Coupled chemical-dynamical data assimilation

ESA/ESTEC Contract

Team

Dr Richard Ménard (P.I.) (1)
Dr Pierre Gauthier (1)
Dr Jean de Grandpre (1)
M. Alain Robichaud (1)
Dr Yves Rochon (2)
M. Cecillien Charrette (1)

Dr Simon Chabrillat (3)
Dr Dominique Fonteyn (3)

Dr Thomas von Clarmann (5)

Prof Jack McConnell (4)
Dr Jacek Kaminski (4)

Dr Martin Charron (1)
M. Alexander Kallaur (1)
Dr Yan Yang (2)

Dr Paul Vaillancourt (1)
Dr Monique Tanguay (1)

With the participation of Paul-André Beaulieu(1), Quentin Errera(3), Sylvain Ménard(1), Mike Neish(2) and Cathy Xie(1)

Environment Canada
(1) 2121 Transcanada Highway
Dorval, Qc, H9P 1J3
CANADA

(2) 4905 Dufferin Street
Toronto, Ont., M3H 5T4
CANADA

(3) **Belgisch Instituut voor Ruimte-Aëronomie**
Institut d'Aéronomie de Belgique (BIRA-IASB)
3, avenue Circulaire
1180 Brussels, BELGIUM

(4) **York University**
Department of Earth and Atmospheric Science
4700 Keele Street, Toronto, Ont. M3J 1P3
CANADA

(5) **Institut für Meteorologie und Klimaforschung**
Universität Karlsruhe
Forschungszentrum Karlruhe
GERMANY

SPARC Data Assimilation Workshop, Toronto, September 4 2007

Environment Canada Environnement Canada

FIMK

YORK U

.be

Canada

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)

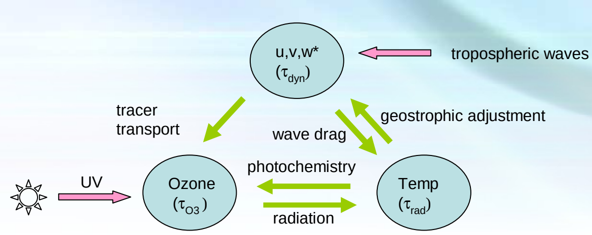
- Early beginnings of DA
  3D Var , OI (data window 6 hr)

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 <u>causality</u> and physical laws

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

Data assimilation methods are based on <u>information</u> content and its transfer (time, space, variables)

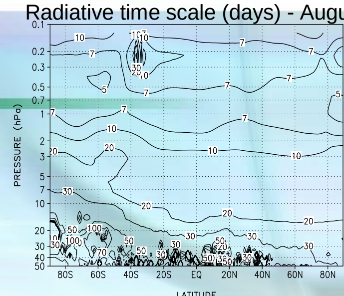
flow of information ≠ causality

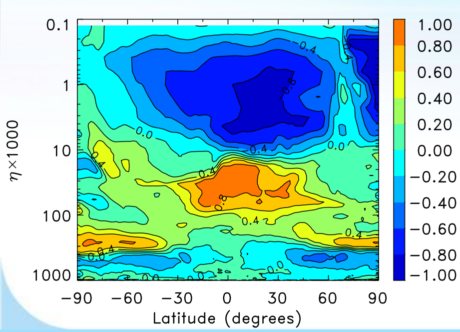
e.g. deducing winds from chemical tracer observations

Cross-error covariance Temperature-Ozone

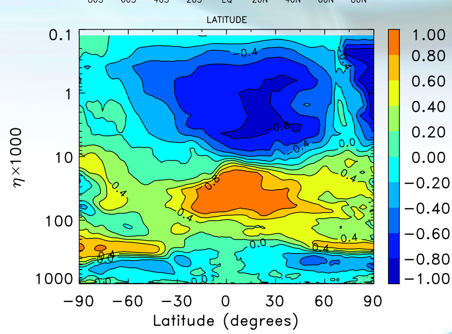
Method: 6-hr differences (CQC)

Radiative time scale (days) - August





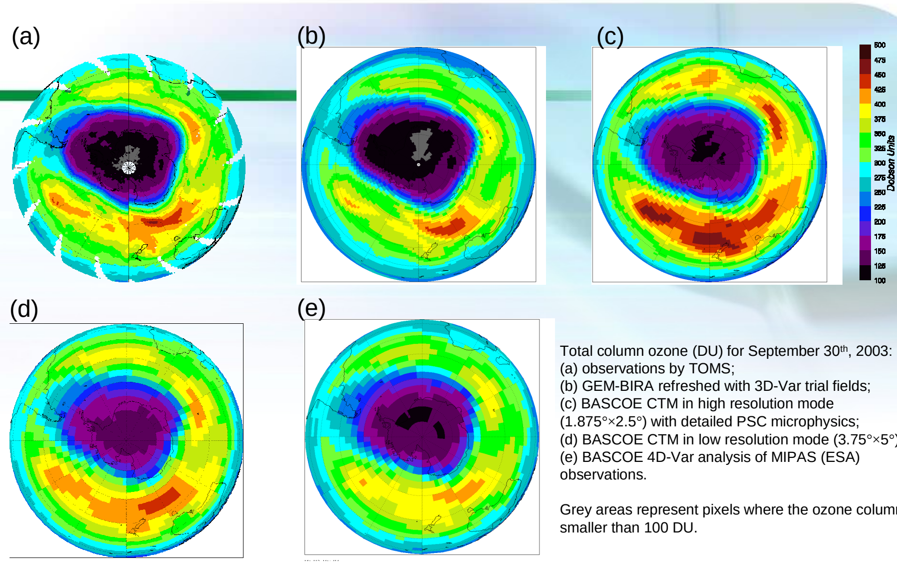
without ozone-radiation interaction



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

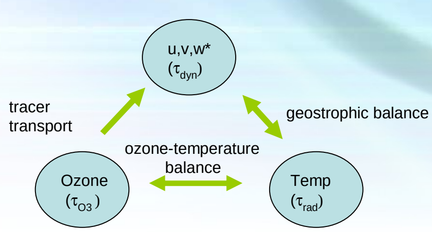


Total column ozone (DU) for September 30th, 2003:
(a) observations by TOMS;
(b) GEM-BIRA refreshed with 3D-Var trial fields;
(c) BASCOE CTM in high resolution mode (1.875°×2.5°) with detailed PSC microphysics;
(d) BASCOE CTM in low resolution mode (3.75°×5°);
(e) BASCOE 4D-Var analysis of MIPAS (ESA) 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° x 1.5° 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 and 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_2
- 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

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

- 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_2O, CO_2, O_3, N_2O, CH_4, CFC-11 -12 -113 -114 sulfate aerosols, sea salt, and dust.
  So far O3 and H2O advected species are online

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

Chemistry

Either

- Ozone climatology (Fortuin and Kelder 1998)

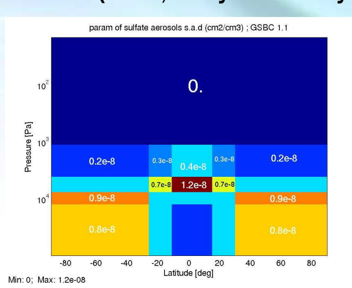
- Parametrization of water vapor due to methane oxidation (ECMWF) with a height dependent relaxation time scale ~ 100 days at the stratopause, ~ 2000 days at 10 hPa, infinite at the tropopause

or

BASCOE chemistry

- **57 chemical species, all advected (S-L)**
- **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 reactions; 7 heterogeneous reactions**
- **52 photodissociation reactions, *J* interp from tables**
- **Photochemical rates are taken from JPL-2002**
- **Solver generated by KPP (Sandu and Sander, 2006)**
- **Numerical method: 3^{rd} – order Rosenbrock**
- **45-min timesteps divided into sub-timestep**

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



- **PSC : T < 194 K → NAT PSC with s.a.d. = 1.e-7 cm^2/cm^3**
  T < 186 K → ICE PSC with s.a.d. = 1.e-6 cm^2/cm^3
  (+ loss of H2O/HNO3 due to sedimentation)

Ozone-radiation

- Assimilation of temperature

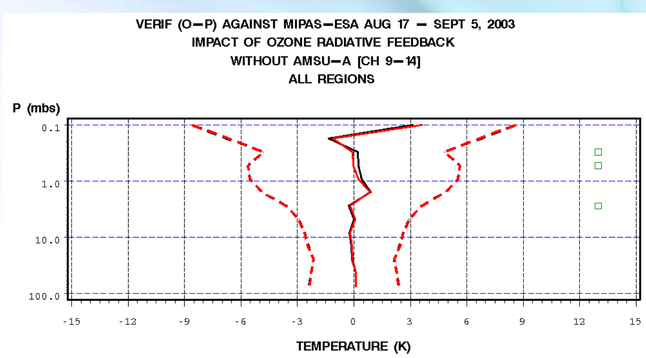
  Impact on analyses
  Impact on 10-day forecasts

- Assimilation of ozone and temperature

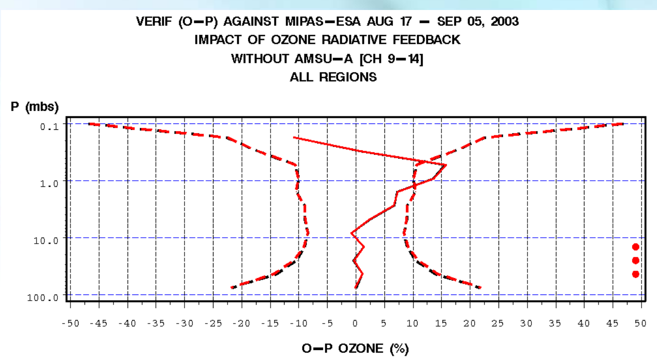
  Impact on analyses
  Impact on 10-day forecasts

Assimilation of Temperature: Impact on analyses

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



red : ozone-radiation black : no interaction



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

|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---------------------| ANALYSES

|---------------| (24hr)

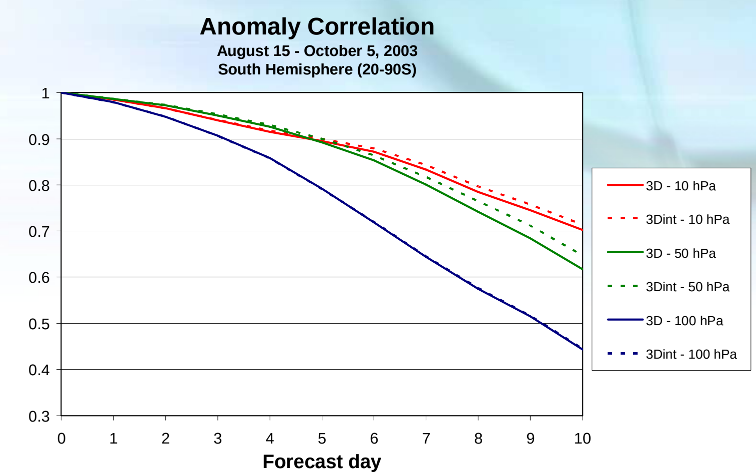
|------------------------------| (48hr) FORECAST

| ---| (72hr)

ANOMALY CORRELATION *r*

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

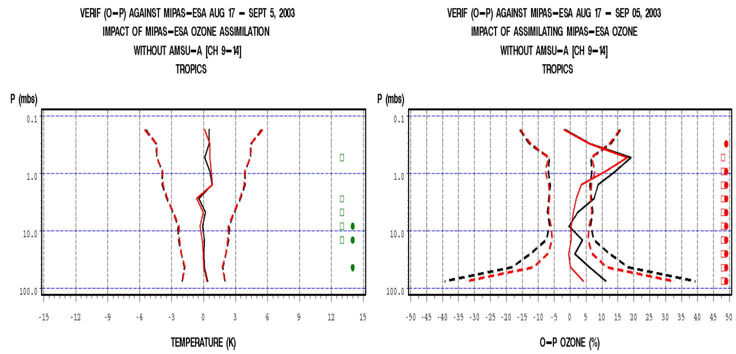
04/09/2007 Coupled chemical-dynamical data assimilation Page 23



04/09/2007 Coupled chemical-dynamical data assimilation Page 24

Assimilation of Ozone and Temperature: Impact on analyses

tropics

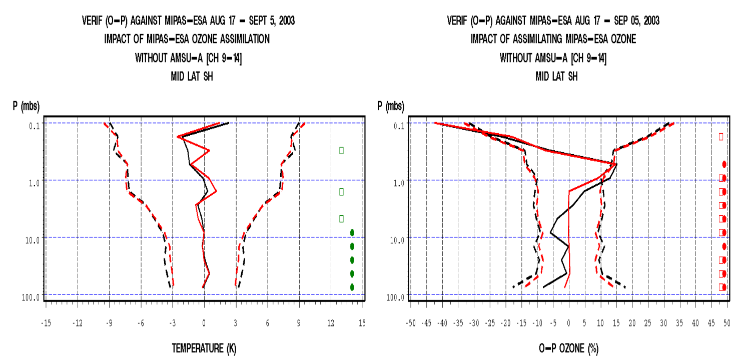


ozone-radiation interaction on

red : temperature + ozone assimilation

black : temperature only assimilation

mid-latitudes SH

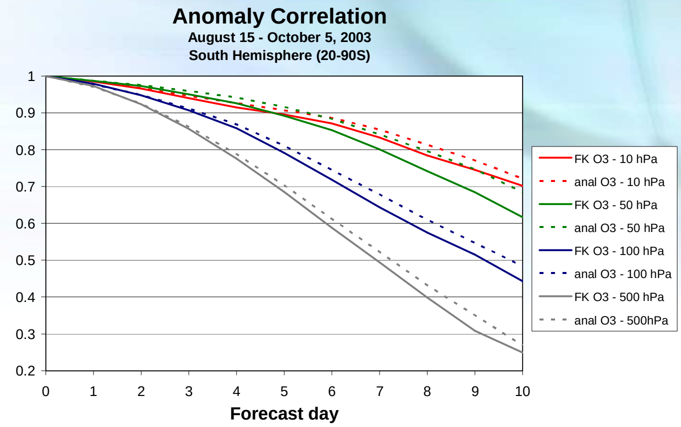


ozone-radiation interaction on

red : temperature + ozone assimilation

black : temperature only assimilation

Assimilation of Ozone and Temperature: Impact on forecasts



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 developped 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. $\overline{(\mathbf{y} - H(\mathbf{x}_b))} = \overline{\mathbf{y}}$

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

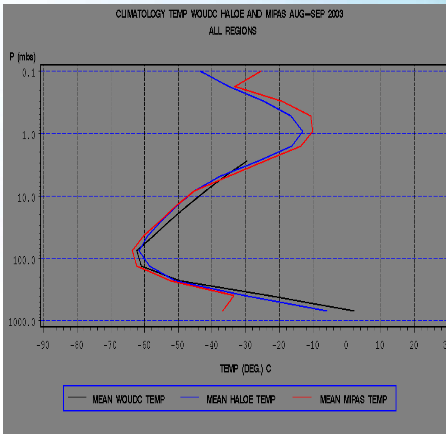
Can we use the same assumption in the stratosphere ?

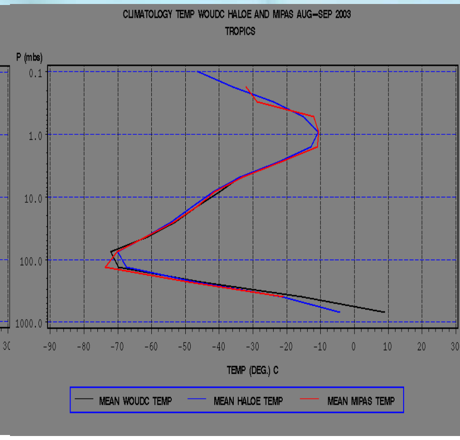
- Radiosondes measurements typicaly reach not much higher than 30 hPa
- Large uncertainties in stratospheric modeling due to gravity wave drag parametrization

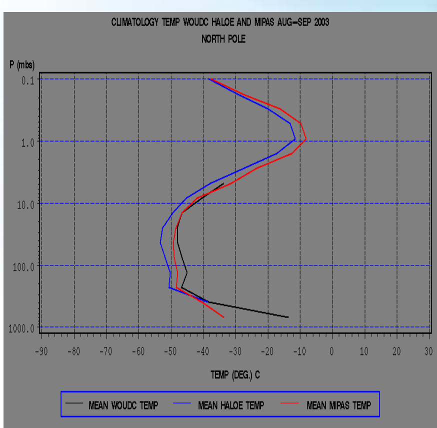
Anchoring the reference solution with MIPAS obs.

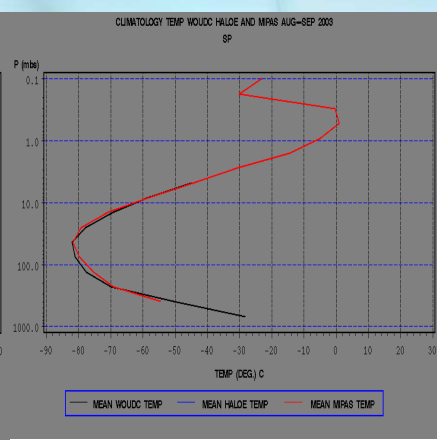
Assimilation of MIPAS temperatures used to anchor the solution and develop the bias correction coefficient

Quality of MIPAS temperature observations







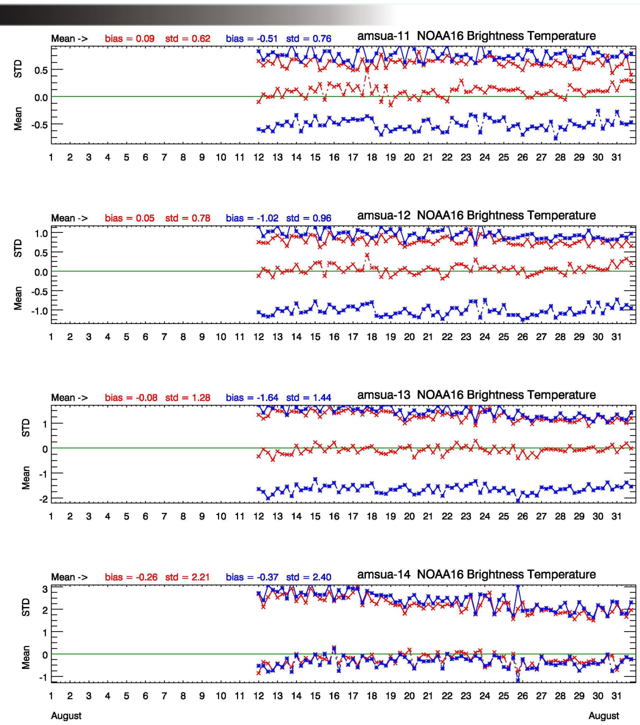


HALOE and WOUDC have limited coverage here so cannot conclude

No HALOE date here

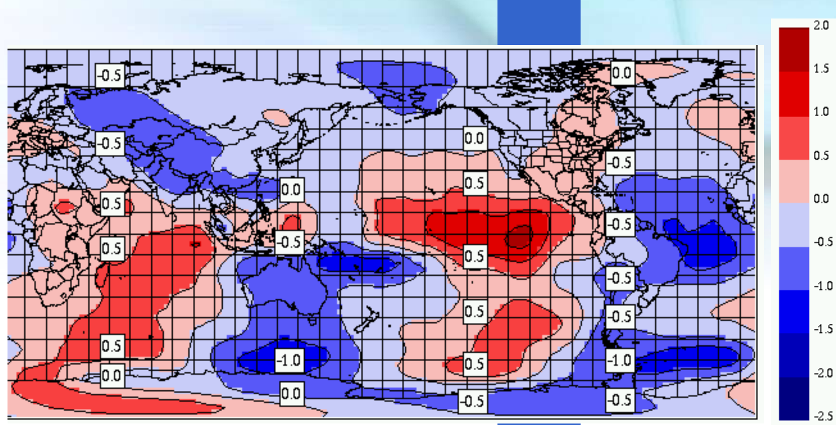
Experiments: bias correction of stratospheric radiances (A3es0319)

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



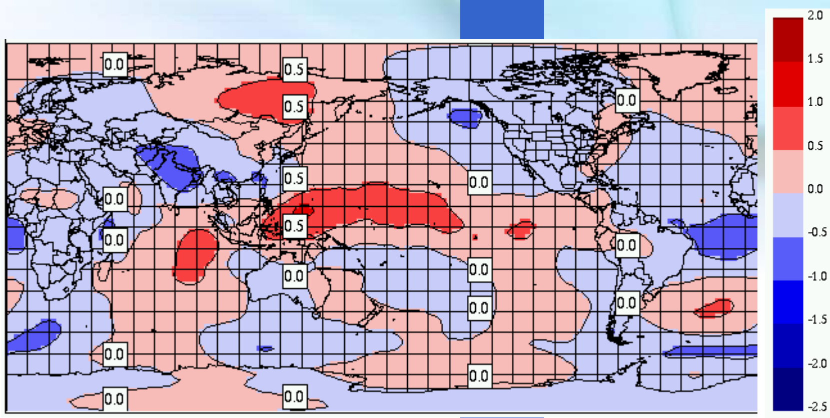
Mean analysis temperature increments at

No bias correction of AMSU-a channels 11-14 (September 2003)



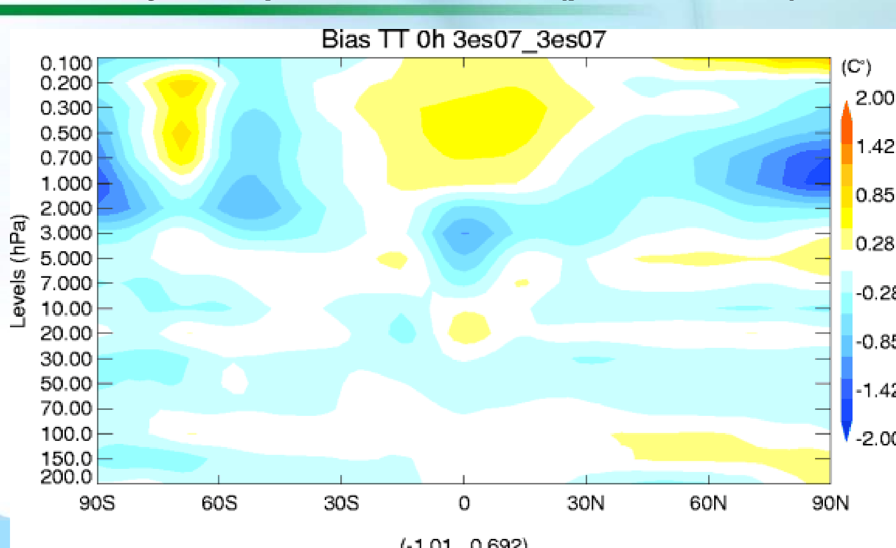
Mean analysis temperature increments at

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



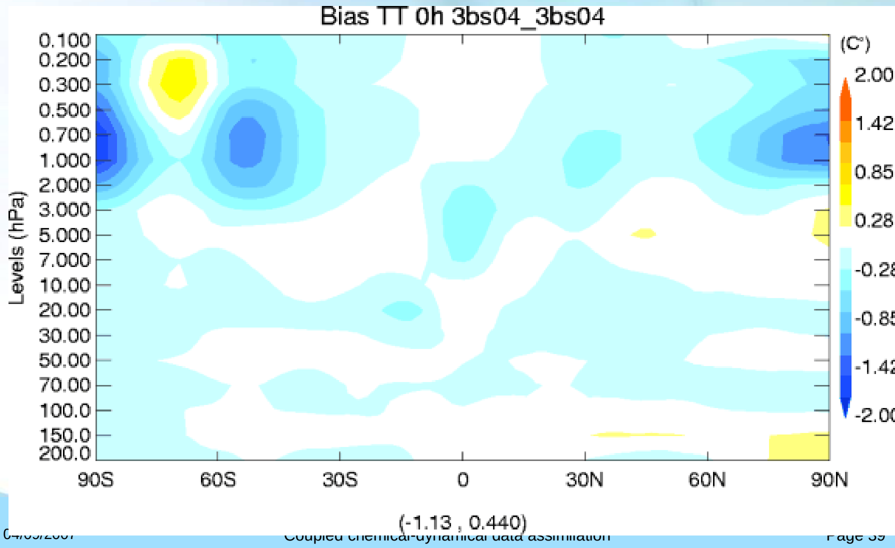
Experiment without any bias correction

Mean analysis temperature increments (previous results)



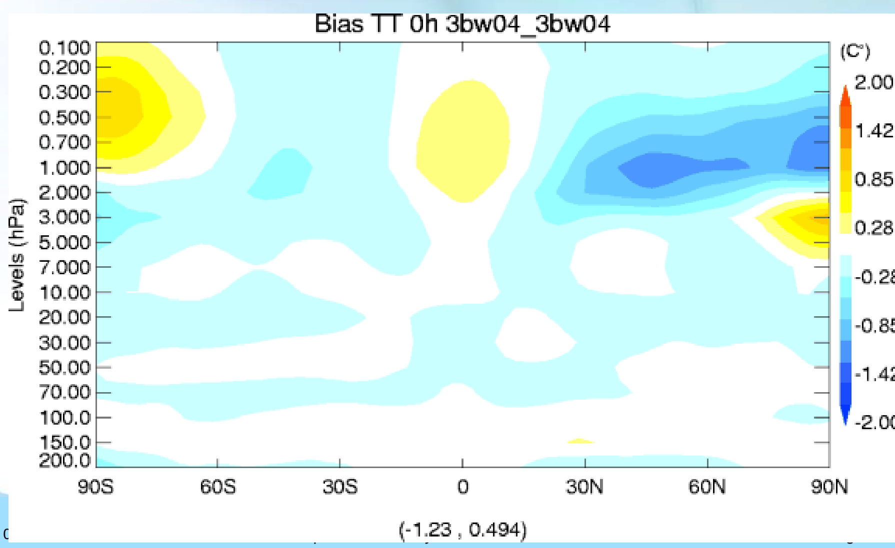
Experiment with the revised bias correction

Mean analysis temperature increments (September 2003)



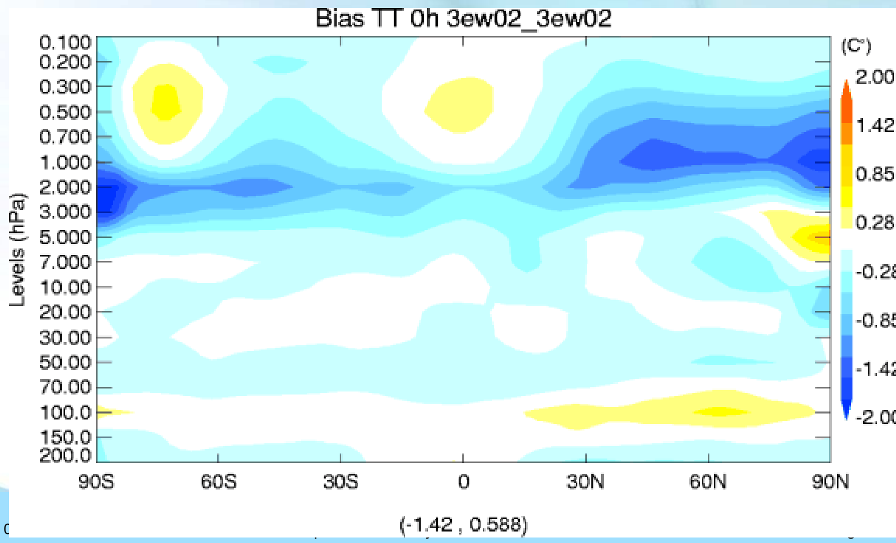
Revised bias correction (winter)

Mean analysis temperature increments (January 2003)



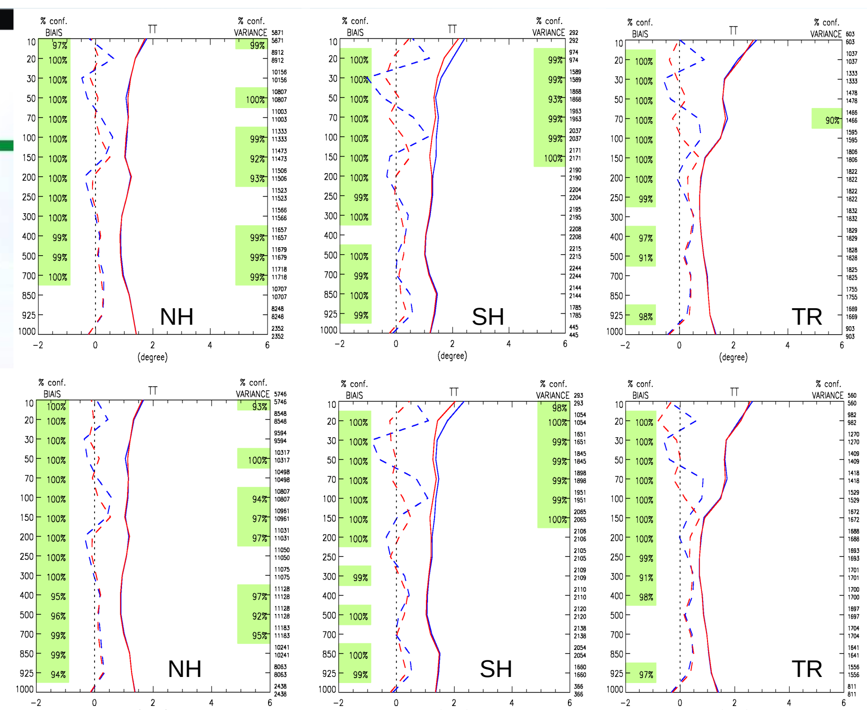
Without bias correction (winter)

Mean analysis temperature increments (January 2003)



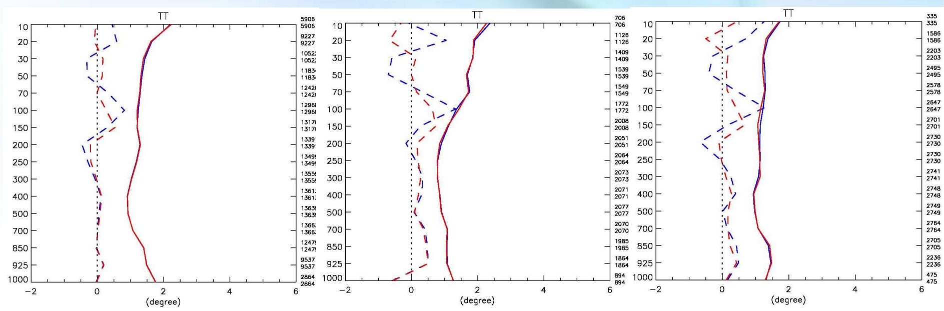
Aug 11th – Sept 5th

Sept 6th – Sept 30th



Validation against radiosondes

Winter period (62 cases in January 2003)



northern hemisphere tropics southern hemisphere

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
Environment Canada
Environnement Canada
FIMK
YORK U
.be
Canada