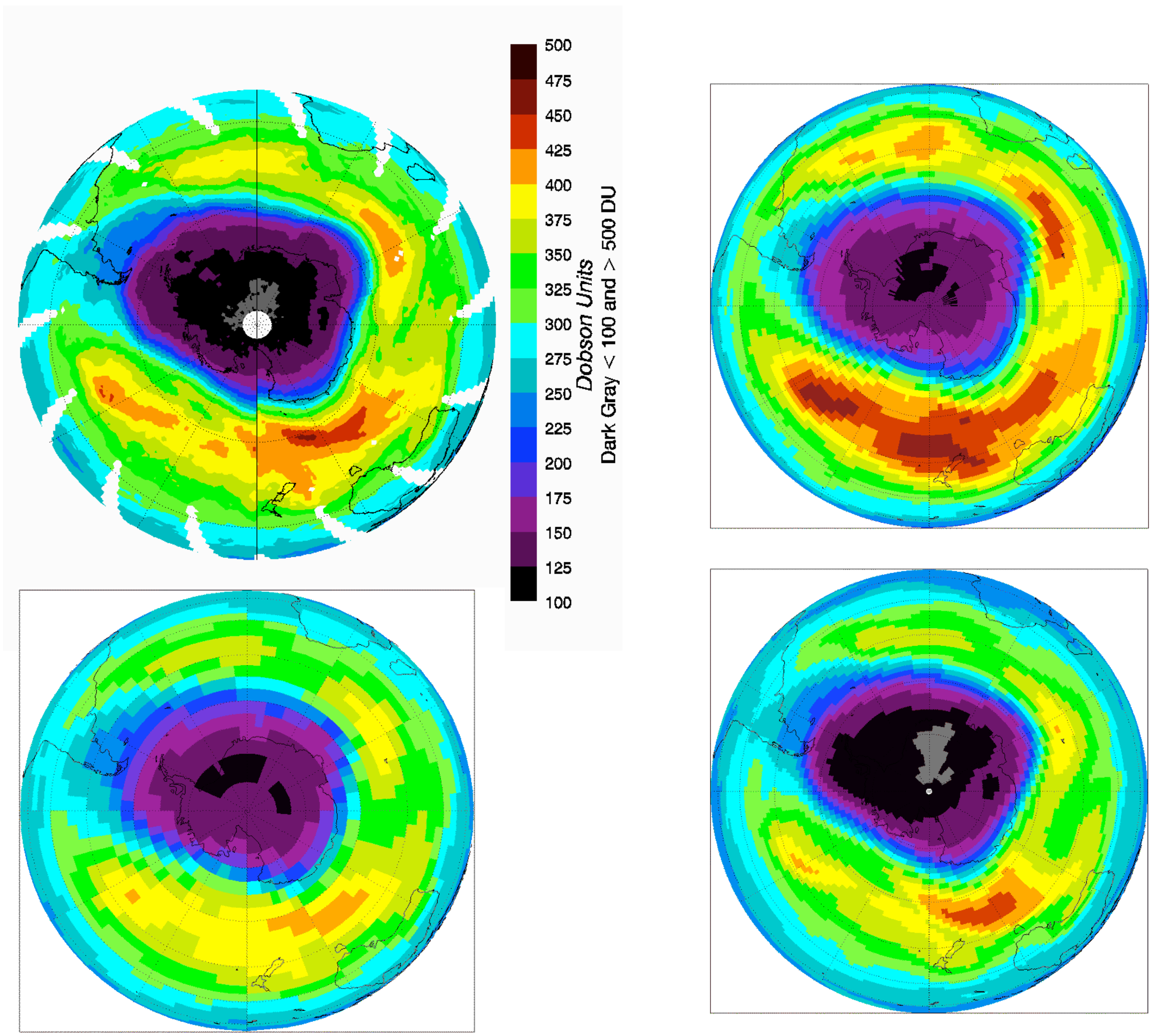
# Simulation of total column ozone

**TOMS obs.**

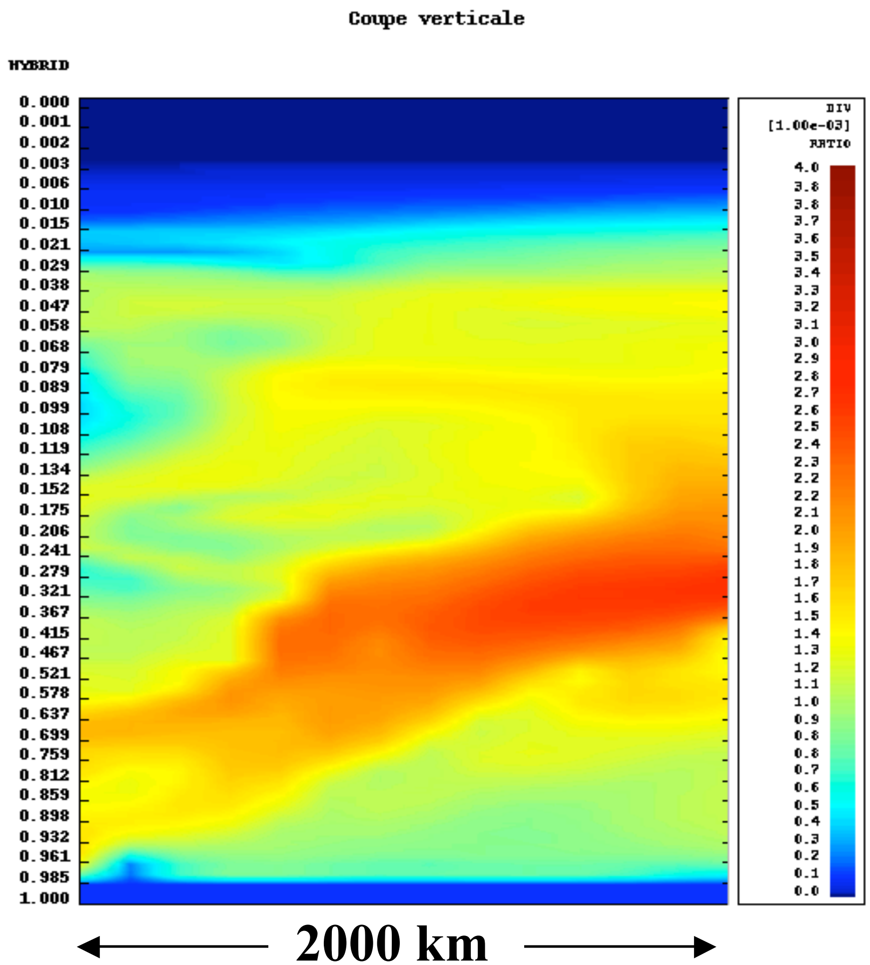
**best BASCOE CTM**

**best BASCOE product**

**first GEM-BIRA simulation**



# Tropopause folding event March 14th 2006
# Ratio $HNO_3/O_3$




**see A. Robichaud's poster**

- **3D-Var extensions**
  - **Constituent observations**
  - **BUFR format for chemical species:  WMO proposal**
  - **Observation error standard deviations**
  - **Observation quality check**
  - **Preconditioning: Variable transformations**
  - **Background error covariances**
  - **Analysis splitting and others**

# Preconditioning: Variable transformations

- **Univariate or multivariate (in two modes) constituent assimilation.**
- **Multivariate: Basic infrastructure implemented for addition of constituent variable transformations (i.e. application of balance operators).**
- **Possible variable transformation for ozone:**

$$\delta \boldsymbol{O}_3 = \delta \boldsymbol{O}_3' + \delta \boldsymbol{O}_3^b = \delta \boldsymbol{O}_3' + F(\mathrm{T}, \boldsymbol{O}_3)\delta \mathrm{T} + G\delta \boldsymbol{\o}$$

$$= \delta \boldsymbol{O}_3' + F(\mathrm{T}, \boldsymbol{O}_3)\delta \mathrm{T}' + G'(\mathrm{T}, \boldsymbol{O}_3)\delta \boldsymbol{\o}$$

$$\delta \boldsymbol{x}_p = \begin{bmatrix} \delta\psi \\ \delta\chi \\ \delta \mathrm{T} \\ \delta \ln \mathrm{q} \\ \delta O_3 \\ \delta \mathrm{p}_\mathrm{s} \end{bmatrix} = \mathbf{M} \cdot \delta \boldsymbol{x} = \begin{bmatrix} \mathbf{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{E} & \mathbf{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \boldsymbol{T} & \mathbf{0} & \mathbf{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{I} & \mathbf{0} & \mathbf{0} \\ \mathbf{G'} & \mathbf{0} & \mathbf{F} & \mathbf{0} & \mathbf{I} & \mathbf{0} \\ \mathbf{S} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \delta\psi \\ \delta\chi' \\ \delta \mathrm{T}' \\ \delta \ln \mathrm{q} \\ \delta O_3' \\ \delta \mathrm{p'}_\mathrm{s} \end{bmatrix}$$

## Anomaly correlation – a measure of forecast skill

Correlation between forecast and analysis as a function of length of forecast

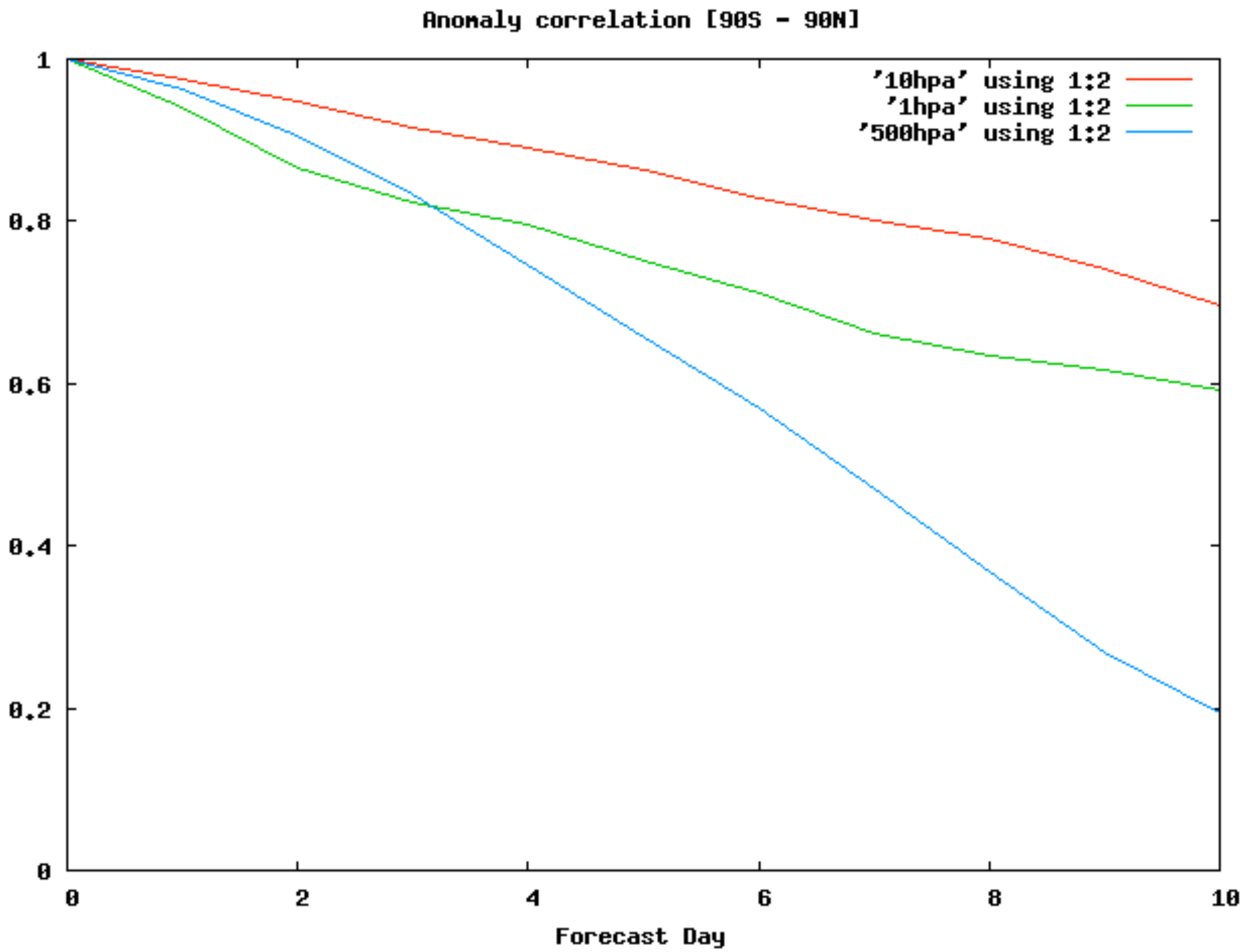
$f_\tau'(t) = f_\tau(t) - C$ ; $a_\tau'(t) = a_\tau(t) - C$

$$\text{AnoCor} = [< (f_\tau' - <f_\tau'>)(a_\tau' - <a_\tau'>) >] \; [< (f_\tau' - <f_\tau'>)^2 \; < (a_\tau' - <a_\tau'>)^2 >]^{-1/2}$$

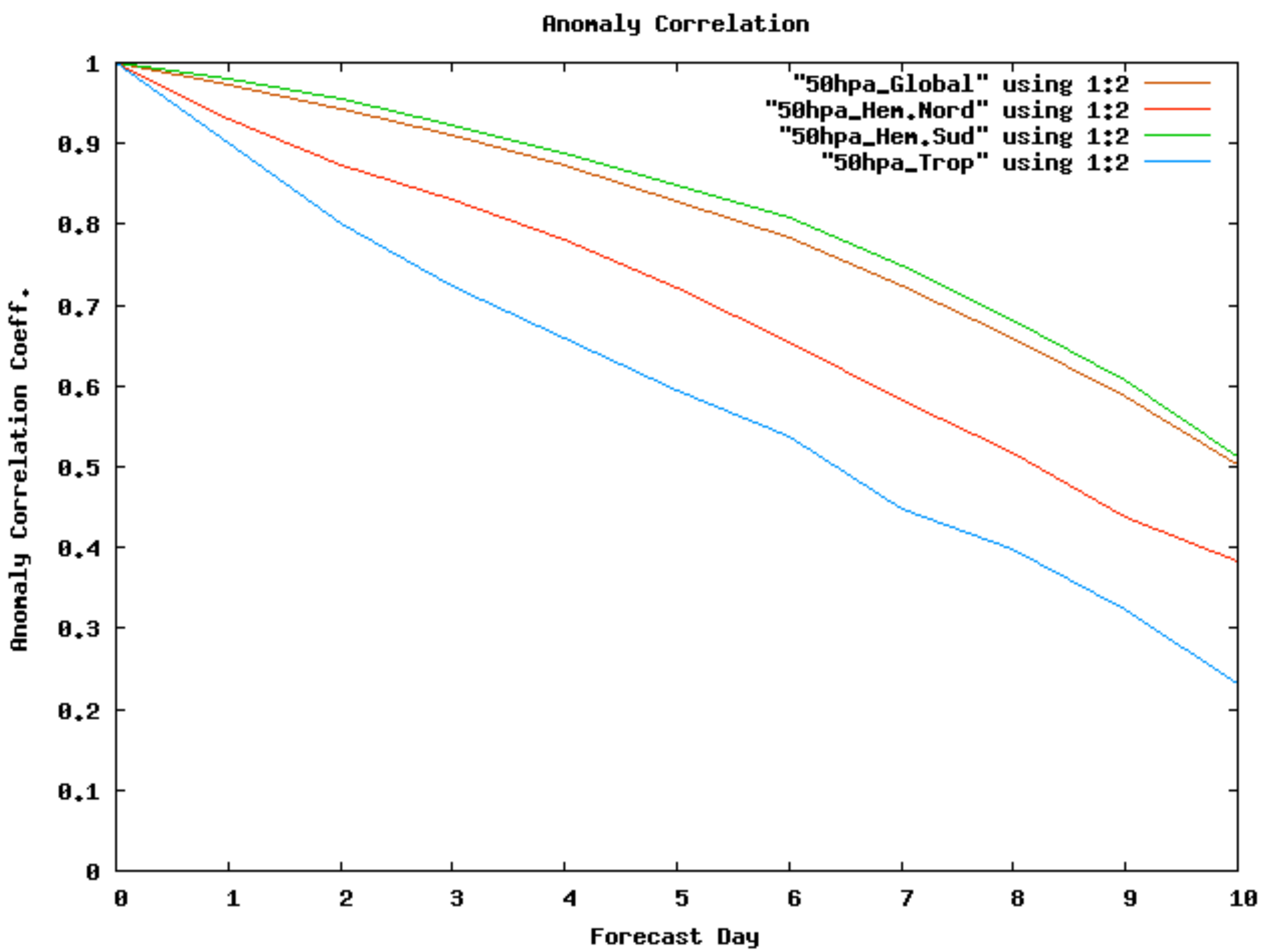
¬ ensemble of forecast (10 days) is needed

¬ used in NWP to monitor improvement in model or assimilation

# Temperature correlation (global) anomaly

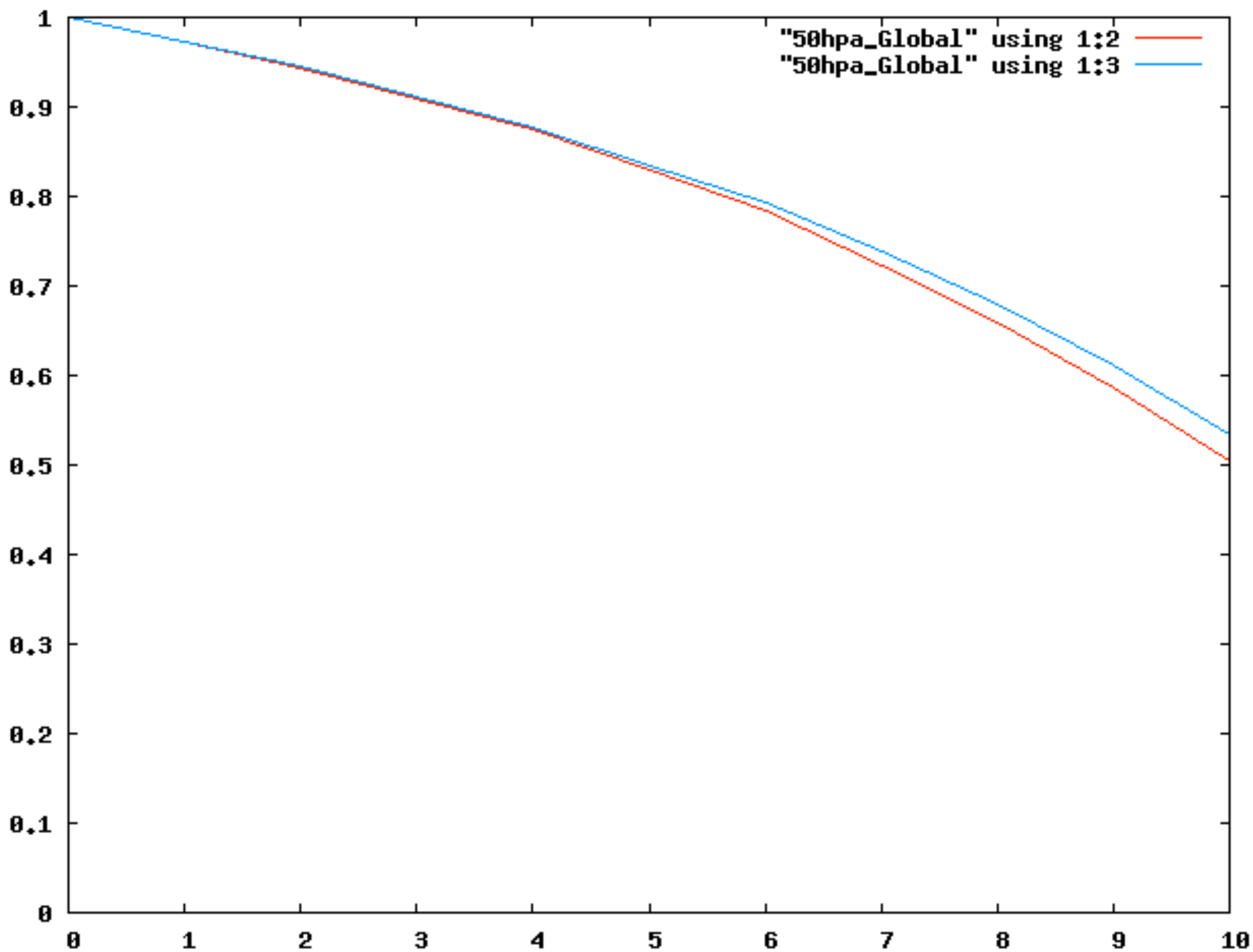


## by regions



Anomaly Correlation
"50hpa_Global" using 1:2
"50hpa_Hem.Nord" using 1:2
"50hpa_Hem.Sud" using 1:2
"50hpa_Trop" using 1:2
Anomaly Correlation Coeff.
Forecast Day
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
1
2
3
4
5
6
7
8
9
10

# Ozone-radiation interaction



## Impact of bias corrected radiances

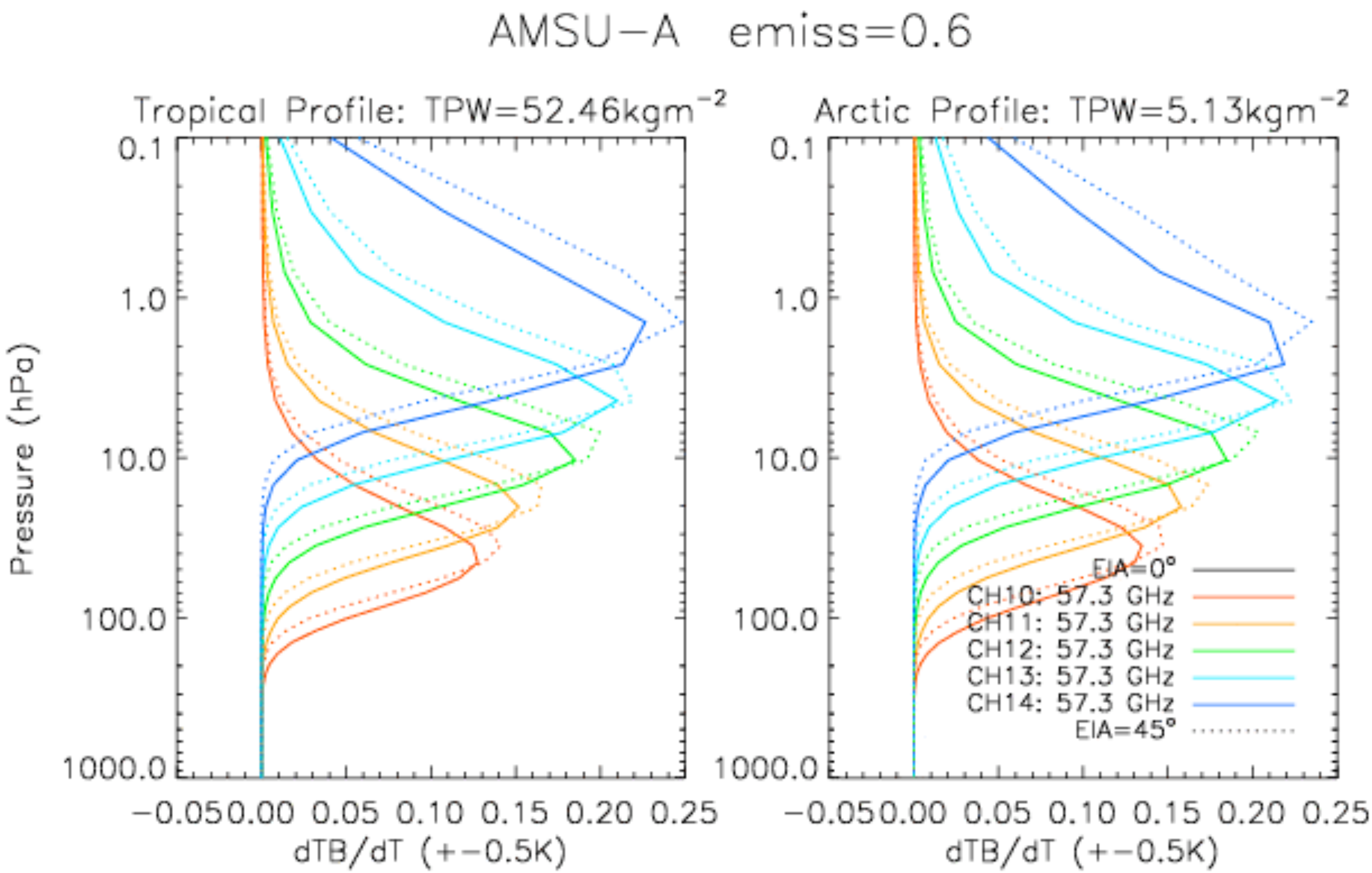
- All experiments are in FGAT mode with 4D data thinning
- Changes in the assimilation system often leads to changes in the model bias
- Bias correction scheme for AMSU-a data
  - Innovation statistics: $\overline{(\mathbf{y} - H(\mathbf{x}_b))} = \overline{\mathbf{y}}$

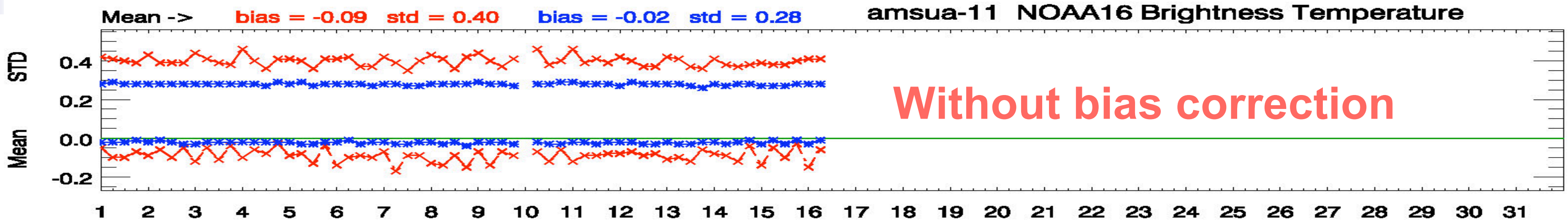
Set $\mathbf{y} = \mathbf{y}_c + \tilde{\mathbf{y}}$ so that $\overline{\tilde{\mathbf{y}} - H(\mathbf{x}_b)} \approx 0$

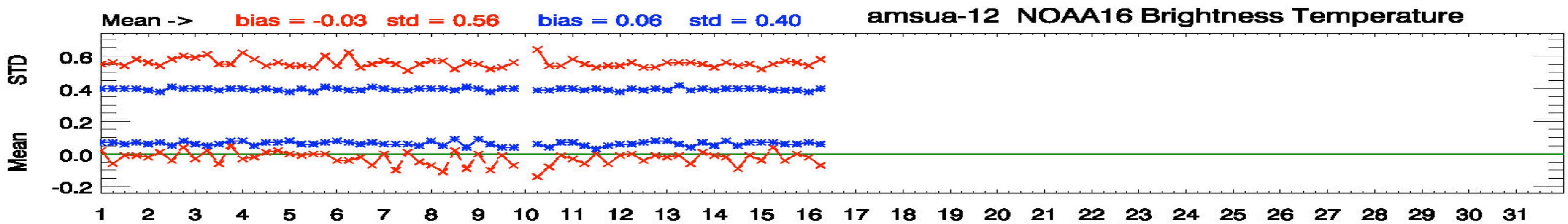
provided $\mathbf{y}_c = \mathbf{y}_c(\alpha_1, \alpha_2, \alpha_3) = \overline{\mathbf{y}}$

Predictors are related to air mass characteristics and scan angle

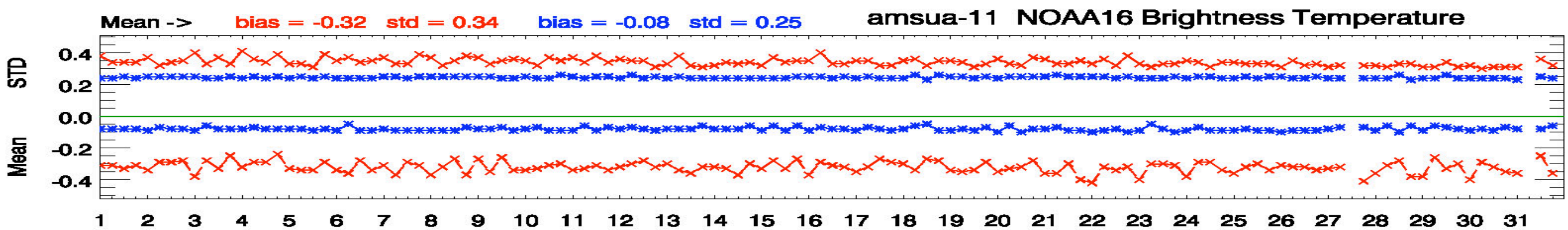
**Jacobians with respect to temperature for channels 10-14 of AMSU-a**

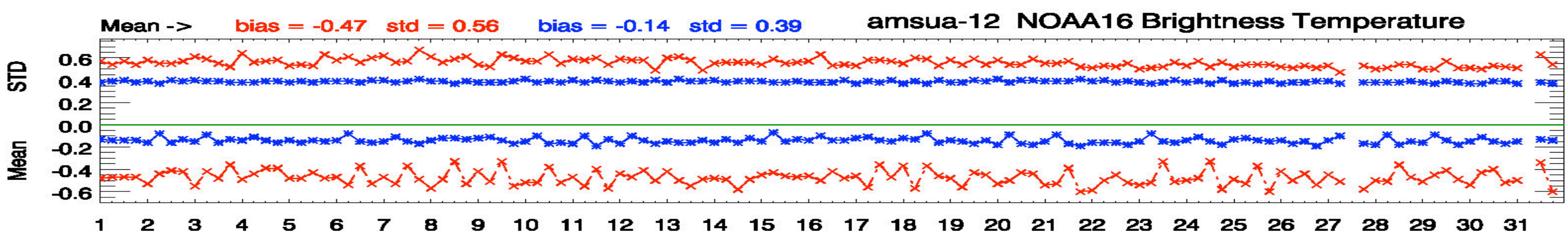




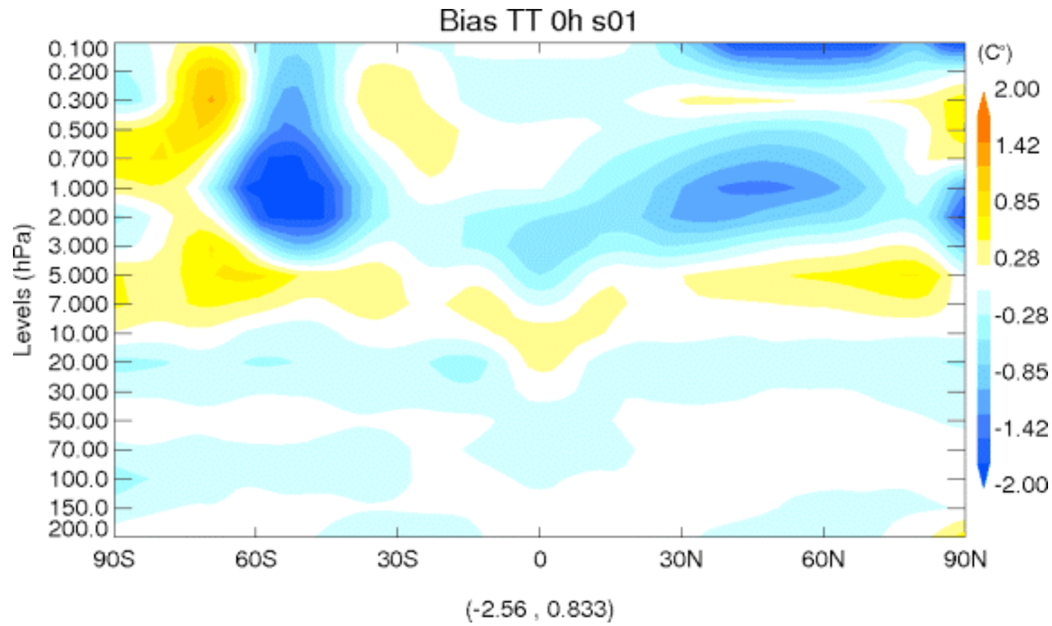




## With bias correction

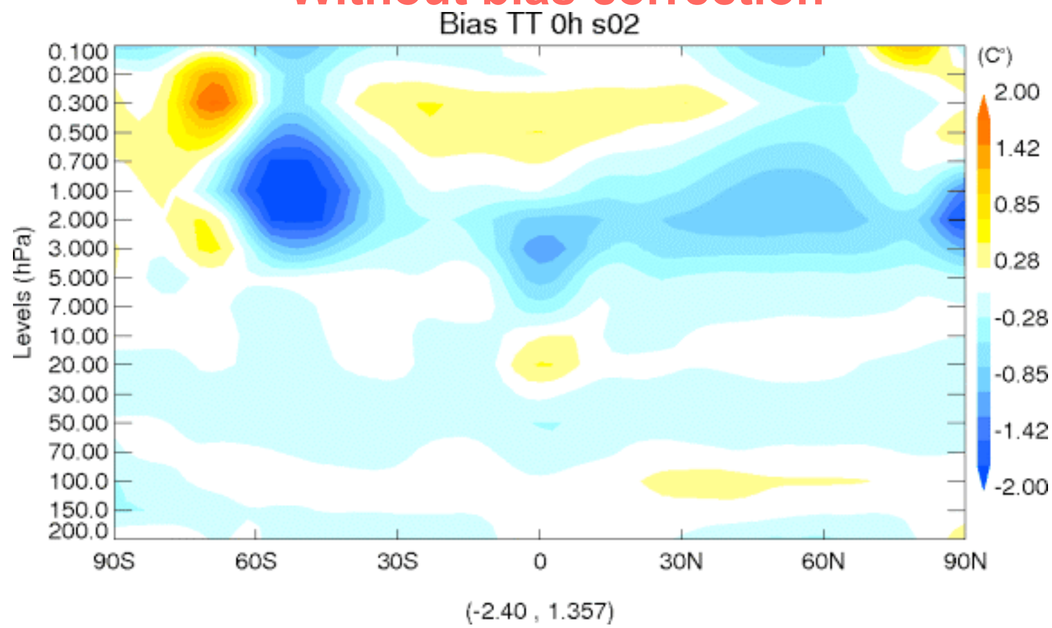


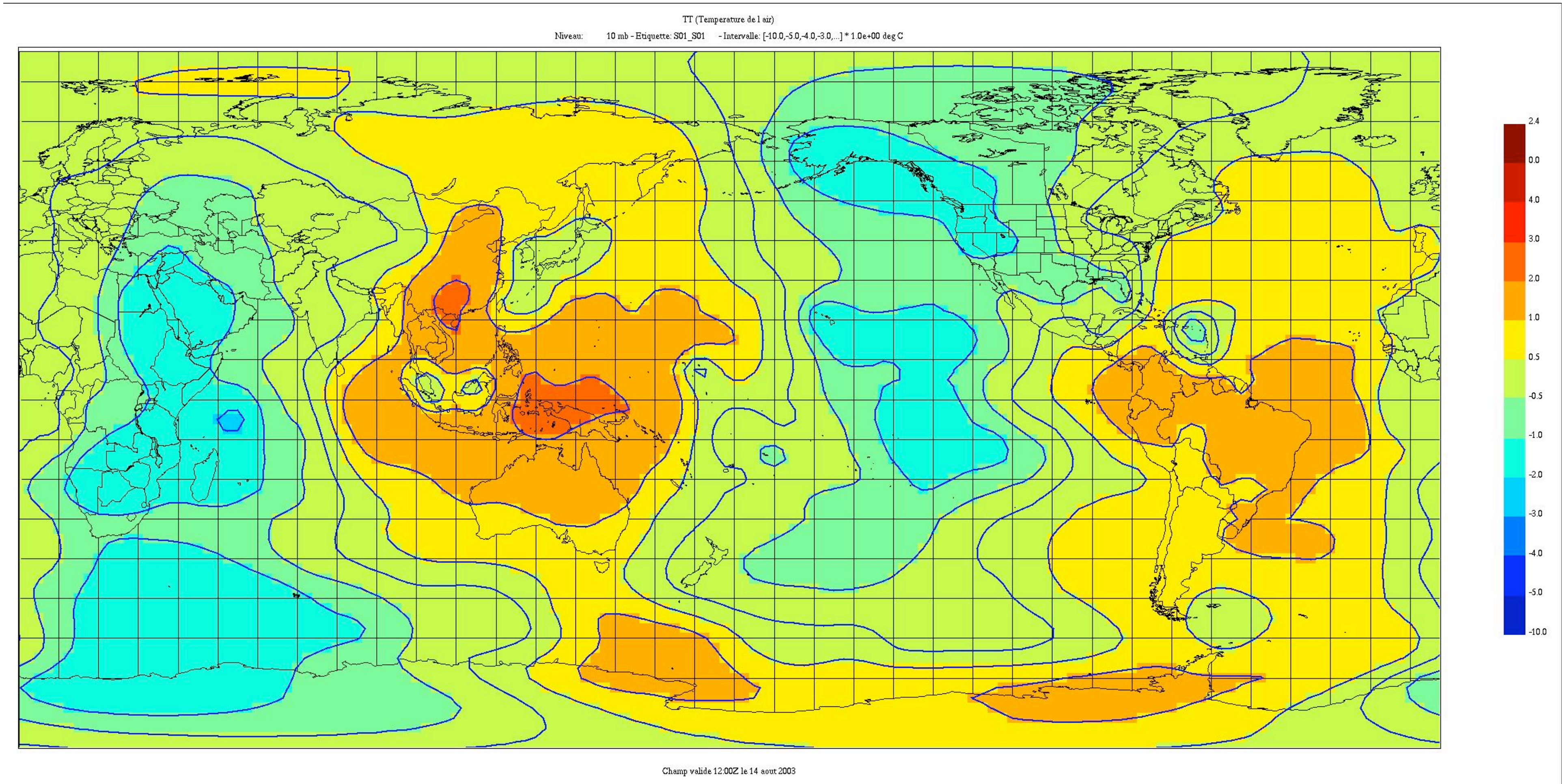
Zonal mean of temperature increments



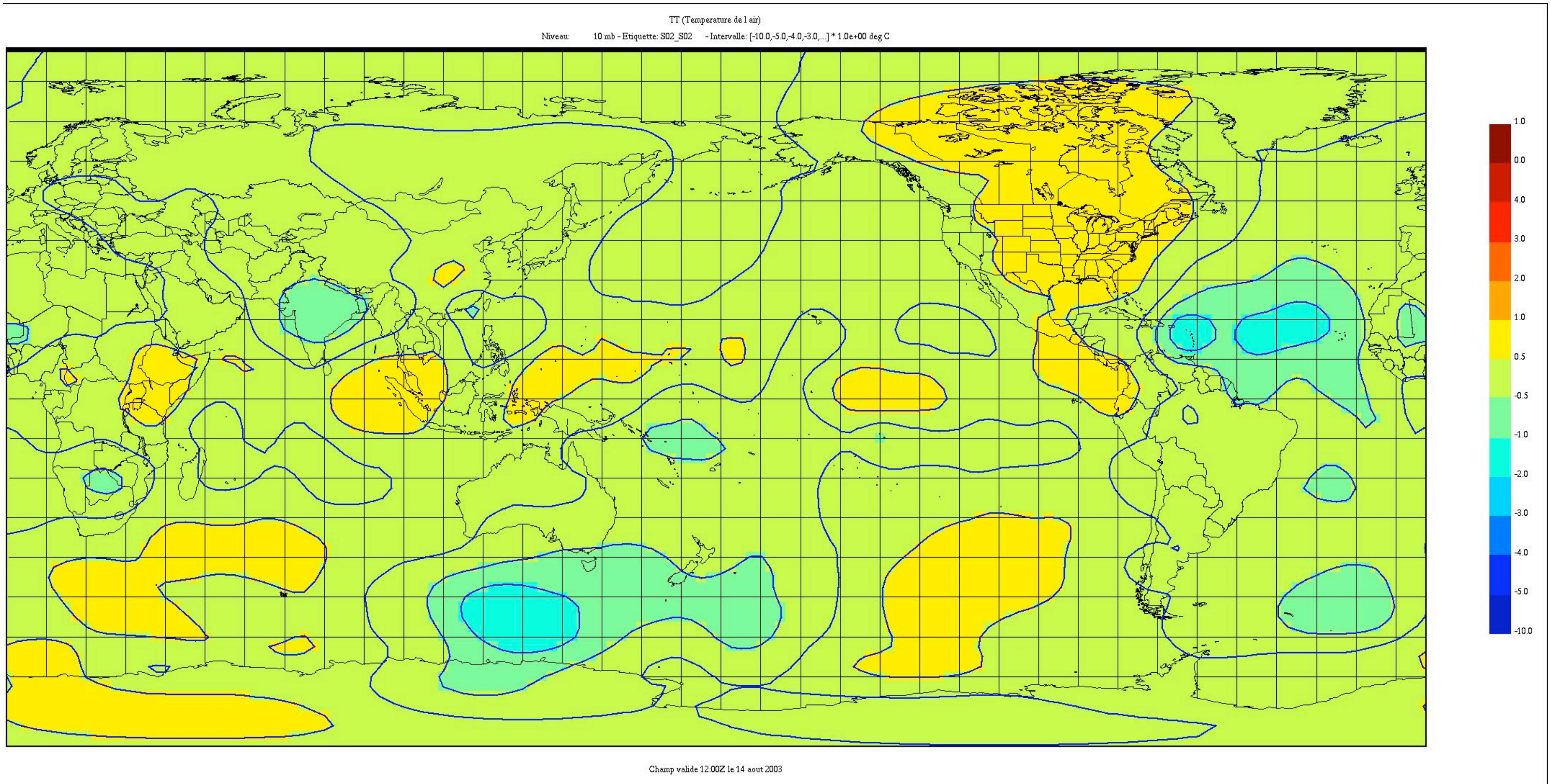

**Without bias correction**



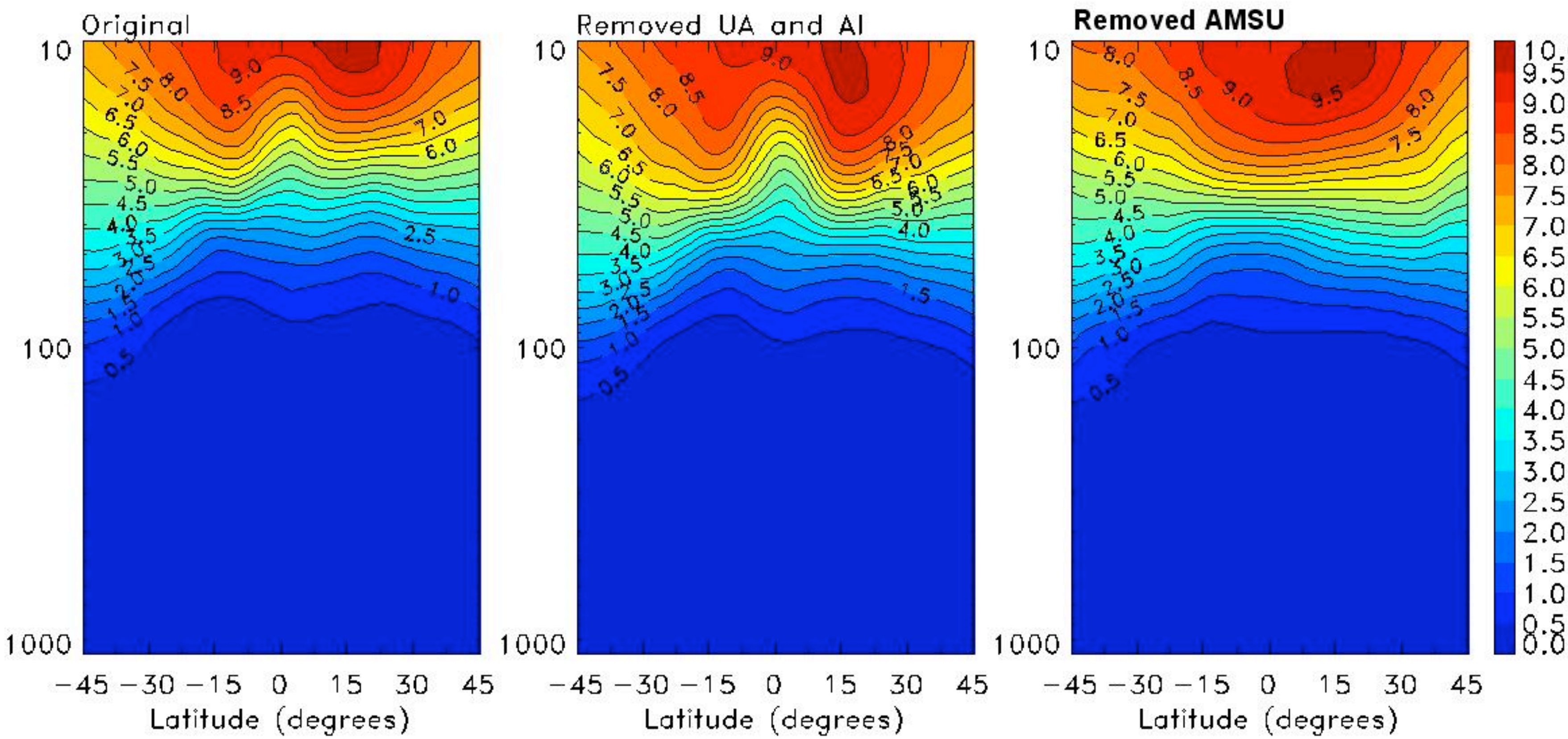
# Mean temperature analysis increments at 10 hPa
## **(with bias correction applied to AMSU-A channels 11-14)**



## Mean temperature analysis increments at 10 hPa
## **(without bias correction applied to AMSU-A channels 11-14)**

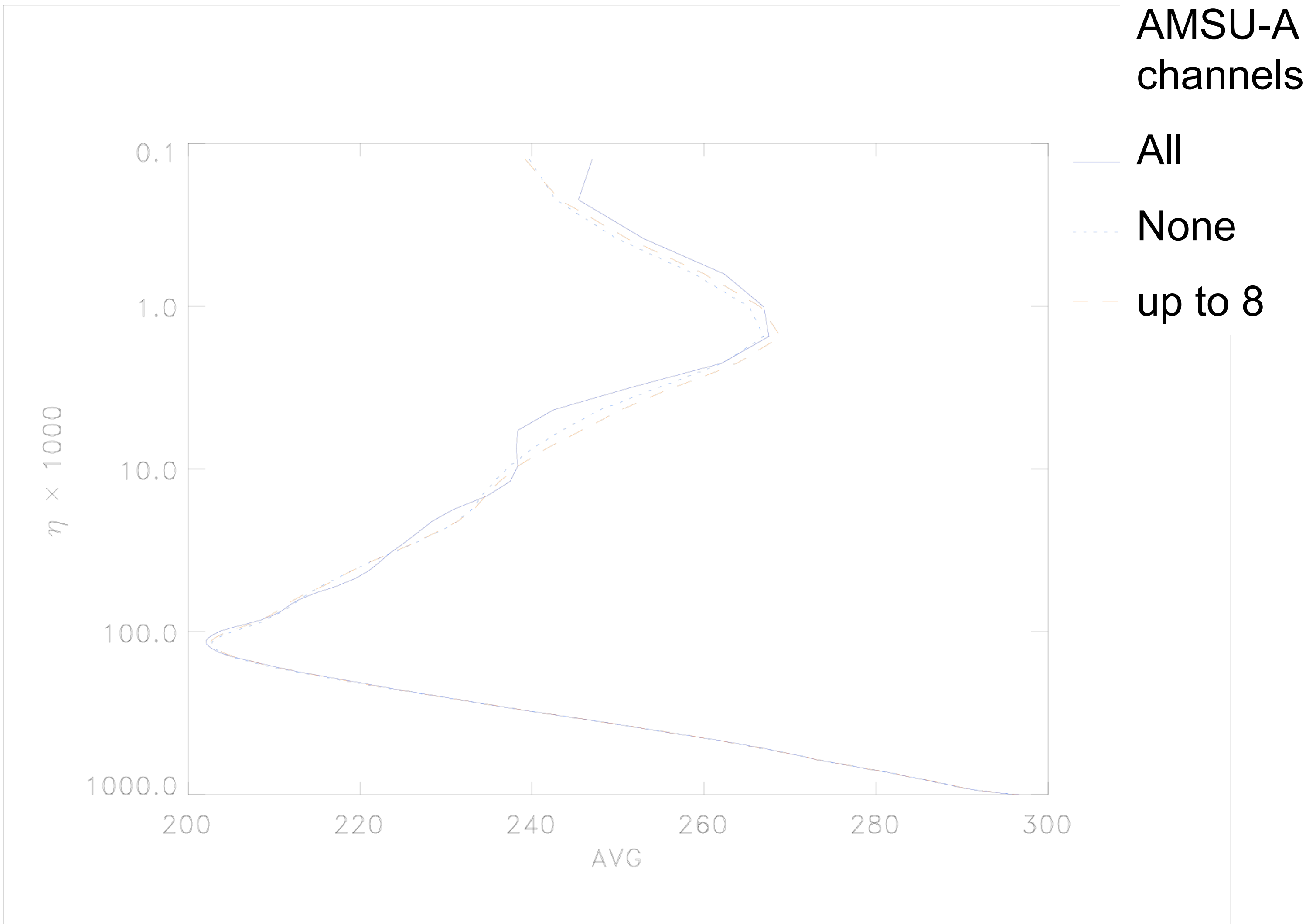


## Coupled Chemical-Dynamical Data Assimilation: Dynamical Assim.: wiggles




So it would seem UA and/or AI improves balance… and AMSU deteriorates balance this in the presence of larger background variances in the middle stratosphere than at lower levels. AH-HA or is it EUREKA?

# Average temperatures at the equator (20-30 Aug. 2003)

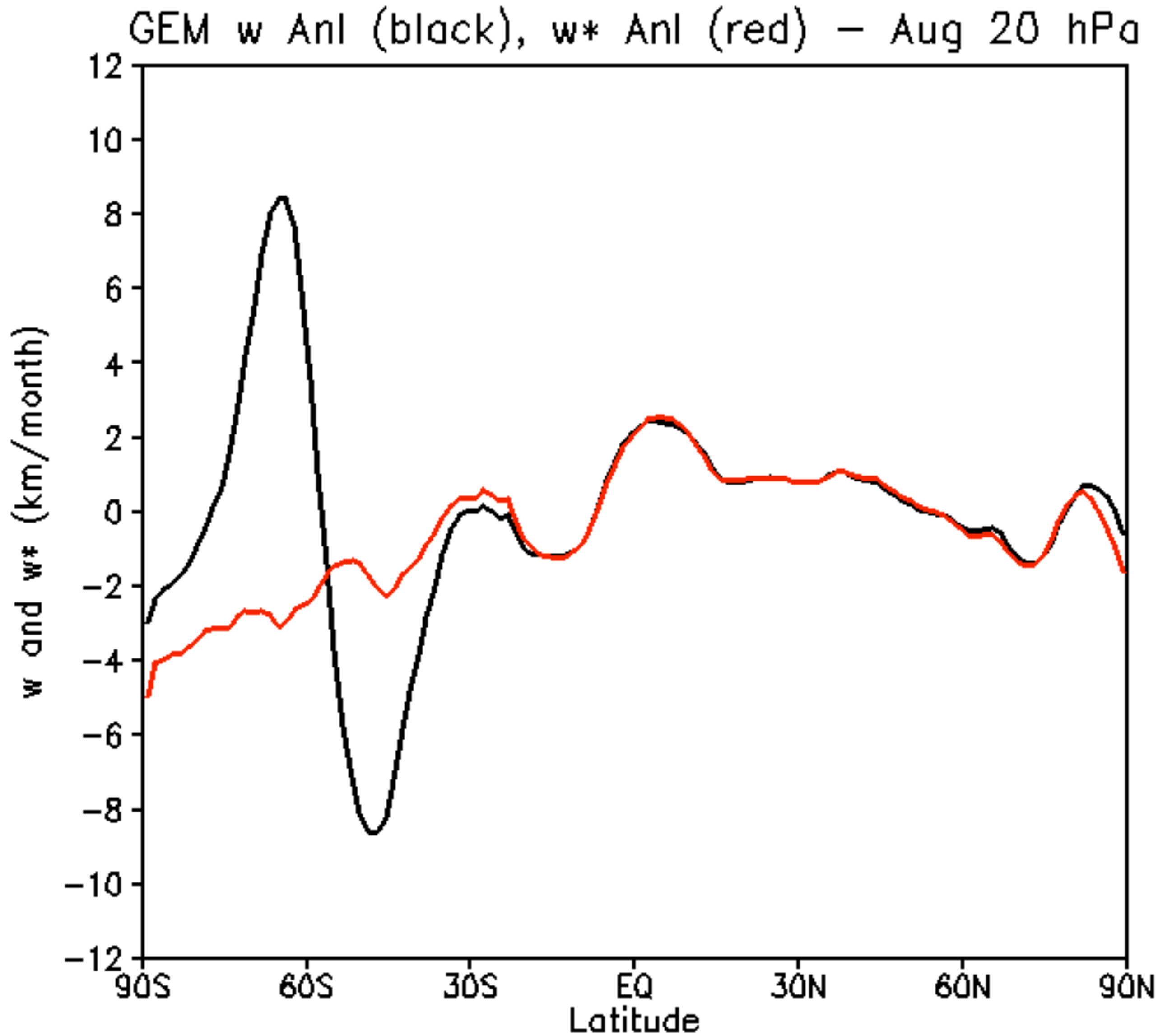


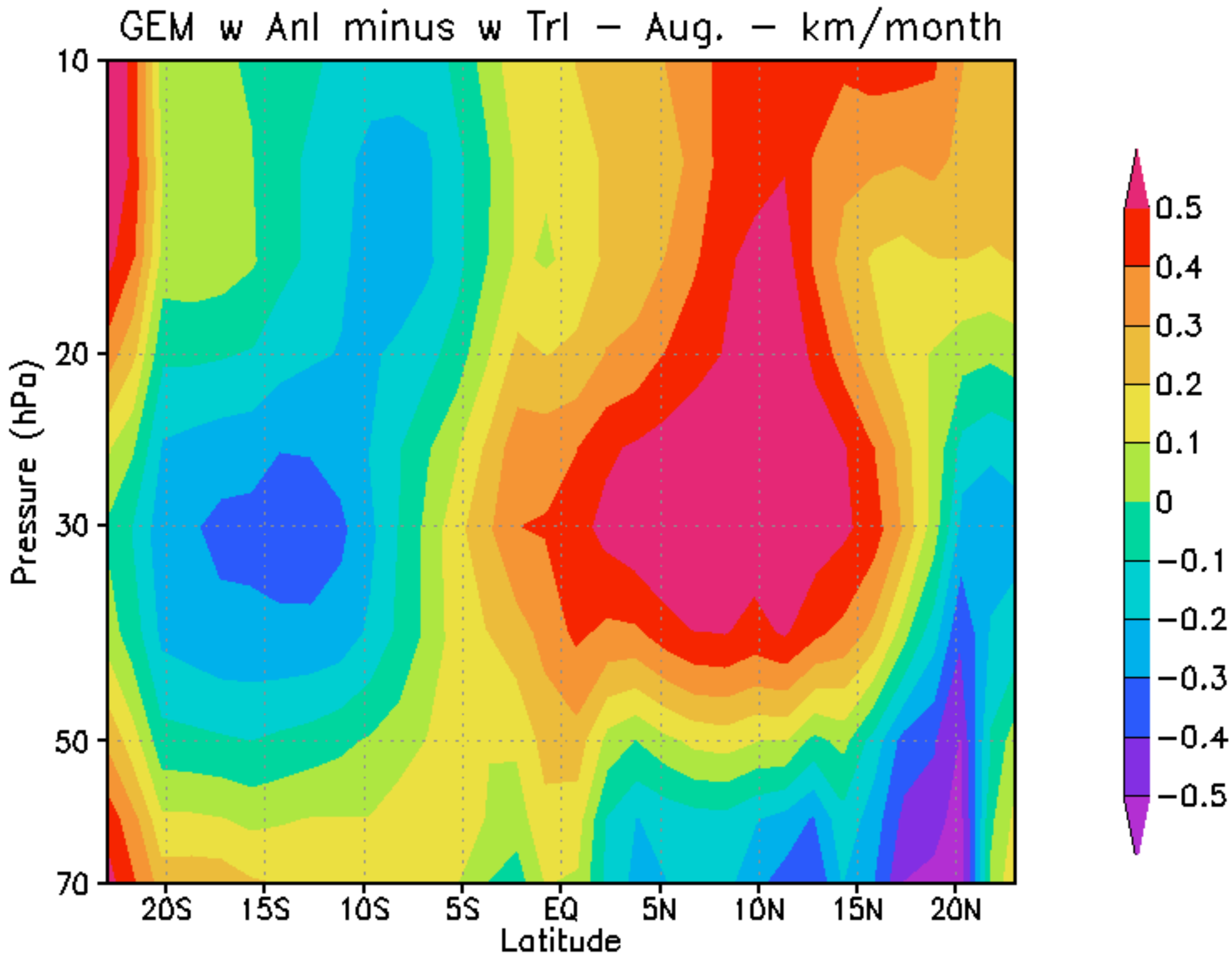
## Changes in stability

Transformed Eulerian mean diagnostic

Neglecting zonal mean temperature advection,

$$(\Gamma_d - \Gamma)\overline{\omega}^* = \overline{Q}$$


GEM w Anl (black), w* Anl (red) – Aug 20 hPa
w and w* (km/month)
Latitude
12
10
8
6
4
2
0
−2
−4
−6
−8
−10
−12
90S
60S
30S
EQ
30N
60N
90N


GEM w Anl minus w Trl – Aug. – km/month
Pressure (hPa)
10
20
30
50
70
20S
15S
10S
5S
EQ
5N
10N
15N
20N
Latitude
0.5
0.4
0.3
0.2
0.1
0
−0.1
−0.2
−0.3
−0.4
−0.5

## Estimation of error variances and correlations

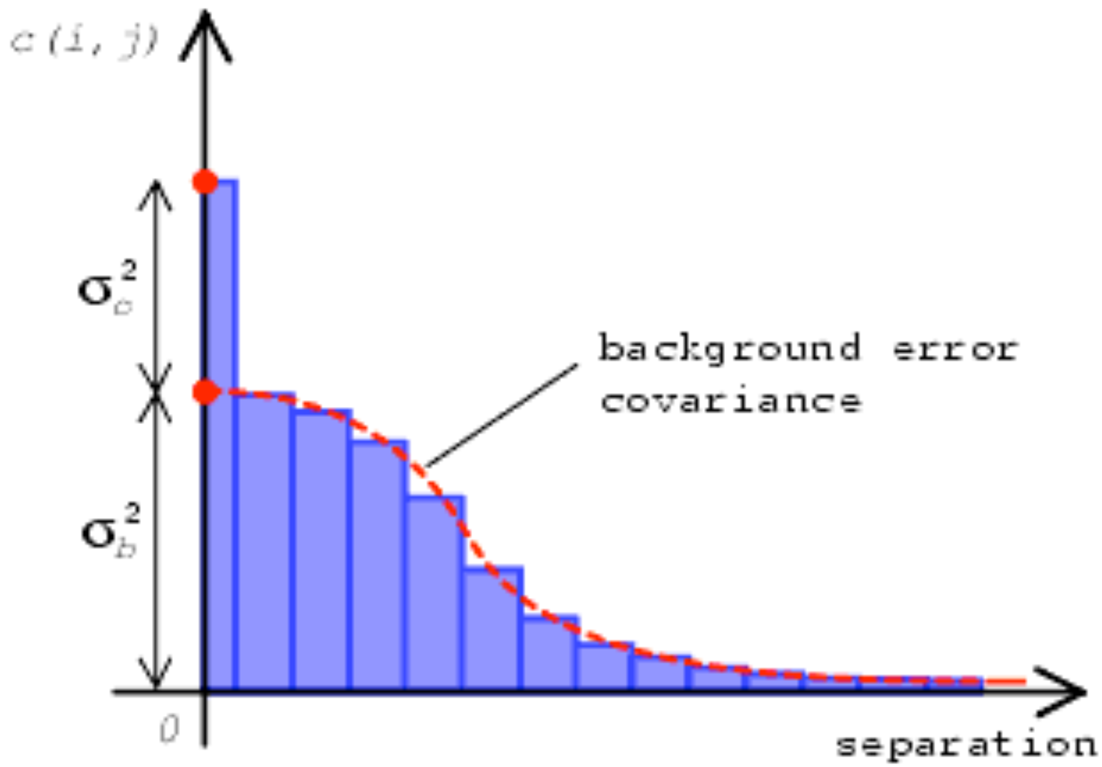
If the observations correspond to model variables:

$$\langle H\varepsilon_b(p) H\varepsilon_b(q)\rangle = \sigma_b(p)\sigma_b(q)\rho(|p-q|)$$

with ρ being the correlation function.

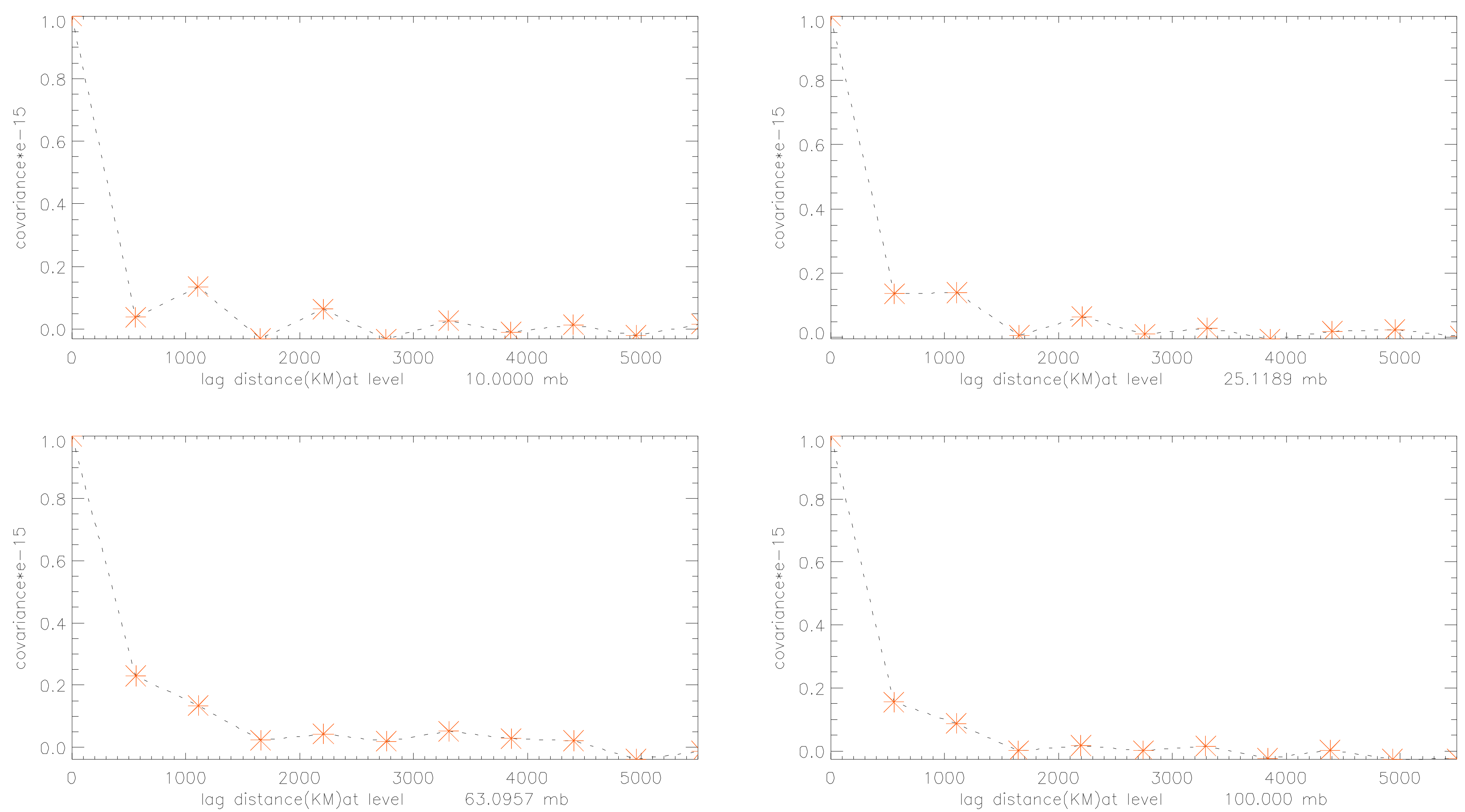
$$I(p,p) = \sigma_o^2 + \sigma_b^2$$

$$I(p,q) = \sigma_b^2 \rho(r)$$

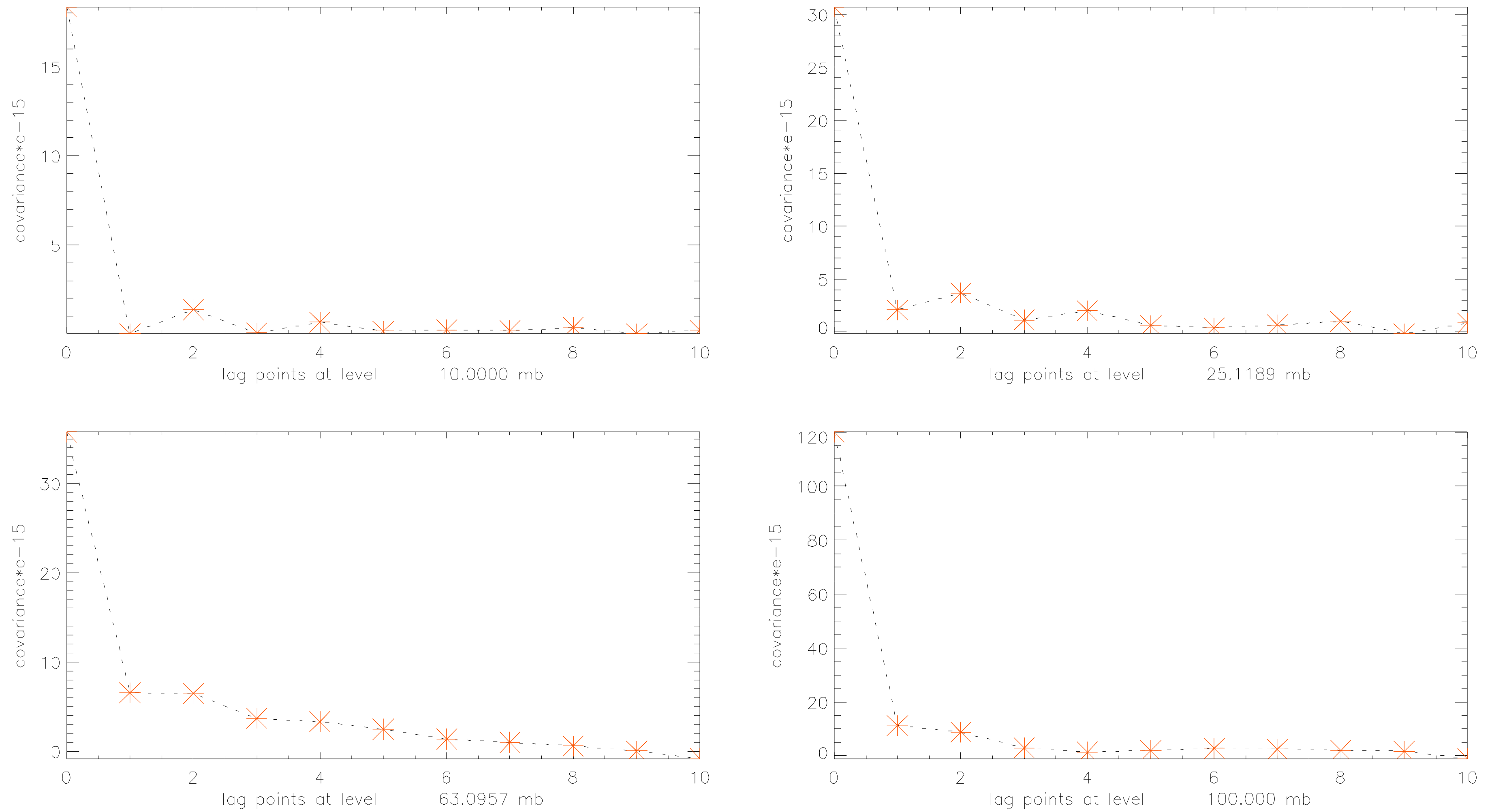



(from Bouttier and Courtier, 2000, ECMWF)

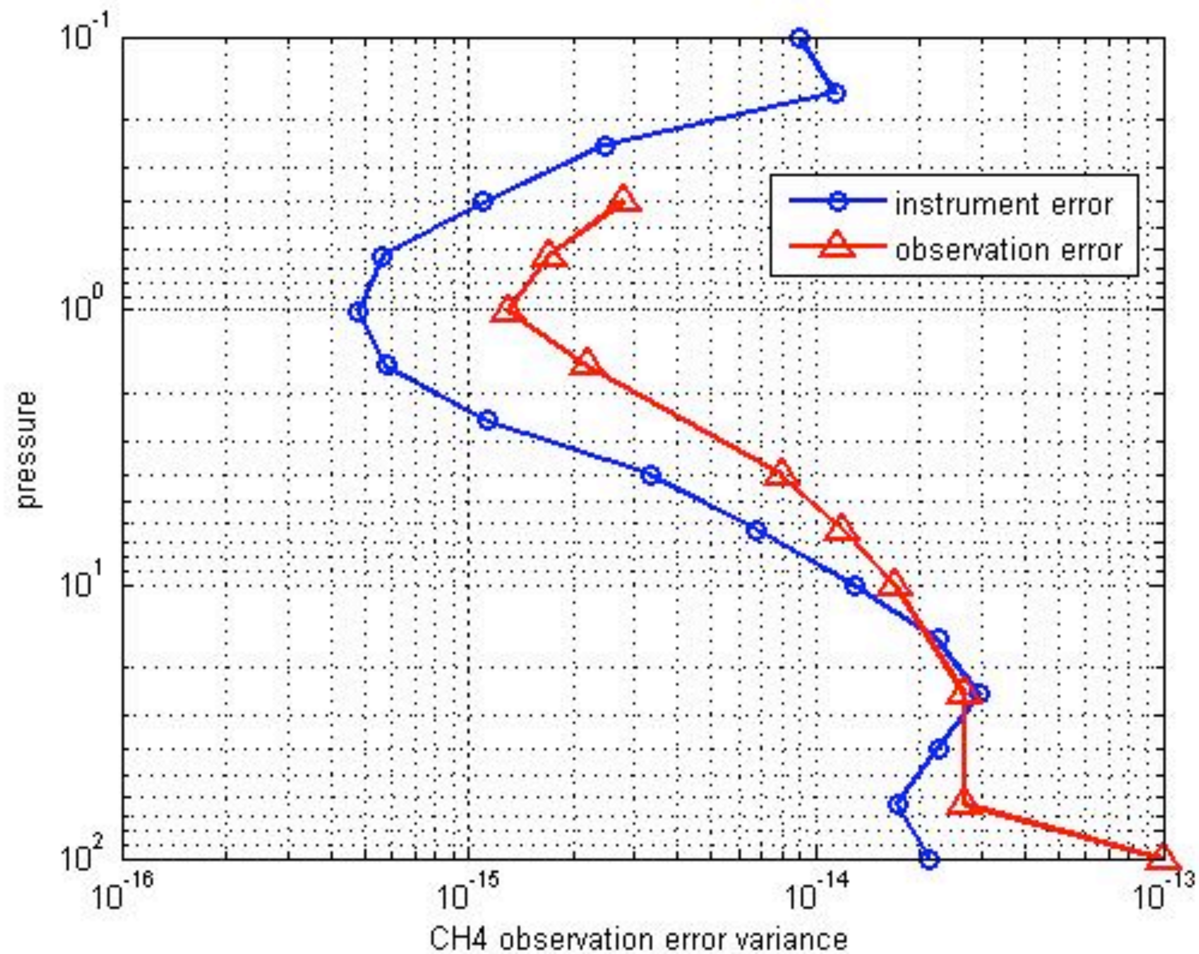
# Along track innovation covariance - ozone assimilation

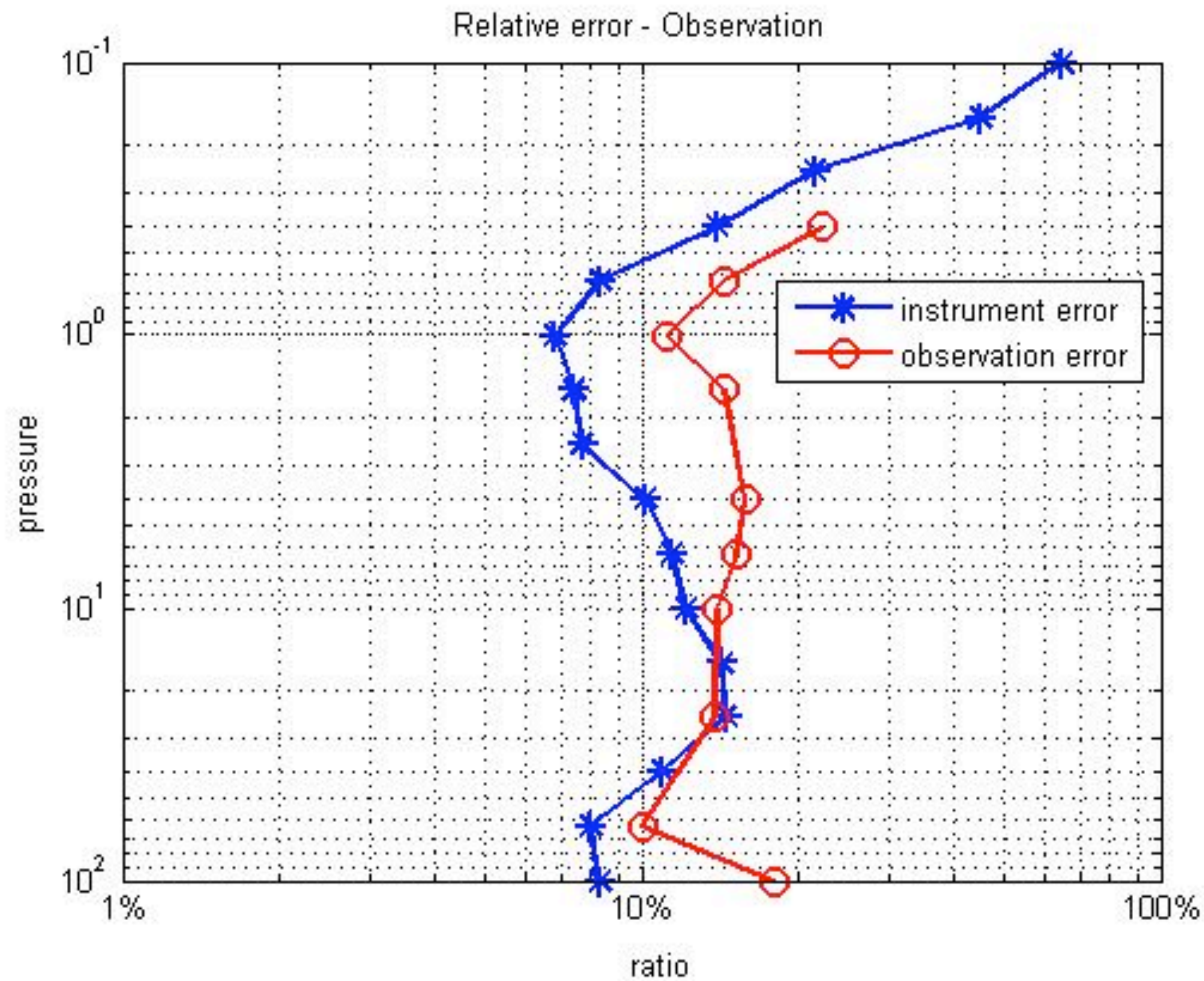


# Along track innovation covariance – methane assimilation

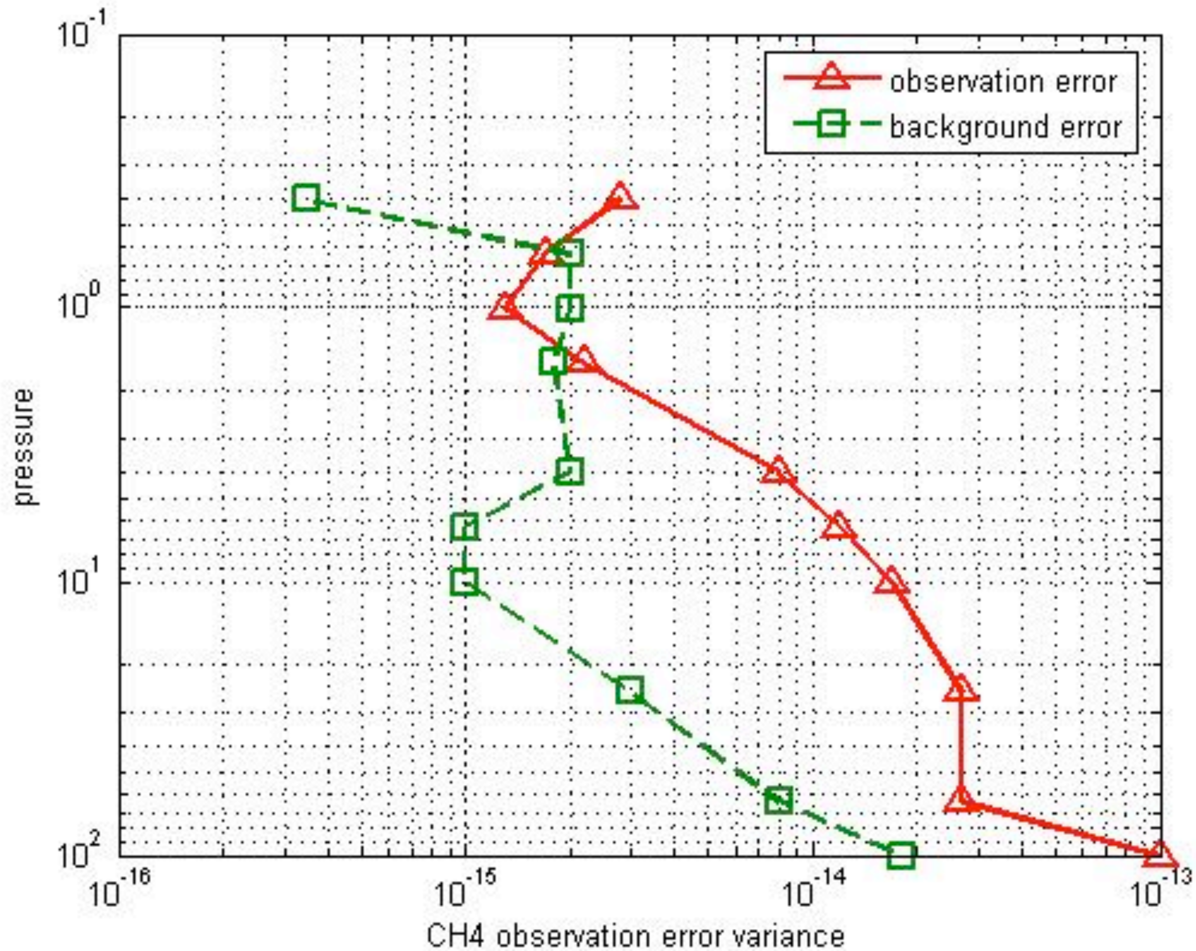


## Error statistics for CH4

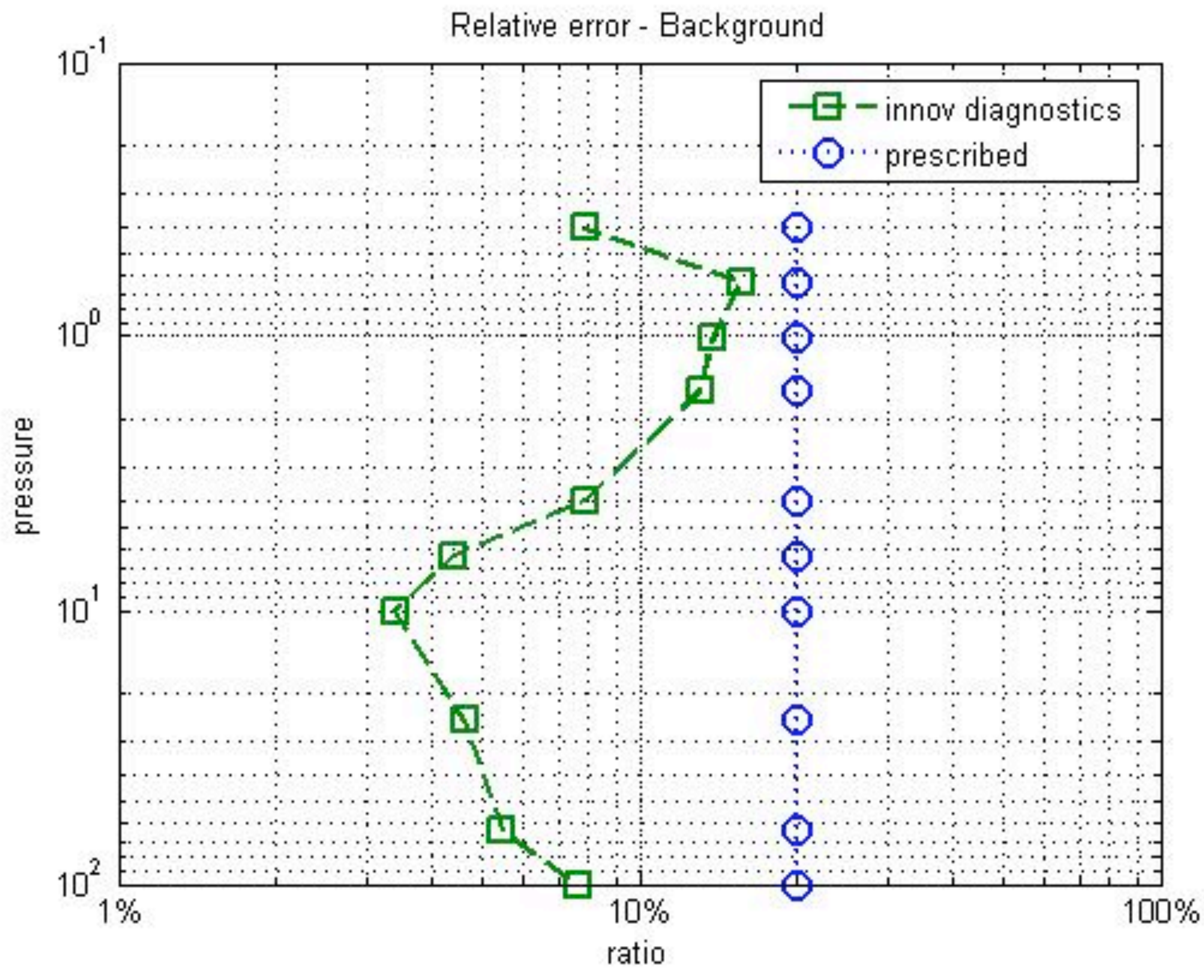




Relative error - Observation
instrument error
observation error
pressure
ratio
1%
10%
100%
$10^{-1}$
$10^{0}$
$10^{1}$
$10^{2}$



observation error
background error
pressure
CH4 observation error variance
$10^{-1}$
$10^{0}$
$10^{1}$
$10^{2}$
$10^{-16}$
$10^{-15}$
$10^{-14}$
$10^{-13}$



Relative error - Background
innov diagnostics
prescribed
pressure
ratio
1%
10%
100%
$10^{-1}$
$10^{0}$
$10^{1}$
$10^{2}$

## Relative error formulation

- observation error that include representativeness error can be formulated with a relative error
- background error does not fit a relative error formulation ( error std proportional to state ) .

## Other approaches to estimate observation error: Desrosiers' method

$$\left\langle OmA\,(OmF)^T \right\rangle = \left\langle \left(\mathbf{y} - \mathbf{H}\mathbf{x}^a\right)\left(\mathbf{y} - \mathbf{H}\mathbf{x}^f\right)^T \right\rangle$$

$$= \left\langle \left(\mathbf{d} - \mathbf{HKd}\right)\mathbf{d}^T \right\rangle = \left(\mathbf{I} - \mathbf{HK}\right)\left\langle \mathbf{dd}^T \right\rangle$$

$$= \mathbf{R}\boldsymbol{\Gamma}^{-1}\overline{\boldsymbol{\Gamma}}$$

$$\left\langle AmF\,(OmF)^T \right\rangle = \left\langle \left(\mathbf{H}\mathbf{x}^a - \mathbf{H}\mathbf{x}^f\right)\left(\mathbf{y} - \mathbf{H}\mathbf{x}^f\right)^T \right\rangle$$

$$= \left\langle \mathbf{HKd}\,\mathbf{d}^T \right\rangle = \mathbf{HK}\left\langle \mathbf{dd}^T \right\rangle$$

$$= \mathbf{HBH}^T\boldsymbol{\Gamma}^{-1}\overline{\boldsymbol{\Gamma}}$$

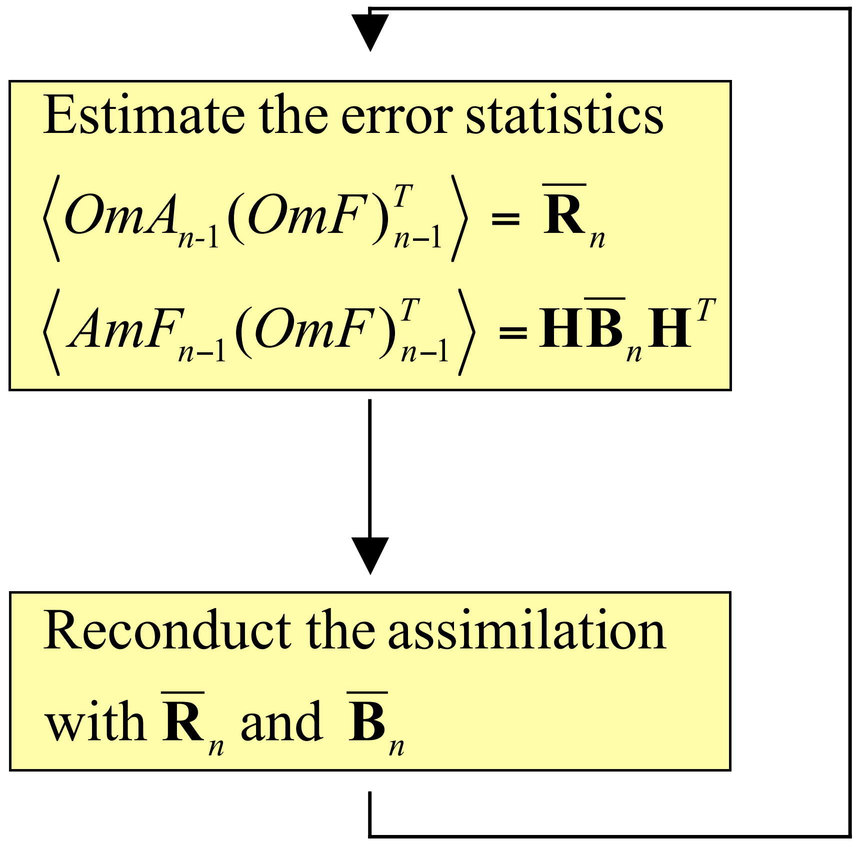
And if condition $\boldsymbol{\Gamma} = \overline{\boldsymbol{\Gamma}}$ is satisfied, then

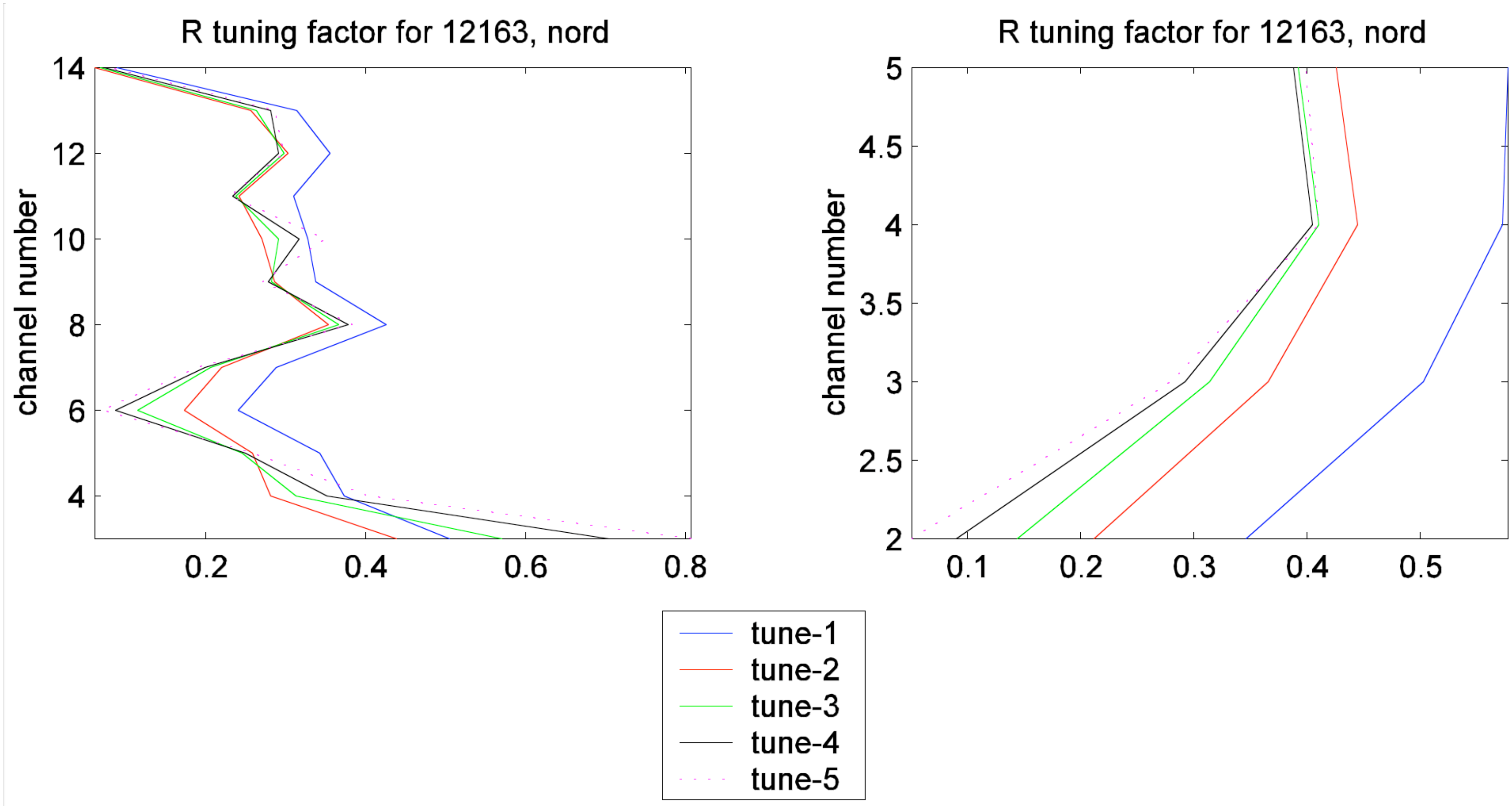
$$\left\langle OmA\,(OmF)^T \right\rangle = \mathbf{R}$$

$$\left\langle AmF\,(OmF)^T \right\rangle = \mathbf{HBH}^T$$

see Y. Yang's poster

# Iterative adjustment
## Tuning of the error statistics






Ratio of estimated error variance over the initially prescribed error variance.
Left panel AMSU-A, right panel AMSU-B. Domain northern hemisphere.

## Short term plans

- Adapt the tropospheric bias correction in the light of AMSU-a radiance bias ch. 11-14
- Monitor other chemical data sets for assimilation (e.g. GOMOS observation, MIPAS-IMK )

## In a broader context

- This study is a first step towards the development of chemical weather capability using operational model and assimilation systems (prototype 2010)

- The operational air quality model is currently being implemented online with GEM – operational by 2008

- Development towards a unified tropospheric-stratospheric GCCM envisioned for 2008