

# Coupled chemical-dynamical data assimilation

## ESA/ESTEC Contract

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*SPARC Data Assimilation Workshop, Toronto, September 4 2007*



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# ESA Invitation to tender

- “Advances in Atmospheric Chemistry and Dynamics Research by Development of Coupled Chemistry-Dynamics Data Assimilation” ESTEC ITT, February 2004
- Objectives:
  - Develop GCCM from state-of-the-art GCM and CTM
  - Analysis of benefits/drawbacks of GCCM-DAS
  - Using dynamical and chemical observations from ENVISAT
- Consortium
  - Environment Canada (Air Quality RD , Meteorological RD)
  - Belgium Institute for Space Aeronomy (BIRA-IASB)
  - York University
  - Institut für Meteorologie und Klimaforschung (IMK)

# Modelling and assimilation of GCM & CTM's

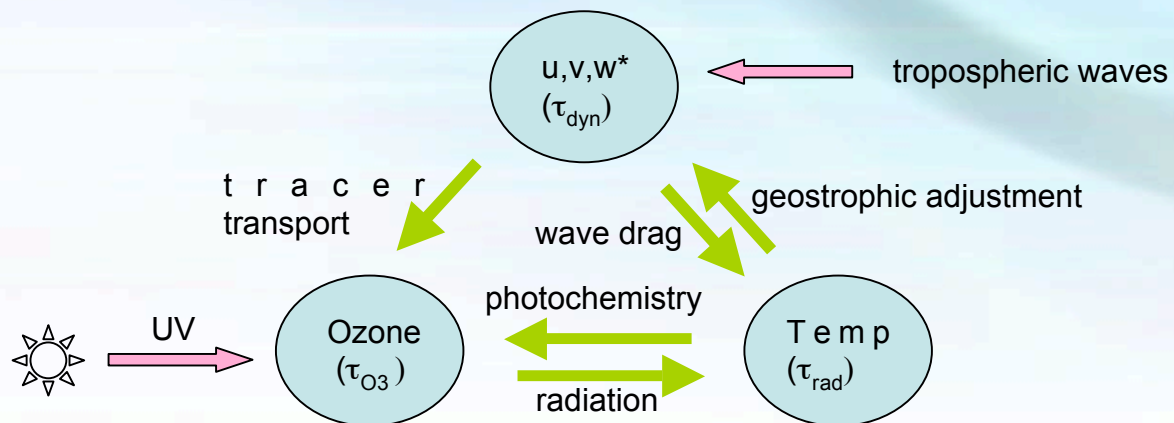
## GCM

- Momentum
- Thermodynamics
- Conservation of mass
- Chemical composition prescribed, except for water (conservation of mass of water; phase change)
- Early beginnings of DA  
3D Var , OI (data window 6 hr)

## CTM

- Momentum (winds) thermodynamics (T), and total mass ( $p_s$ ) is given
- Conservation of mass of individual species, with chemical reactions, and photochemistry
- Early beginnings of DA  
4D Var (data window 24 hr)  
Kalman filter

# Modelling



# Data Assimilation for GCCM ?

**Models are based on causality and physical laws**

*Link between GCM and CTM is  
photochemistry-dynamics-radiation interaction*

**Data assimilation methods are based on  
information content and its transfer  
(time, space, variables)**

***flow of information  $\neq$  causality***

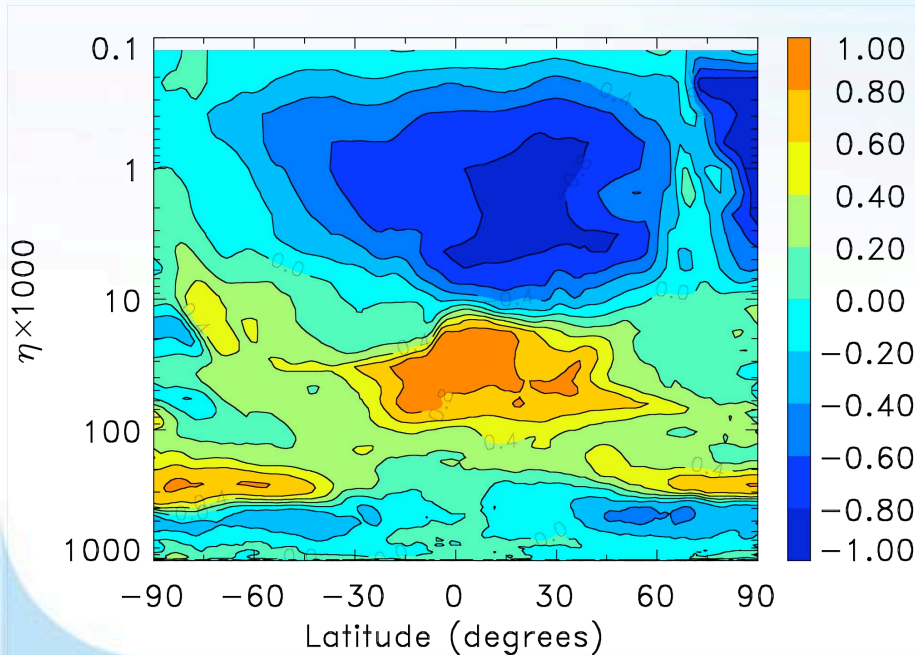
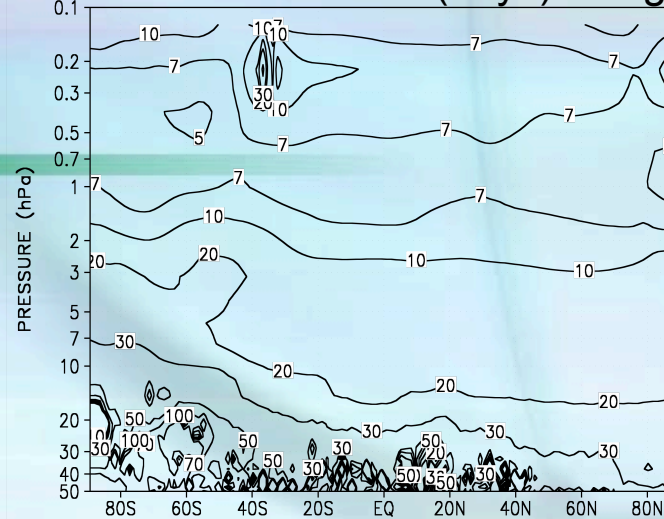
*e.g. deducing winds from chemical tracer observations*



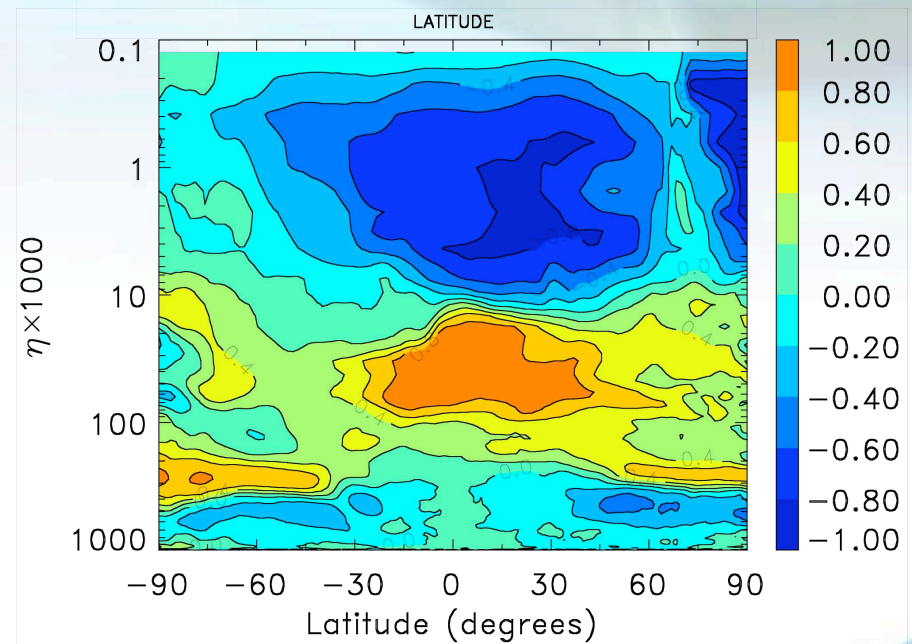
# Cross-error covariance Temperature-Ozone

Method: 6-hr differences (CQC)

### Radiative time scale (days) - August



without ozone-radiation interaction

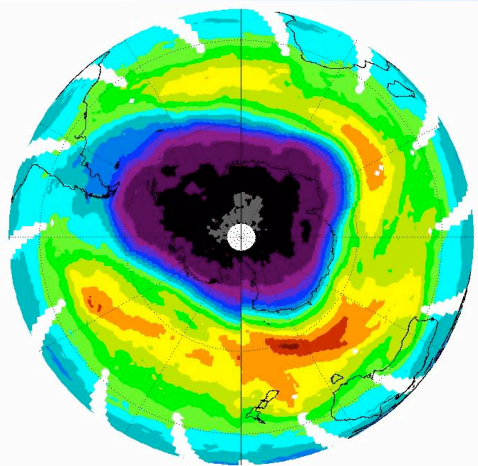


with ozone-radiation interaction

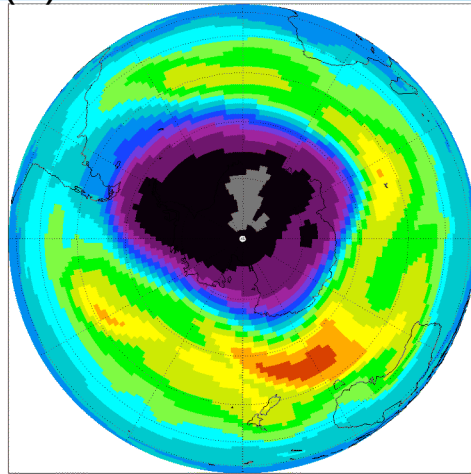
## Things to consider in the design of a DAS for GCCM

- Adjustments that take place on a short-time scale of a few days or less and which results in a balance between variables, can be accounted for in cross-error covariances for the analysis
- Adjustments that take place on longer time scales, or correlations that are not local, should not be incorporated in cross-error covariances, **but** should be properly simulated by the model

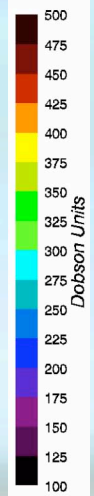
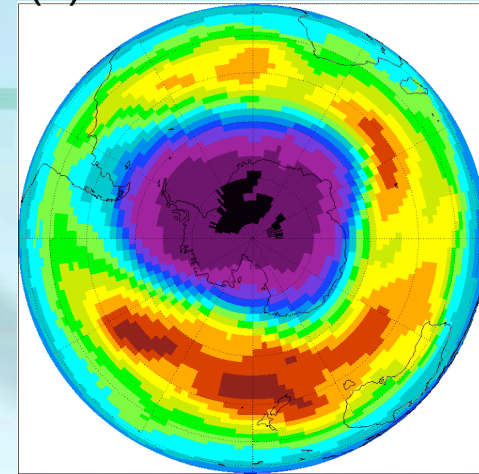
(a)



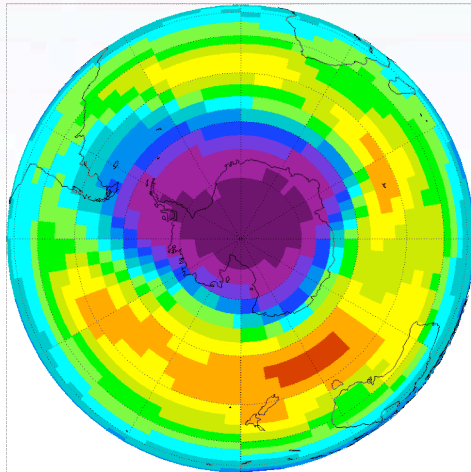
(b)



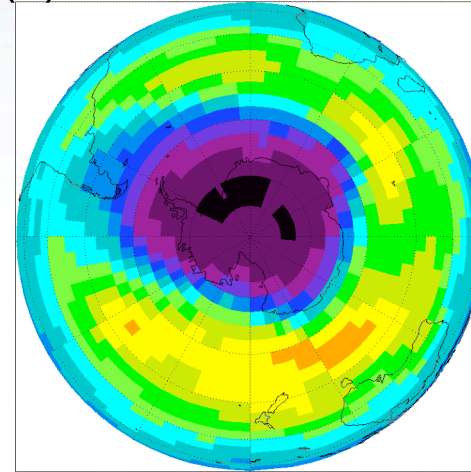
(c)



(d)



(e)



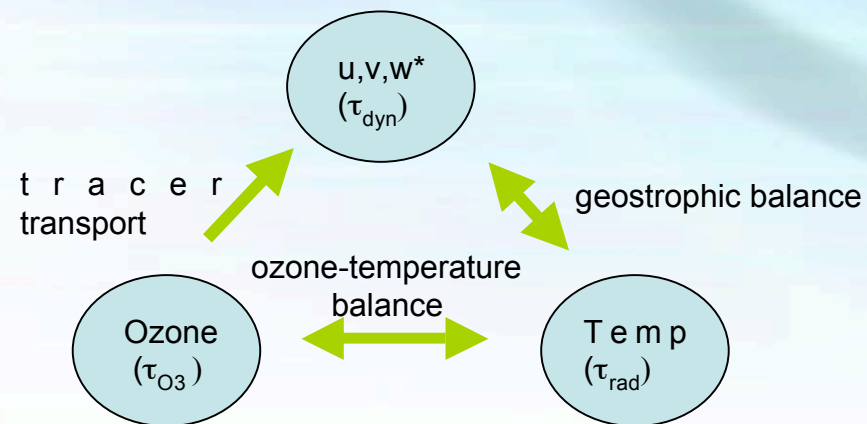
Total column ozone (DU) for September 30<sup>th</sup>, 2003:  
(a) observations by TOMS;  
(b) GEM-BIRA refreshed with 3D-Var trial fields;  
(c) BASCOE CTM in high resolution mode (1.875°×2.5°) with detailed PSC microphysics;  
(d) BASCOE CTM in low resolution mode (3.75°×5°);  
(e) BASCOE 4D-Var analysis of MIPAS (ESA) observations.

Grey areas represent pixels where the ozone column is smaller than 100 DU.



- Model/TLM/Adjoint resolution. We have decided to use same grid for model and analysis
- Four-dimensional variational assimilation should be used to infer wind information from chemical observations
- Error statistics should be consistent with observed-minus-model residuals in order to give the proper weight to the observations
- Stratospheric temperature analyses should be as accurate as possible, have small biases and error standard deviation, and be dynamically consistent

# Flow of information in data assimilation



# Highlights of the study

We have developed a state-of-the-art Global Chemistry Circulation Model (GCCM) running a moderately high resolution  $1.5^\circ \times 1.5^\circ$  with a fully coupled chemistry-dynamics data assimilation system

- ⌘ GCCM made from the operational NWP (GEM used at the Canada Met Service) and a state-of-the-art stratospheric chemistry used in BASCOE, 57 species advected species including heterogeneous chemistry
- ⌘ 3D Var-CHEM handles any cross-covariances between dynamical variables, between chemical variables, and between chemical and dynamical variables
- ⌘ 4D Var-CHEM uses an incremental passive tracer assimilation assumption
- ⌘ We have studied ozone-radiation effect on predictability when both ozone and temperature were assimilated

- ⌘ Multi-specie assimilation with 3D Var, including fast reacting species, e.g. NO<sub>2</sub>
- ⌘ Studied and implemented cross-error covariance between temperature and ozone
- ⌘ Use 4D Var to deduce winds from chemical observations
- ⌘ Evaluate the merit of different MIPAS retrievals (ESA / IMK) for data assimilation as well as GOMOS observations
- ⌘ Investigated the assimilation of MIPAS-ESA temperatures
- ⌘ Developed a method to obtain chemical observation and model error statistics suitable for data assimilation
- ⌘ Improved bias correction scheme for AMSU-a radiances
- ⌘ Performance Evaluation

# The Model

The General Circulation Model used in this study is based on the Canadian operational Global Environmental Multiscale (GEM) model extended to the stratosphere, called GEM-Strato.

The model GEM is a global non-hydrostatic/hydrostatic grid point model developed by Coté et al. (1998) for the purpose of environment prediction, and has the following characteristics:

- ♣ A variable resolution finite element discretization on an Arakawa C grid is used in the horizontal. Second order accuracy in horizontal
- ♣ Hybrid vertical coordinate and non-staggered finite differences
- ♣ Semi-implicit , two-time level semi-Lagrangian advection



## Physics

- θ Turbulence in planetary boundary layer through vertical diffusion, diffusion based on stability and kinetic energy
- θ Kuo-type deep convection
- θ Non-precipitating shallow convection
- θ Sundqvist condensation scheme for stratiform precipitation
- θ Orographic gravity wave drag (Mc Farlane et al 1987)
- θ Surface layer based on Monin-Obukhov similarity theory
- θ Prediction of surface temperature over land, force-restore

θ Radiation scheme : correlated-k method

Computes heating and cooling rates, precision of a line by line RTM of emission and absorption in IR, visible and UV. Can accept 2D or 3D fields of H<sub>2</sub>O, CO<sub>2</sub>, O<sub>3</sub>, N<sub>2</sub>O, CH<sub>4</sub>, CFC-11 -12 -113 -114 sulfate aerosols, sea salt, and dust.

*So far O3 and H2O advected species are online*

θ Non-horographic gravity wave drag due to Hines (1997)

# Chemistry

Either

θ Ozone climatology (Fortuin and Kelder 1998)

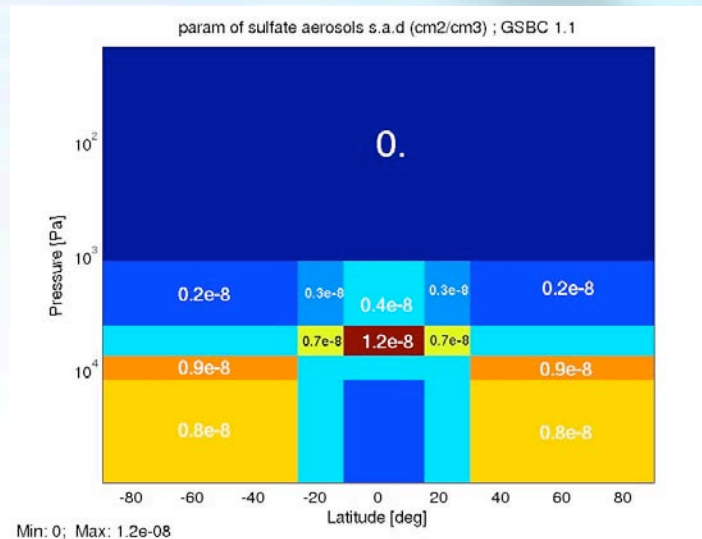
θ Parametrization of water vapor due to methane oxidation (ECMWF) with a height dependent relaxation time scale  
~ 100 days at the stratopause, ~ 2000 days at 10 hPa,  
infinite at the tropopause

or

## *BASCOE chemistry*

- θ 57 chemical species, all advected (S-L)
- θ  $O_x$ ,  $HO_x$ ,  $NO_x$ ,  $ClO_x$ ,  $BrO_x$  and few hydrocarbons
- θ Source species:  $N_2O$ ,  $CH_4$ ,  $H_2O$ , CFCs, HCFCs and Halons
- θ 142 gas-phase reactions; 7 heterogeneous reactions
- θ 52 photodissociation reactions,  $J$  interp from tables
- θ Photochemical rates are taken from JPL-2002
- θ Solver generated by KPP (Sandu and Sander, 2006)
- θ Numerical method: 3<sup>rd</sup> – order Rosenbrock
- θ 45-min timesteps divided into sub-timestep

- θ Heterogeneous chemistry is fully resolved, with simplified parameterizations for surface area densities (s.a.d., badly known anyway)
- θ Sulfate aerosol:



- θ PSC : T < 194 K → NAT PSC with s.a.d. = 1.e-7 cm<sup>2</sup>/cm<sup>3</sup>  
 T < 186 K → ICE PSC with s.a.d. = 1.e-6 cm<sup>2</sup>/cm<sup>3</sup>  
 (+ loss of H<sub>2</sub>O/HNO<sub>3</sub> due to sedimentation)

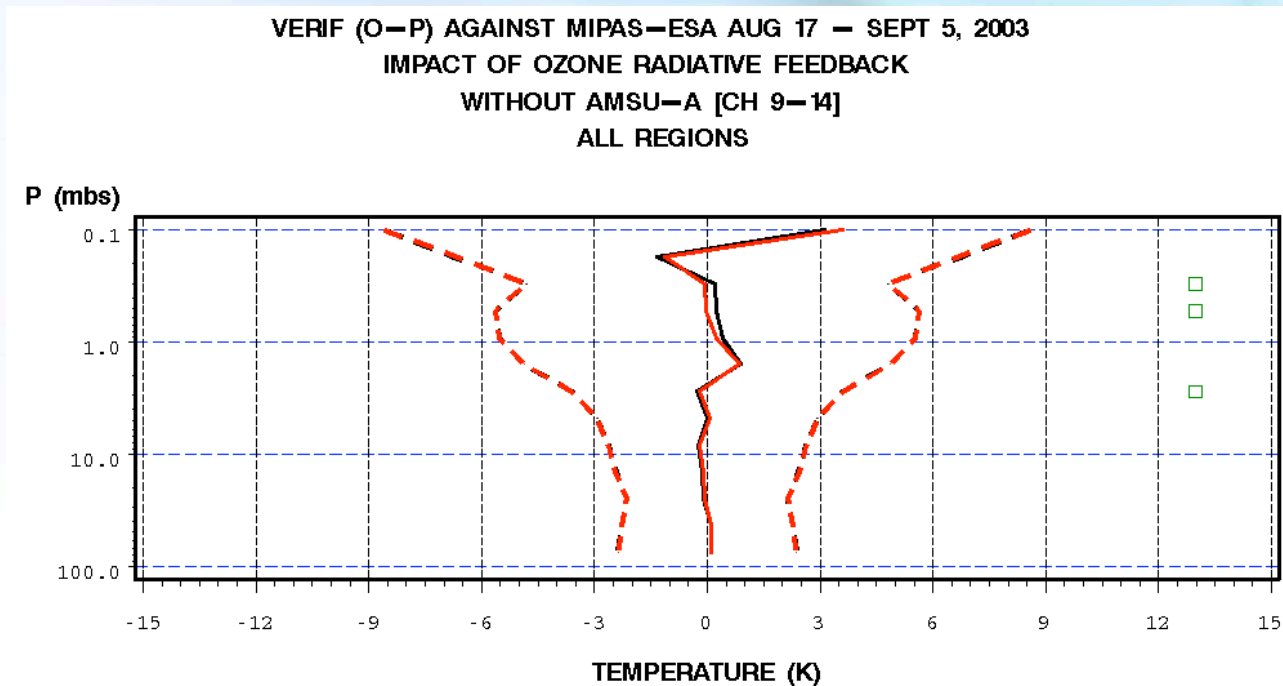


# Ozone-radiation

- Assimilation of temperature
  - Impact on analyses
  - Impact on 10-day forecasts
- Assimilation of ozone and temperature
  - Impact on analyses
  - Impact on 10-day forecasts

# Assimilation of Temperature: Impact on analyses

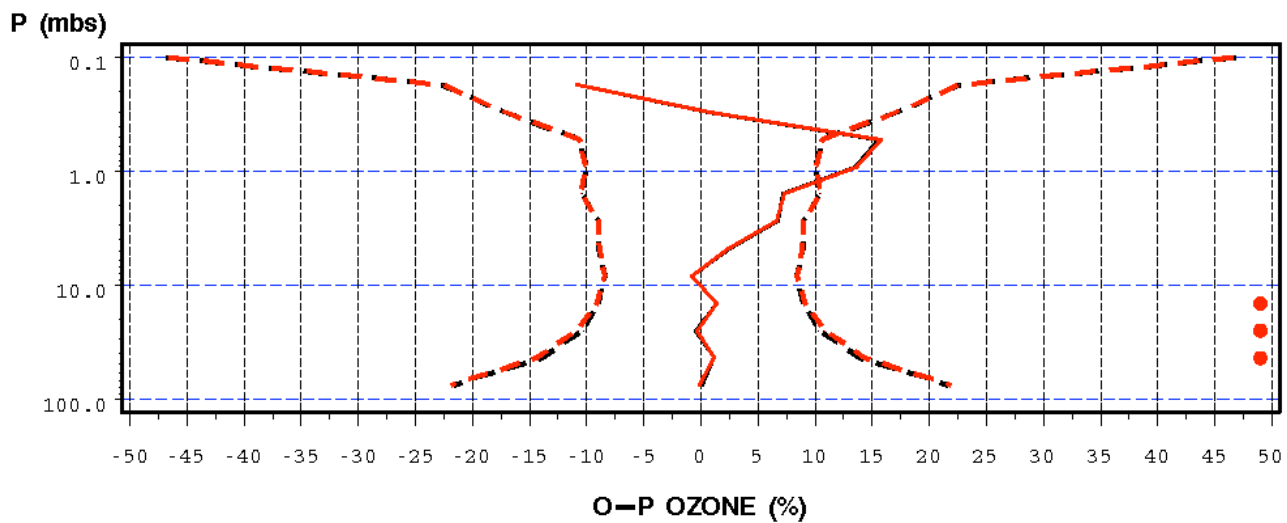
- Assimilation of MIPAS-ESA temperature without AMSU-a channels 9-15



red : ozone-radiation

black : no interaction

VERIF (O-P) AGAINST MIPAS-ESA AUG 17 - SEP 05, 2003  
IMPACT OF OZONE RADIATIVE FEEDBACK  
WITHOUT AMSU-A [CH 9-14]  
ALL REGIONS



red : ozone-radiation

black : no interaction

## Assimilation of Temperature: Impact on forecasts

### Anomaly correlation

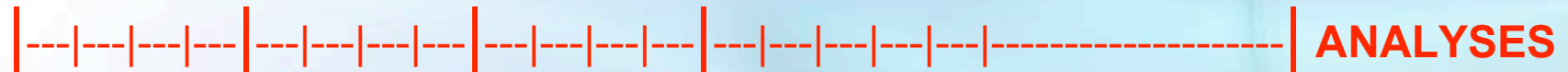
- Ensemble of 10-day forecast launched each 12 hrs
- August 15 – October 5, 2003
- Correlation between forecast-climate anomalies and analysis-climate anomalies valid at the same time
- WMO standard, measure of predictability

11/08

12/08

13/08 .....

05/10



-----| (24hr)

-----| (48hr)

-----| (72hr)

**FORECAST**

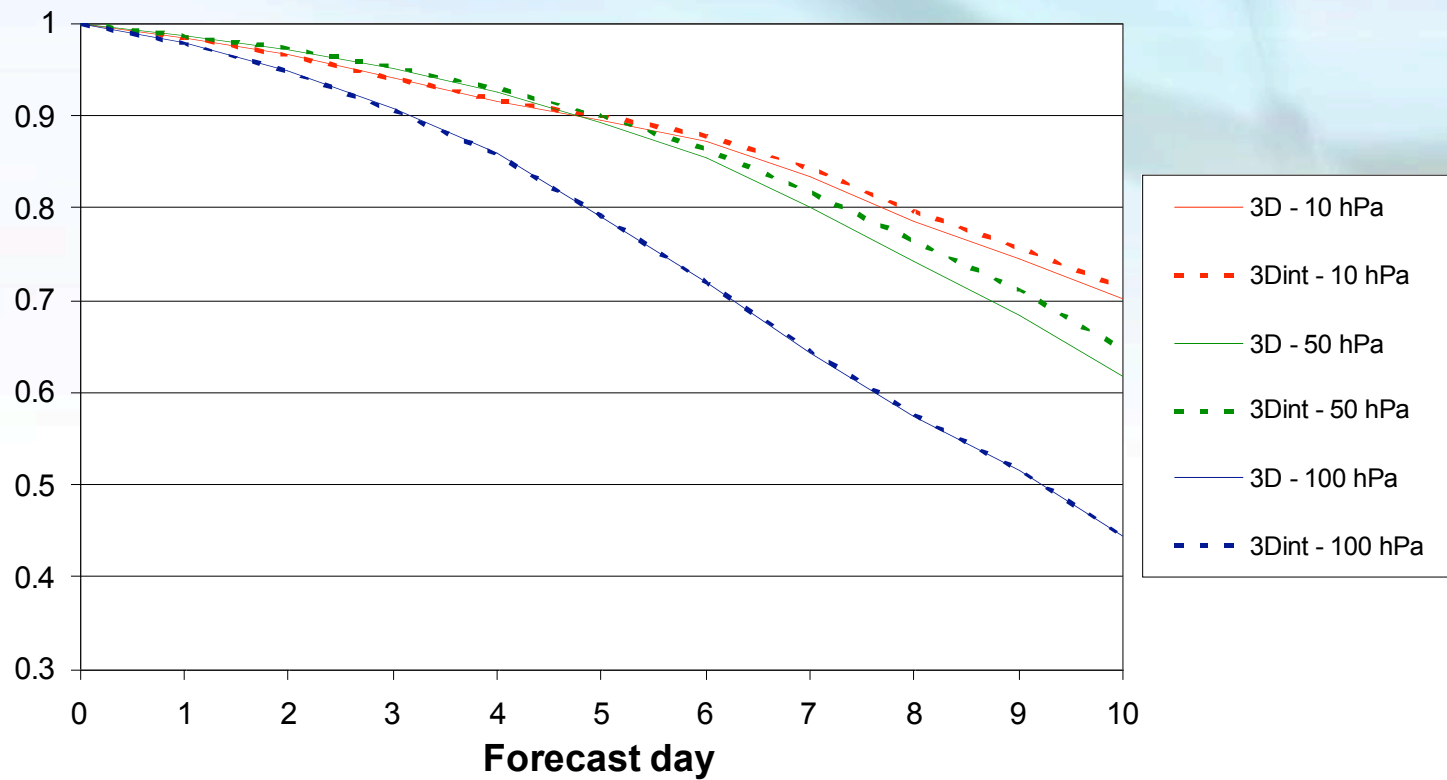
### ANOMALY CORRELATION $r$

$$r = \frac{\sum_{i=1}^n (x_f - x_c - M_{f,c})_i (x_v - x_c - M_{v,c})_i \cos \varphi_i}{\sqrt{\sum_{i=1}^n (x_f - x_c - M_{f,c})_i^2 \cos \varphi_i} \sqrt{\sum_{i=1}^n (x_v - x_c - M_{v,c})_i^2 \cos \varphi_i}}$$



## Anomaly Correlation

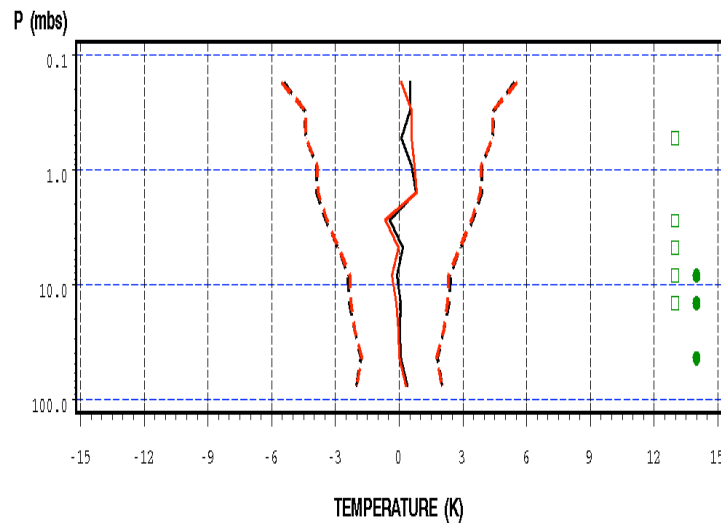
August 15 - October 5, 2003  
South Hemisphere (20-90S)



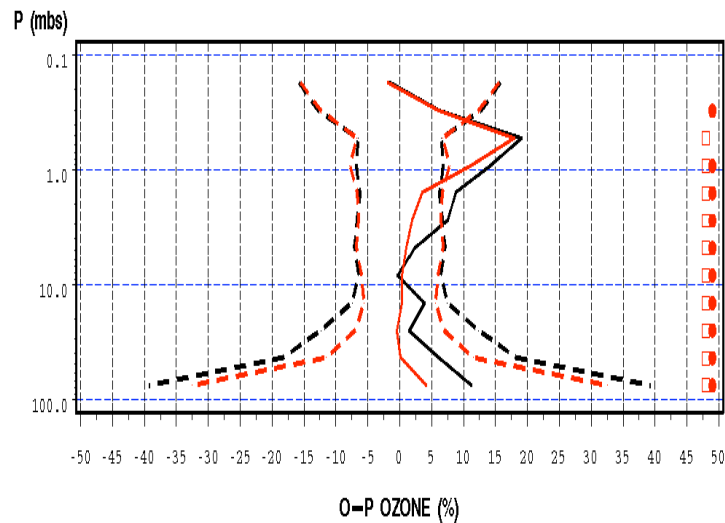
# Assimilation of Ozone and Temperature: Impact on analyses

tropics

VERIF (O-P) AGAINST MIPAS-ESA AUG 17 - SEPT 5, 2003  
IMPACT OF MIPAS-ESA OZONE ASSIMILATION  
WITHOUT AMSU-A [CH 9-14]  
TROPICS



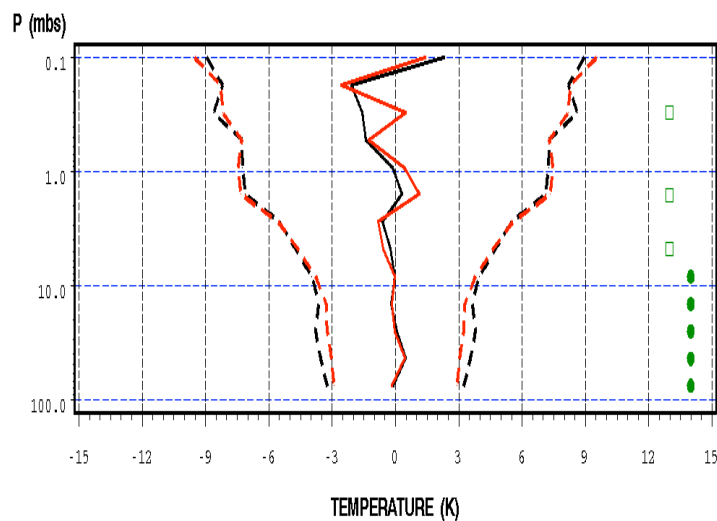
VERIF (O-P) AGAINST MIPAS-ESA AUG 17 - SEP 05, 2003  
IMPACT OF ASSIMILATING MIPAS-ESA OZONE  
WITHOUT AMSU-A [CH 9-14]  
TROPICS



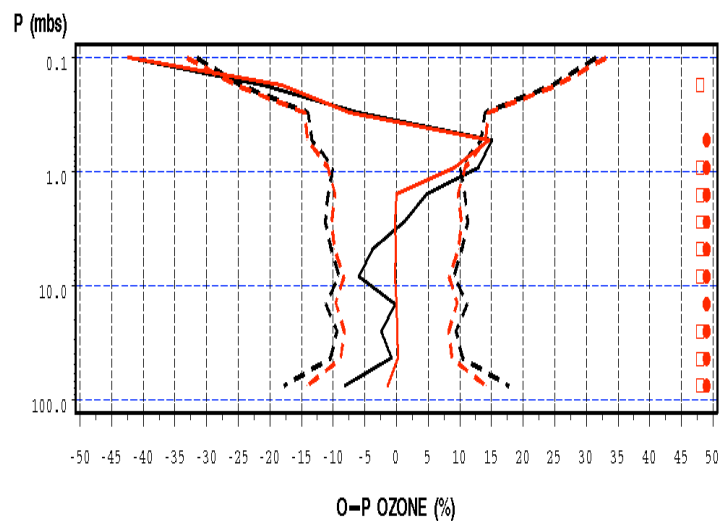
ozone-radiation interaction on  
red : temperature + ozone assimilation  
black : temperature only assimilation

## mid-latitudes SH

VERIF (O-P) AGAINST MIPAS-ESA AUG 17 - SEPT 5, 2003  
 IMPACT OF MIPAS-ESA OZONE ASSIMILATION  
 WITHOUT AMSU-A [CH 9-14]  
 MID LAT SH



VERIF (O-P) AGAINST MIPAS-ESA AUG 17 - SEP 05, 2003  
 IMPACT OF ASSIMILATING MIPAS-ESA OZONE  
 WITHOUT AMSU-A [CH 9-14]  
 MID LAT SH

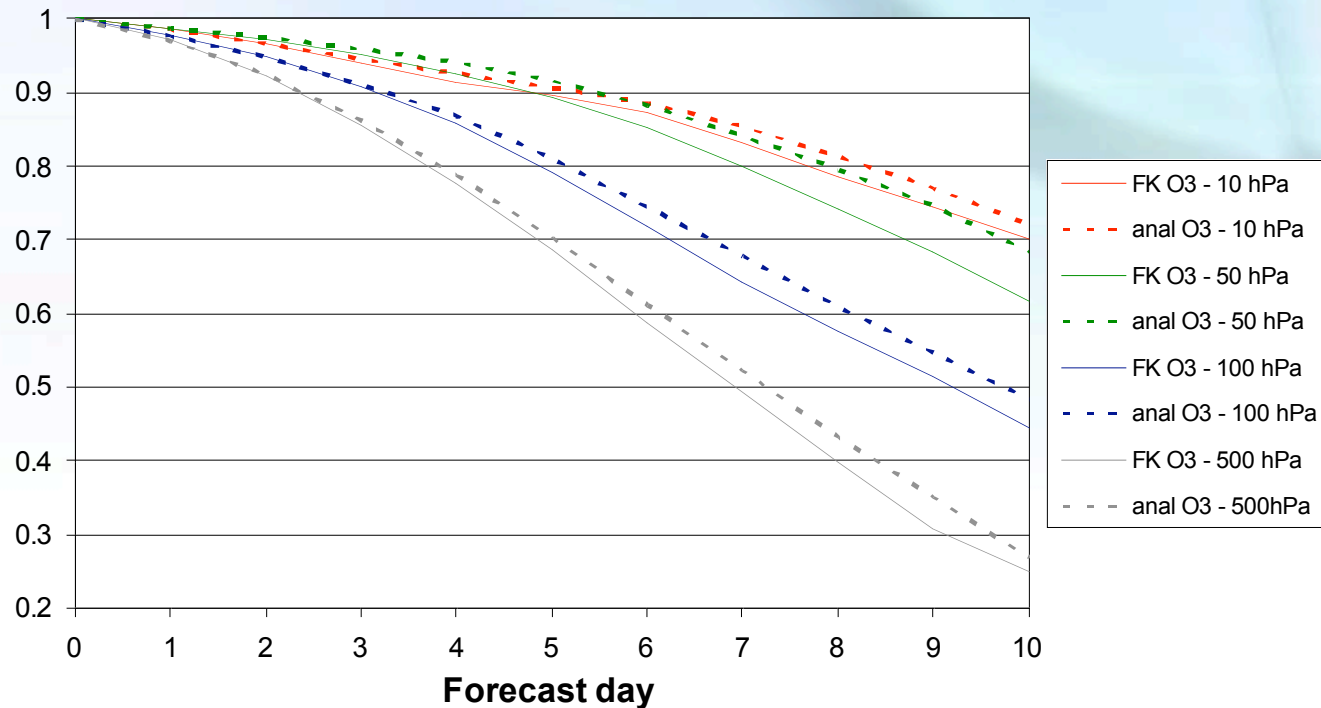


ozone-radiation interaction on  
**red** : temperature + ozone assimilation  
**black** : temperature only assimilation

# Assimilation of Ozone and Temperature: Impact on forecasts

## Anomaly Correlation

August 15 - October 5, 2003  
South Hemisphere (20-90S)



**GCM** assimilation of temperatures using climatological ozone (solid curves)  
**GCCM** assimilation of temperature and ozone from MIPAS (dashed curves)

# Conclusions

## Temperature assimilation

- The impact of ozone radiative feedback on temperature analyses is not significant
- The impact of using an ozone interactive model on temperature predictability is weak. It contributes to increasing the predictability particularly between 10 and 50 hPa
- On 10-day forecast RMS and bias is slightly improved with ozone radiation feedback

## Temperature and ozone assimilation

- The impact of ozone radiative feedback on temperature analysis is significant on temperature in the summer hemisphere where the ozone-radiation interaction is important
- Significant improvement on ozone analyses is observed in all regions
- Systematic improvement of temperature predictability particularly in the lower stratosphere where changes are significant. This improvement comes from a better representation of ozone radiative heating in the lower stratosphere region. This radiative forcing persists throughout the forecast period due to the large ozone photochemical lifetime which is much larger than the radiative timescale in the region



## BIAS correction on AMSU-a channels

Bias correction has been developed in meteorology, on a pre-existing observation network (radiosondes, aircraft data, surface obs.) that provided an already good quality model forecast. Comparing observed radiances against simulated radiances of the model forecast lead to systematic errors that was attributed solely to measurement bias, i.e.  $\overline{(\mathbf{y} - H(\mathbf{x}_b))} = \bar{\mathbf{y}}$

Set  $\mathbf{y} = \mathbf{y}_c + \tilde{\mathbf{y}}$  so that  $\overline{\tilde{\mathbf{y}} - H(\mathbf{x}_b)} \approx 0$   
provided  $\mathbf{y}_c = \mathbf{y}_c(\alpha_1, \alpha_2, \alpha_3) = \bar{\mathbf{y}}$

Predictors are related to air mass characteristics and scan angle

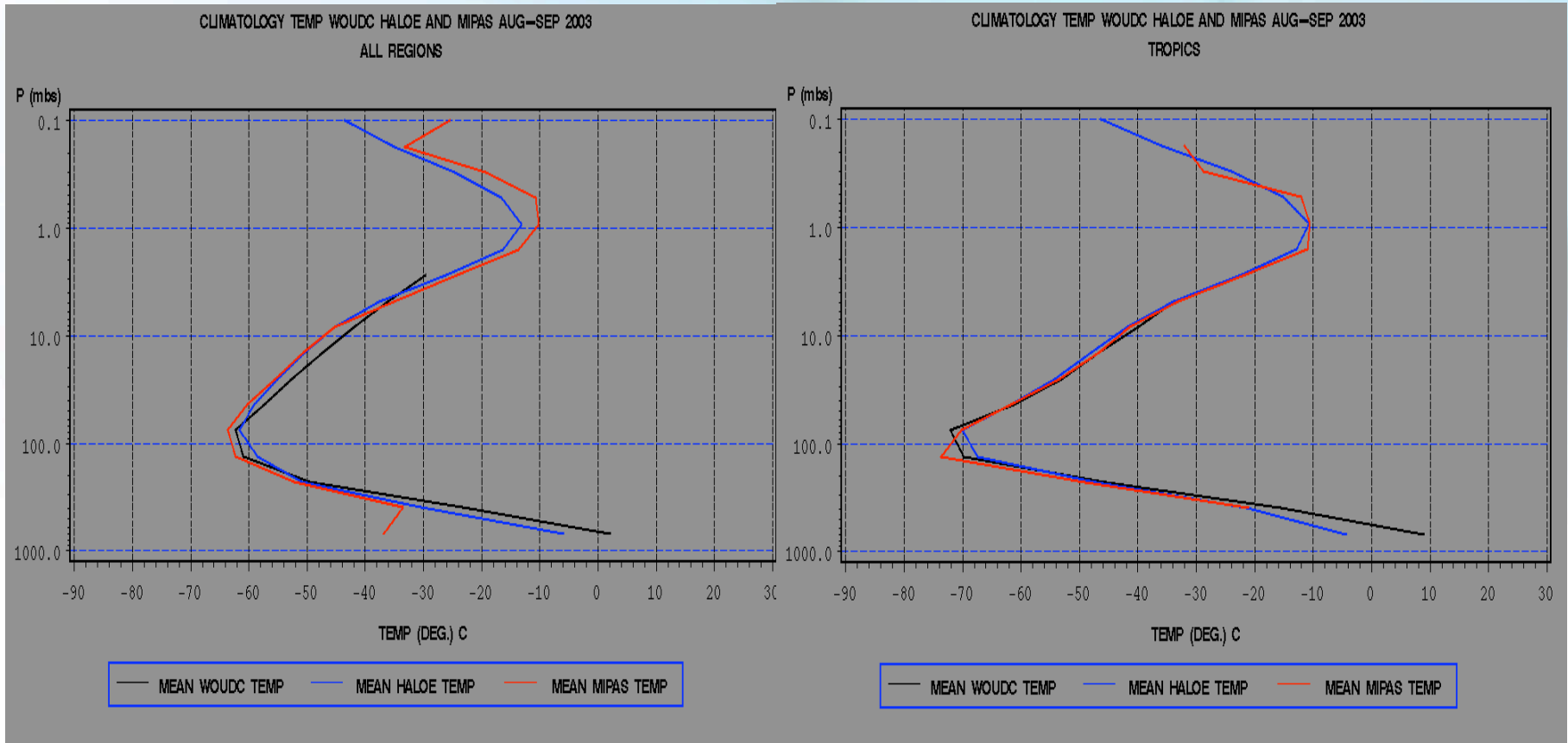
## Can we use the same assumption in the stratosphere ?

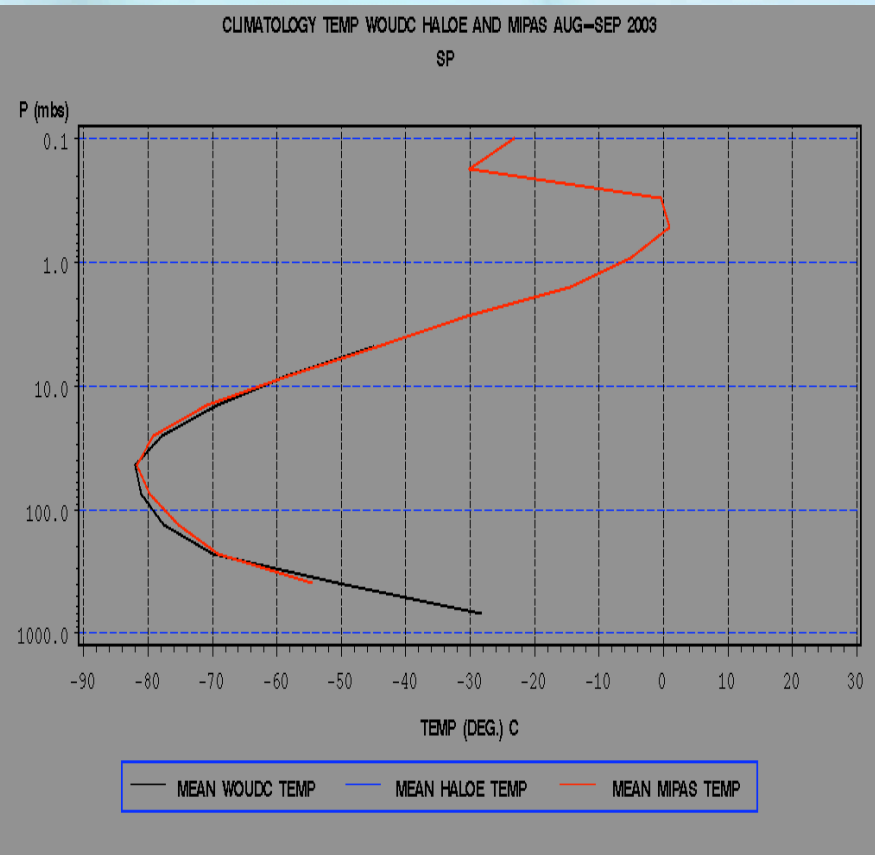
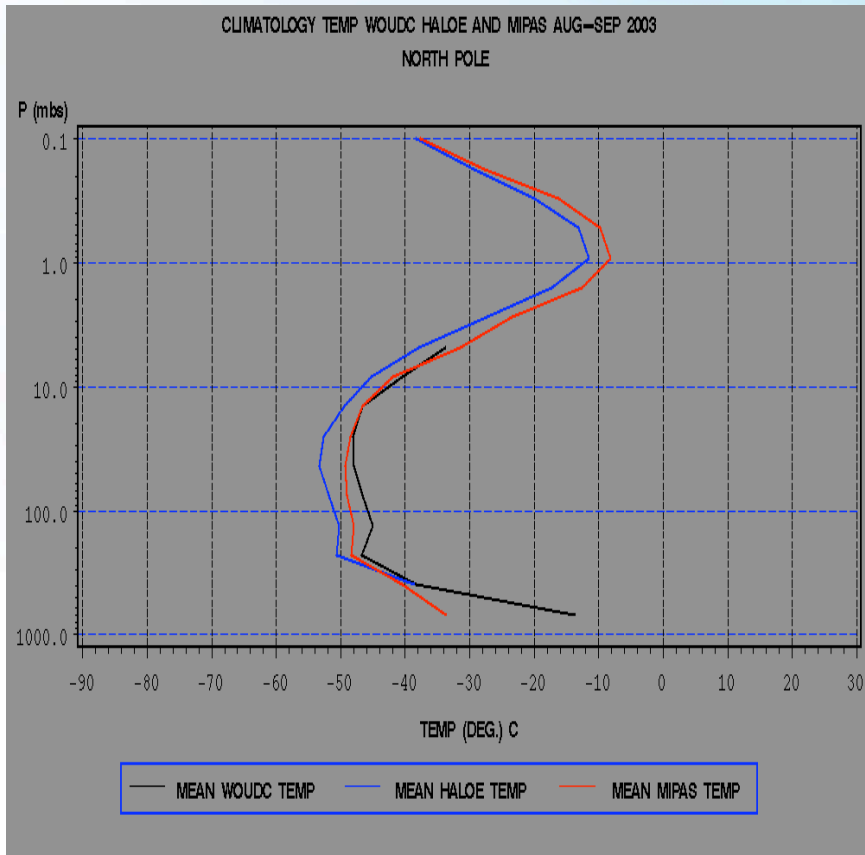
- Radiosondes measurements typically reach not much higher than 30 hPa
- Large uncertainties in stratospheric modeling due to gravity wave drag parametrization

## Anchoring the reference solution with MIPAS obs.

*Assimilation of MIPAS temperatures used to anchor the solution  
and develop the bias correction coefficient*

# Quality of MIPAS temperature observations



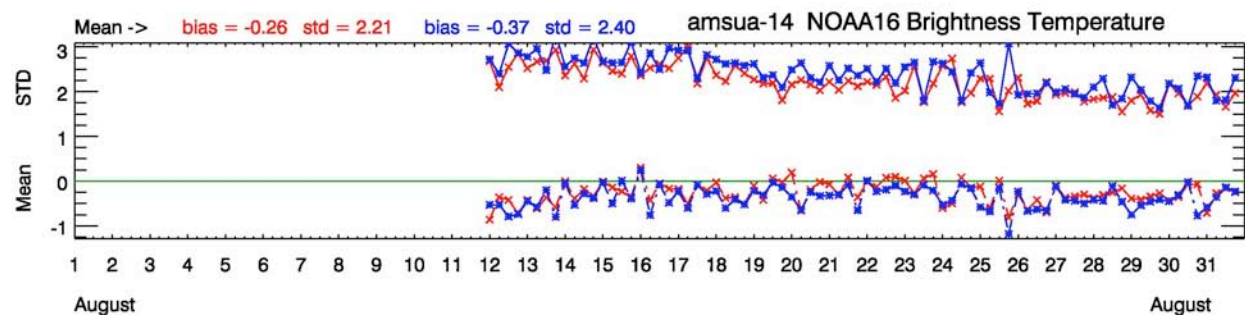
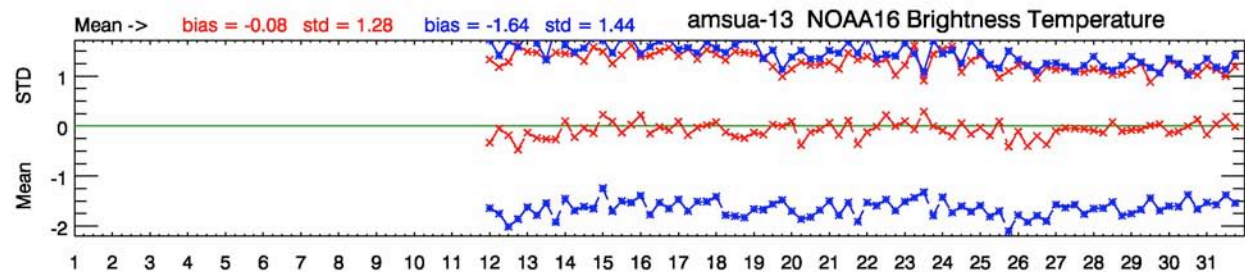
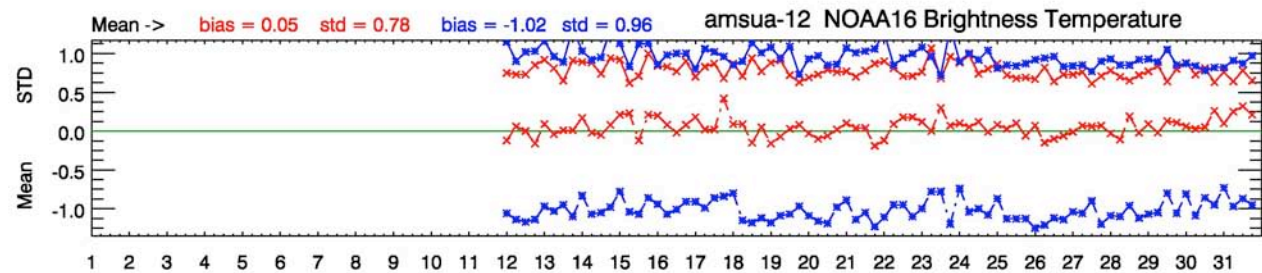
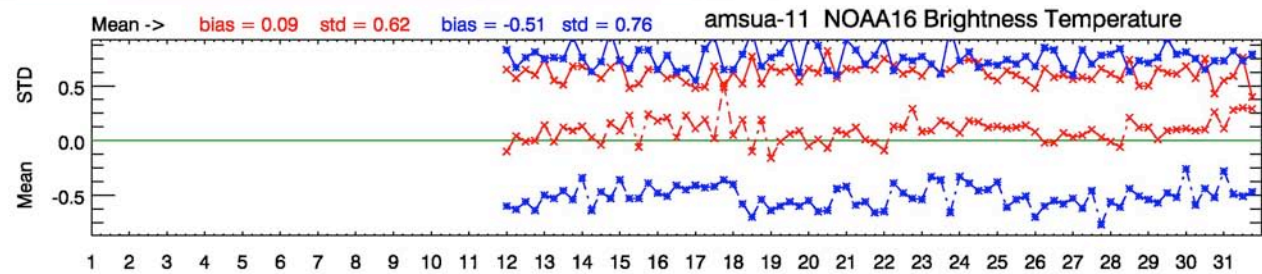


HALOE and WOUDC have limited coverage here so cannot conclude

No HALOE data here

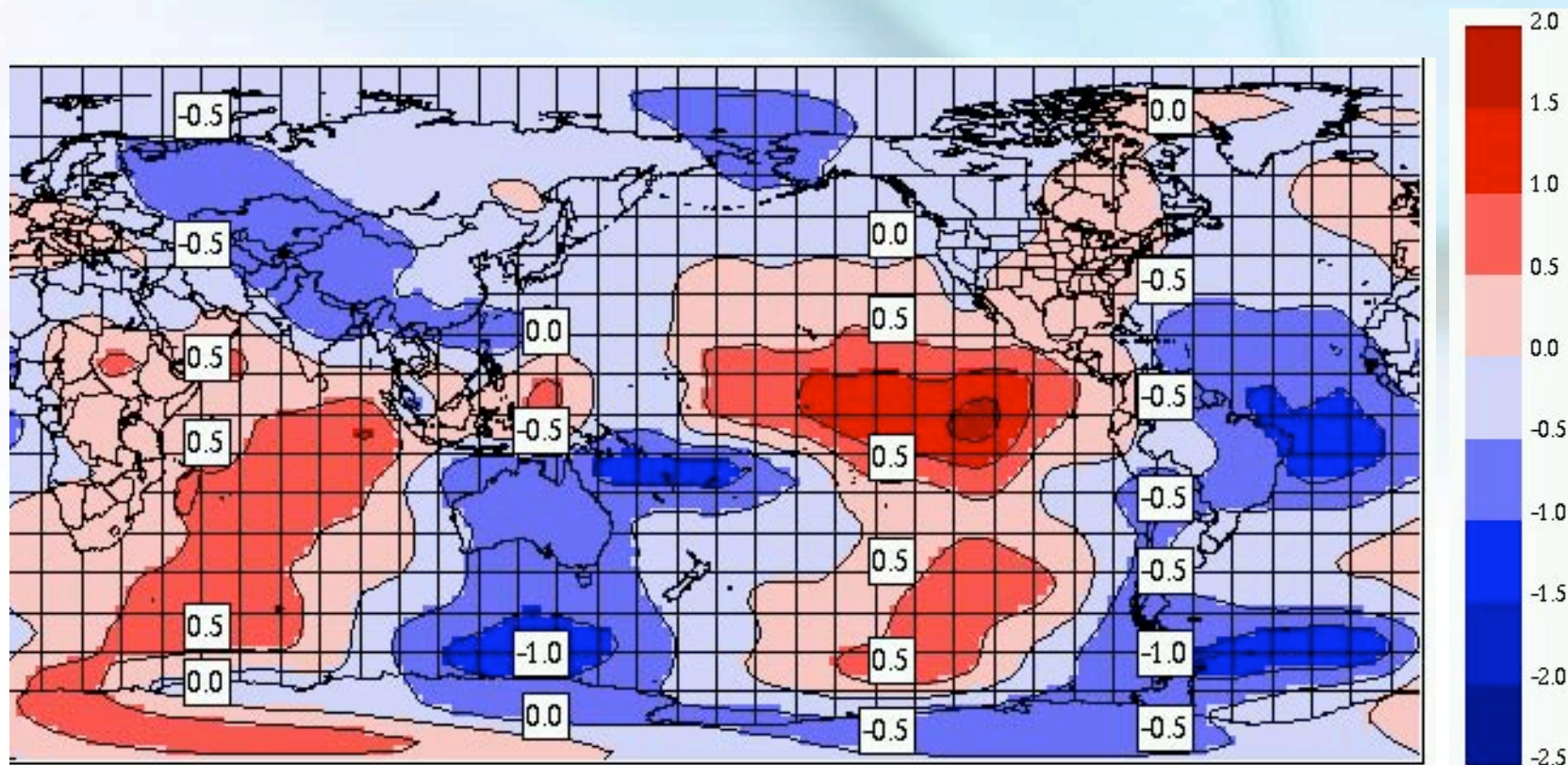
# Experiments: bias correction of stratospheric radiances (A3es0319)

O-P: without bias correction  
O-P: with revised bias correction



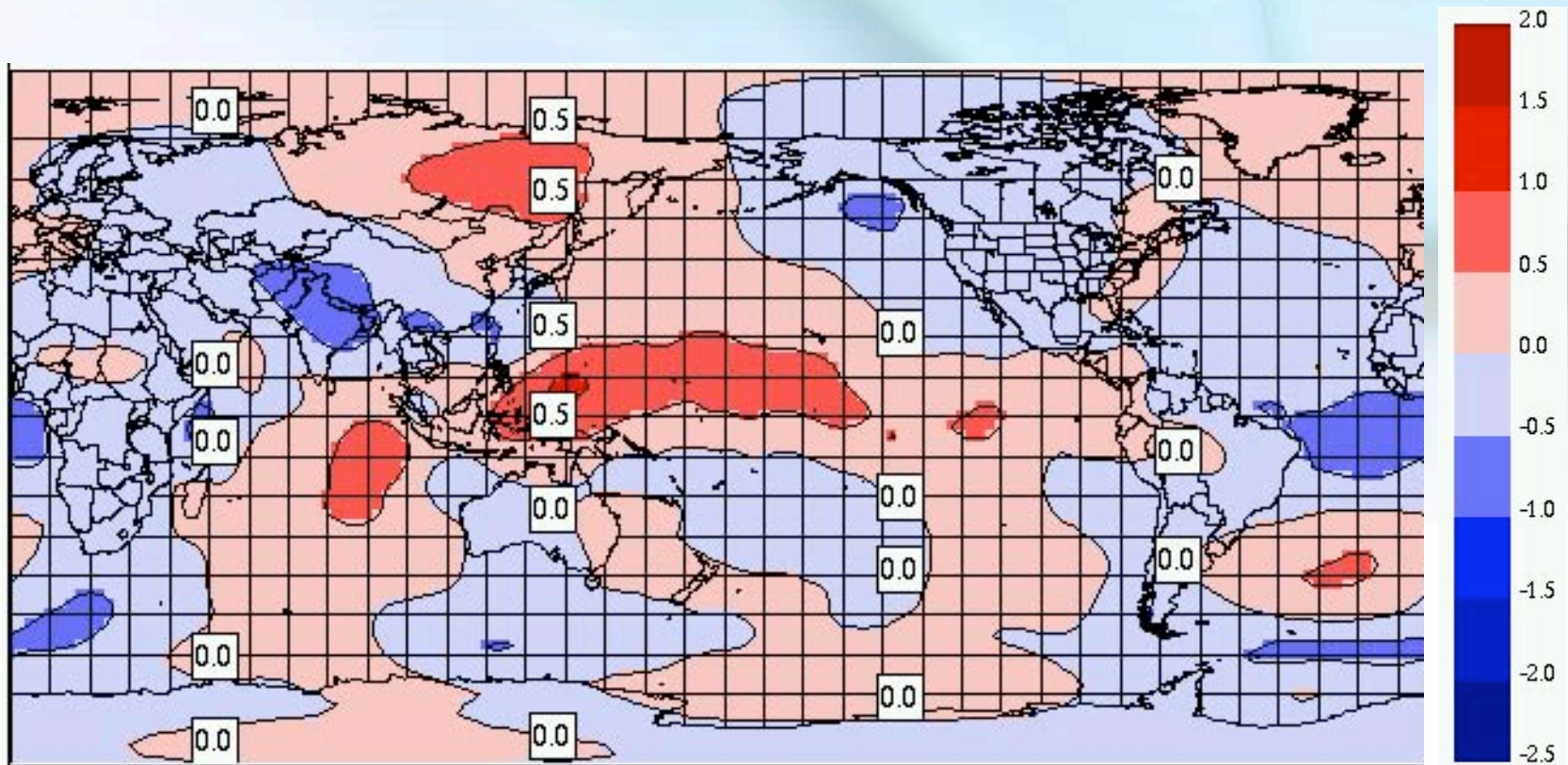


Mean analysis temperature increments at 10 hPa  
No bias correction of AMSU-a channels 11-14 (September 2003)



## Mean analysis temperature increments at 10 hPa

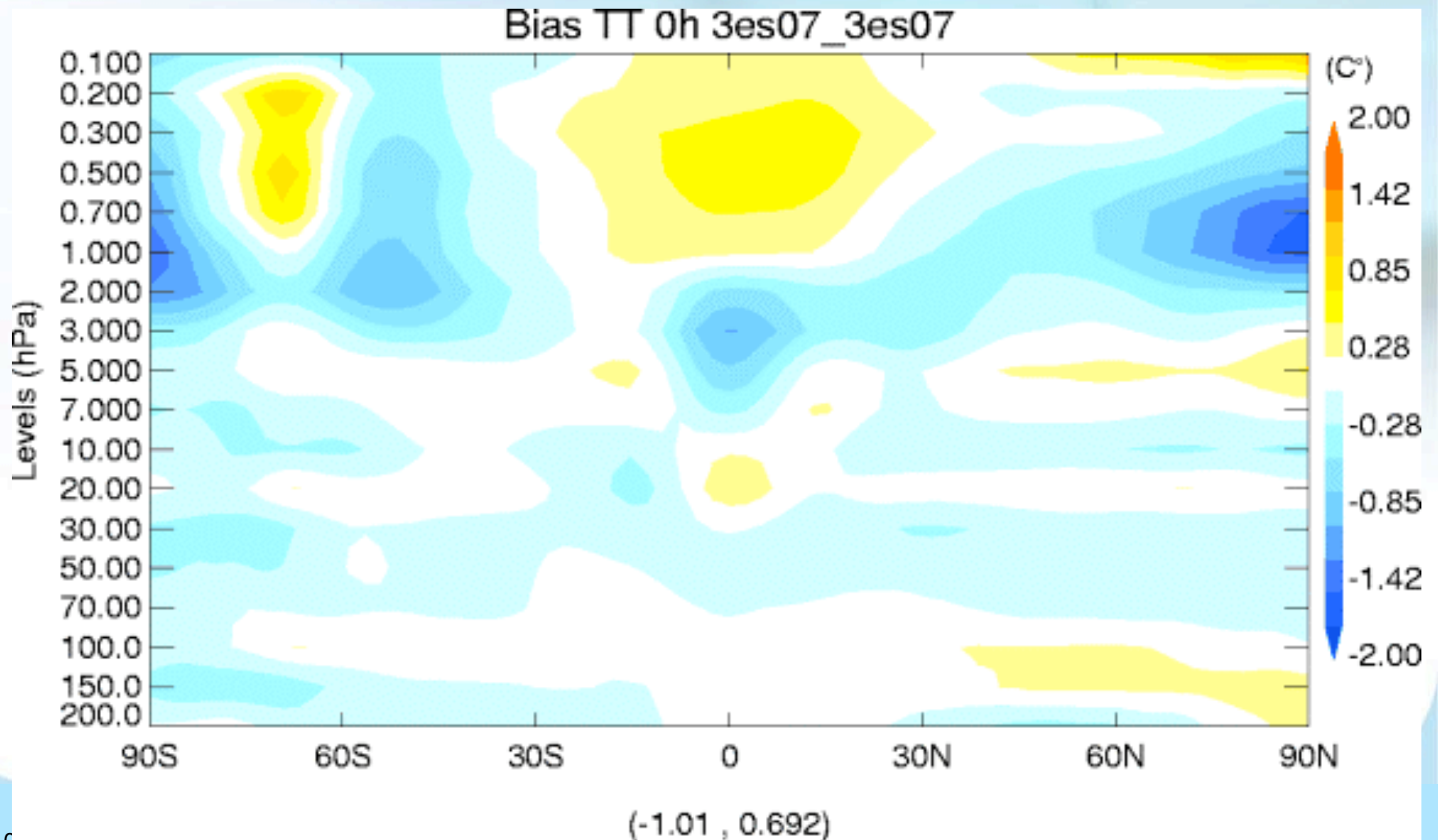
With revised bias correction of AMSU-a channels 11-14 (September 2003)





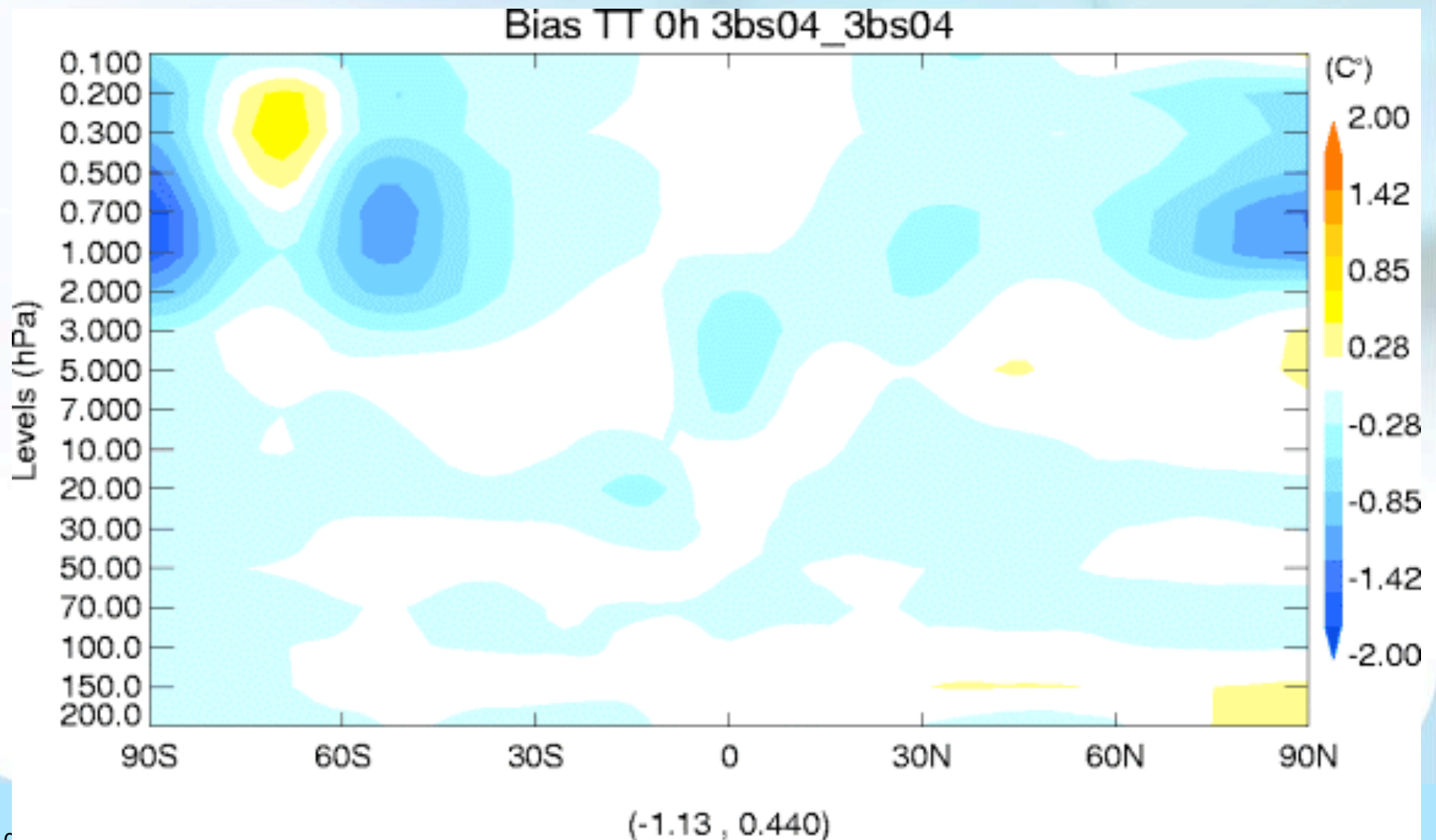
# Experiment without any bias correction

## Mean analysis temperature increments (previous results)



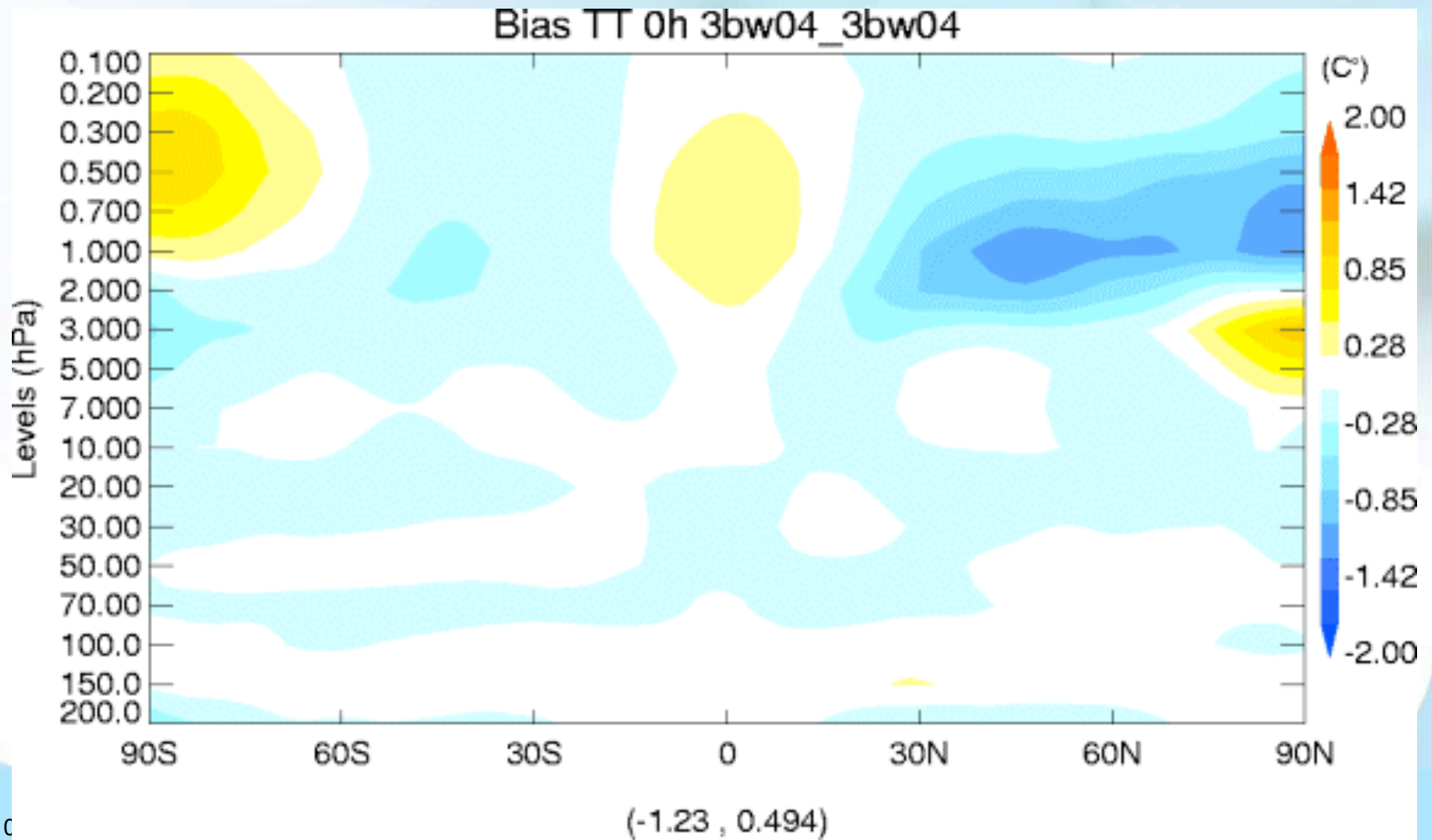
# Experiment with the revised bias correction

Mean analysis temperature increments (September 2003)



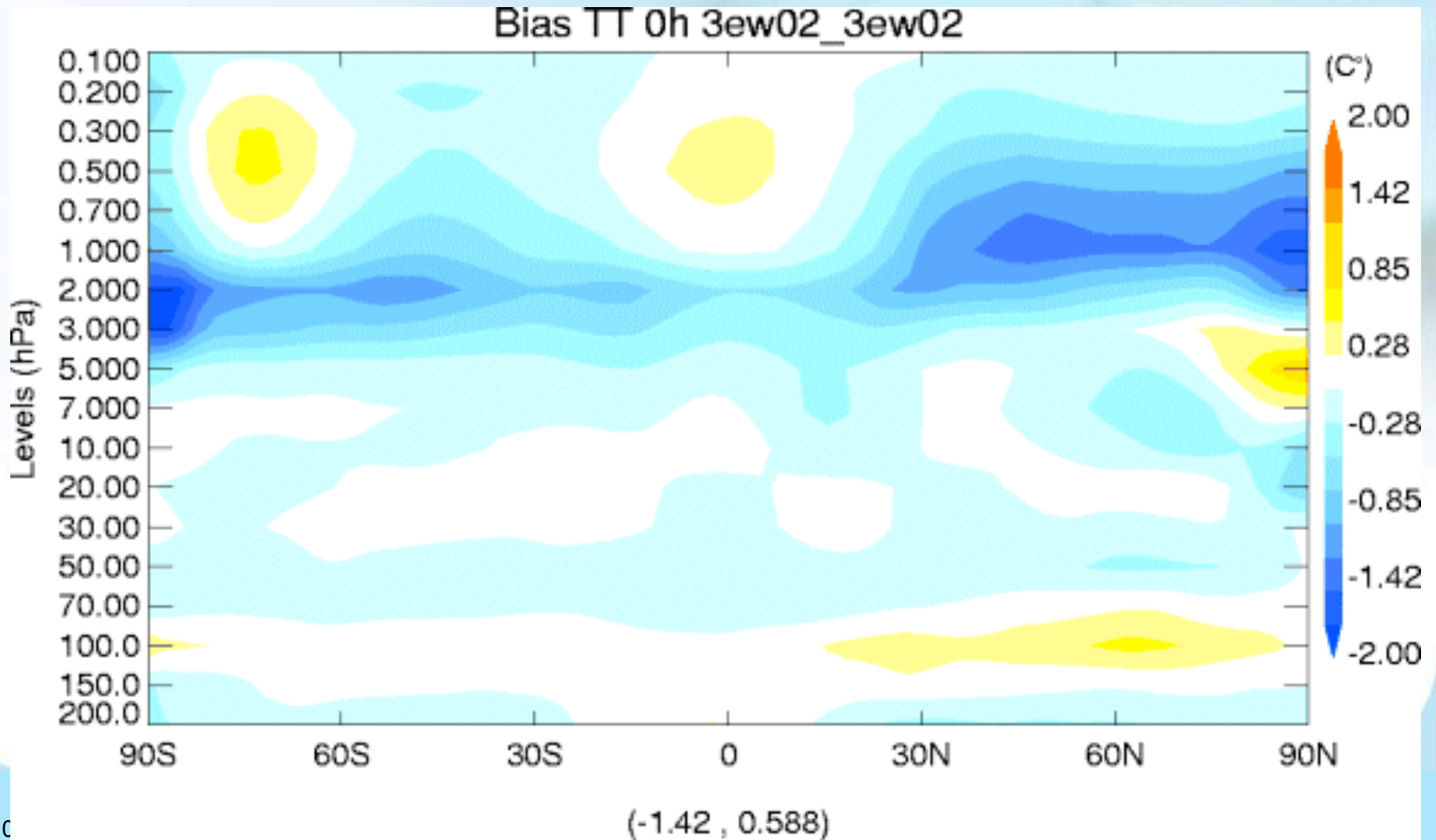
# Revised bias correction (winter)

Mean analysis temperature increments (January 2003)



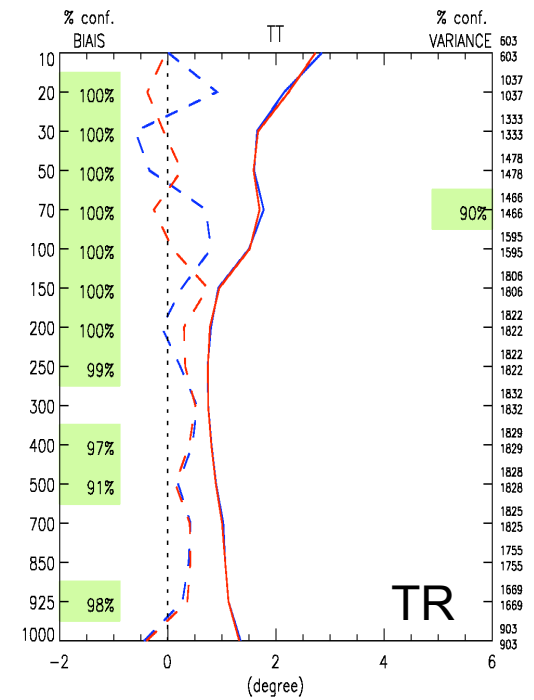
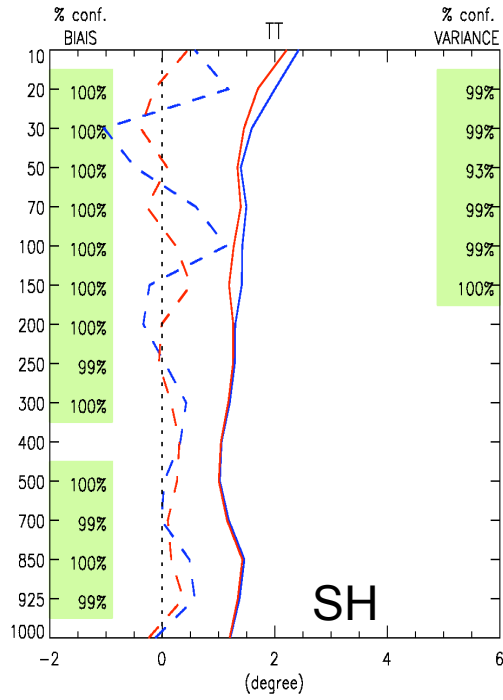
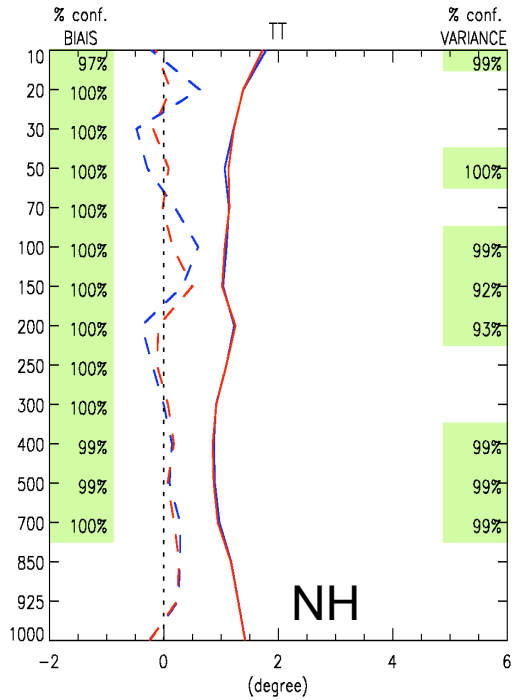
# Without bias correction (winter)

Mean analysis temperature increments (January 2003)

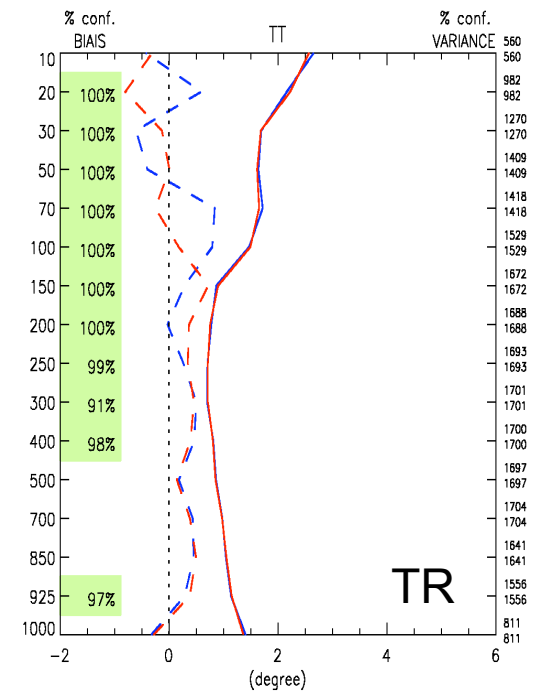
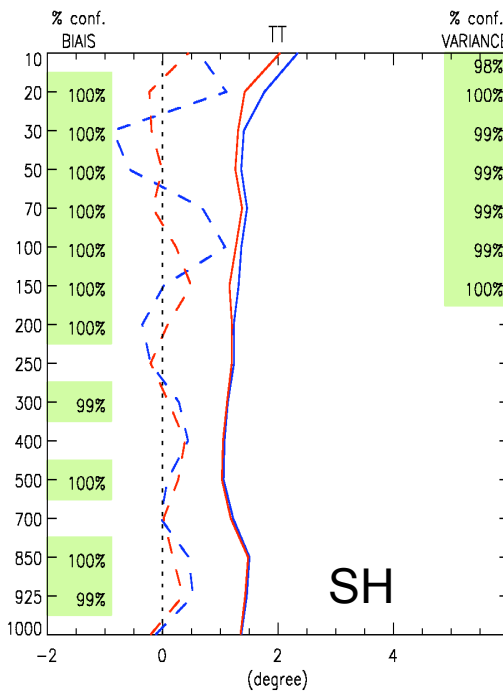
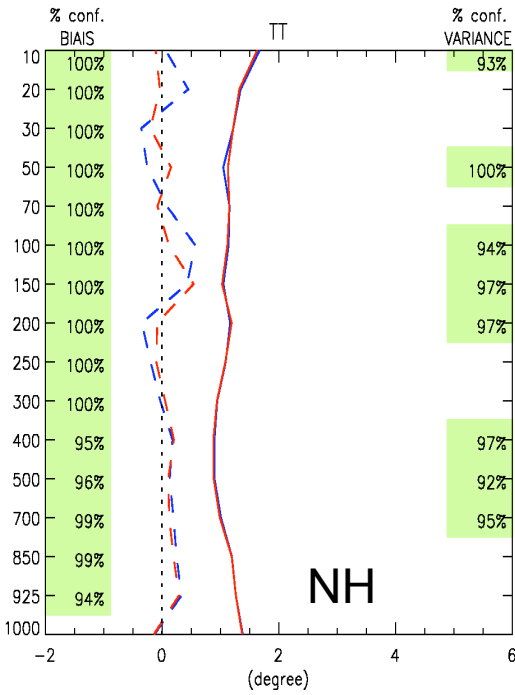




Aug 11<sup>th</sup> – Sept 5<sup>th</sup>



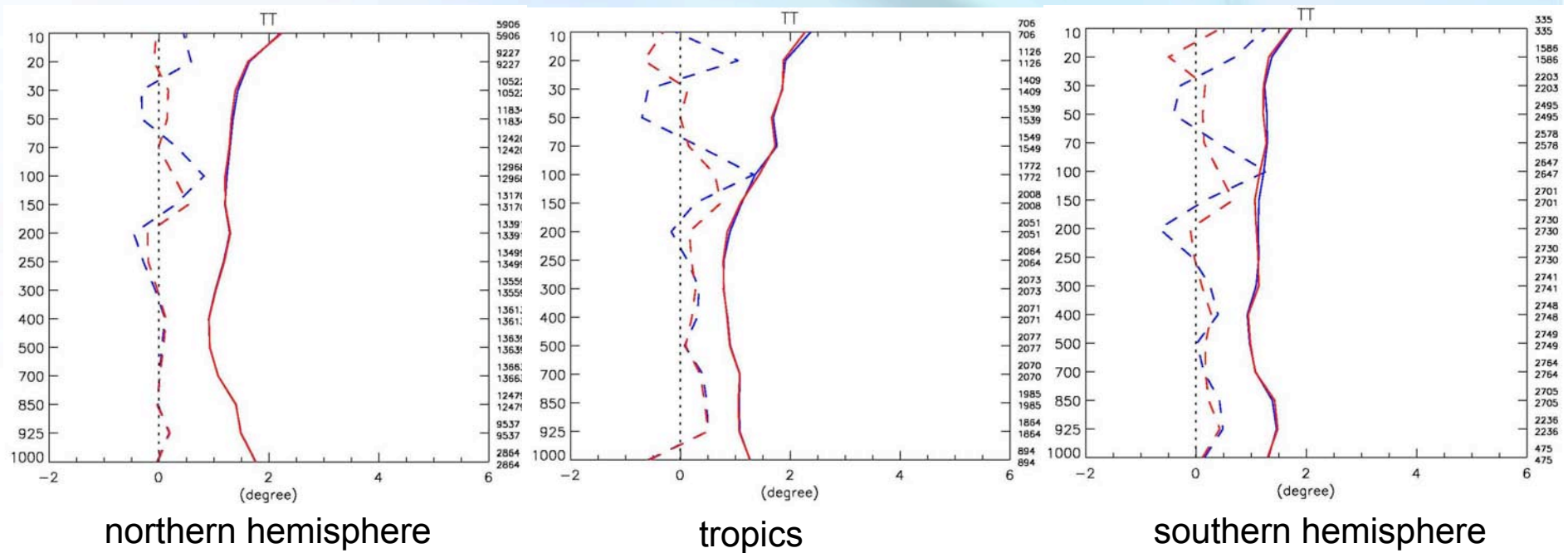
Sept 6<sup>th</sup> – Sept 30<sup>th</sup>



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# Validation against radiosondes

## Winter period (62 cases in January 2003)



## Conclusions

- The revised bias correction improves the monitoring statistics, the mean analysis increments, except in the sponge layer near the poles
- Comparison with independent observations also shows improvement
- Bias correction (obtained in August 2003) is used successfully in winter 2003

Merci

Thank you



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