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International study group

Added-value of chemical data assimilation in the stratosphere and upper-troposphere

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College Park, September 2, 2015

International Team

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- *Sergey Skachko* (BIRA, Belgium)
- *Michiel van Wheele* (KNMI, Netherlands)

Multi-disciplinary

- ❖ Chemical Data Assimilation
- ❖ Observations
- ❖ Chemical transport modeling
- ❖ Diagnostics
- ❖ Processes
- ❖ Ozone-radiation interaction

Links with

- ❑ SPARC Data Assimilation workgroup
- ❑ SPARC Data Initiative workgroup
- ❑ SPARC Renanalysis workgroup
- ❑ SPARC High-Energy-Particle Precipitation in the Atmosphere (HEPPA) workgroup
- ❑ Ozone-CCI (Climate Change Initiative)

Chemical Data Assimilation (CDA)

CDA for reanalysis

- integrate multi-species from multi-sensors
- resolve sampling issues

CDA to estimate ozone loss

- discriminate transport effects from chemistry effects

CDA to capture poorly modeled processes

- capture production and transport (descent) of NO_2

CDA as an initial value estimation

- Stratospheric ozone forecast

CDA coupling to NWP

- Weak coupling: ozone-radiation interaction
- Strong coupling: tracer observations to determine winds

Core CDA system for the project

- Belgium CTM with 4D-Var full chemistry ,
  EnKF tracer ,
  EnKF full chemistry

- Optimality tuned error statistics
  In observation space : $\chi 2$, Desroziers ,
  In model space : NMC , Perturbed assimilation cycles (Fisher 2003)

- Share same elements as the Canadian meteorological DAS
  - Non separable spectral error correlations
  - Observation perturbation EnKF

- Sequential filter – tracer using Prather scheme

- Canadian NWP model GEM with 3D-Var. Linearized ozone chemistry
  Belgium CTM chemistry

Improvement in error covariances

- spectral error covariances (non-separable)
- tuning of the error variances

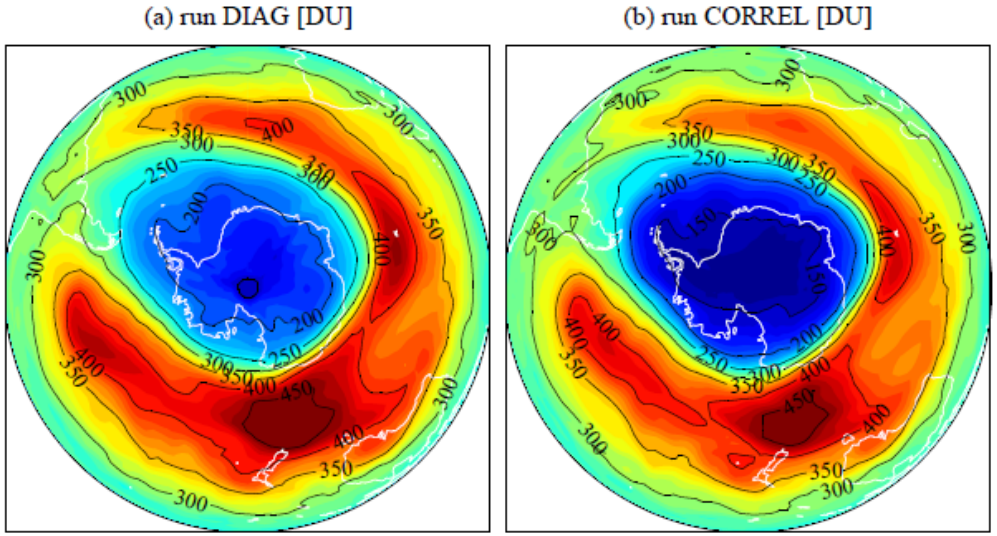


Fig. 6. Total ozone in the Southern Hemisphere on 1 October 2003 obtained by the runs D
Total Ozone Measurement Satellite (TOMS) (c), in Dobson unit (DU).

Errera and Ménard (2012) ACP

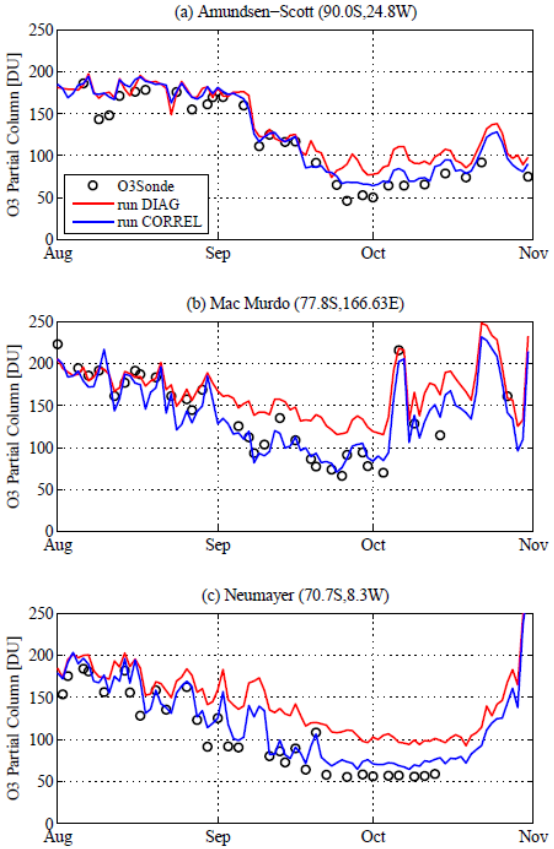


Fig. 5. Time series of the ozone partial column (10–100 hPa) between August and October 2003 obtained above three NDACC stations in Antarctica by the ozone sondes (black circles), and the runs DIAG (red line) and CORREL (blue line), in Dobson unit (DU).

Belgian Assimilation System for Chemical ObsErvations – Var (BASCOE-4Dvar)

BASCOE

- 4D-Var system dedicated to stratospheric chemical observations
- CTM including 58 species, ~200 chemical reactions, PSC parameterization
- **B** matrix: Homogeneous and isotropic correlations (Courtier et al., QJRMS, 1998; Errera and Ménard, ACP, 2012)
- Source of Mesospheric NO_x NOT modelled

Dynamic

- ECMWF ERA-Interim

Resolution

- 3.75° long x 2.5° lat x 37 levels (surf. to 0.1 hPa) x 30 minutes

Assimilation window

- 24h starting at 0Z

Runs

- Assimilation of MLS & MIPAS/ESA: April 2007 – April 2012

Assimilated data in REAN01

Families		*Species*	MLS 2004-present	MIPAS 2002-2012	SCIA 2002-2012	GOMOS 2002-2012	SMR 2001-present	OSIRIS 2001-present
Oxygen		O3	x	x	x	x	x	x
	Hydrogen	H2O	x	x			x	
		CH4		x				
		OH	x					
	Nitrogen	N2O	x	x			x	
		HNO3	x	x				
		NO2		x	x	x		x
		NO		x (IMK/IAA)				
		N2O5		x				
		ClONO2		x				
	Chlorine	ClO	x	x (IMK/IAA)			x	
		HOCl	N/A	x (IMK/IAA)				
		HCl	x					
Bromine		BrO	N/A		x			
	CFCs	CFC11		x				
		CFC12		x				
		...						

In green: assimilated data
In red: Not assimilated

N/A: data available but not suited for assimilation

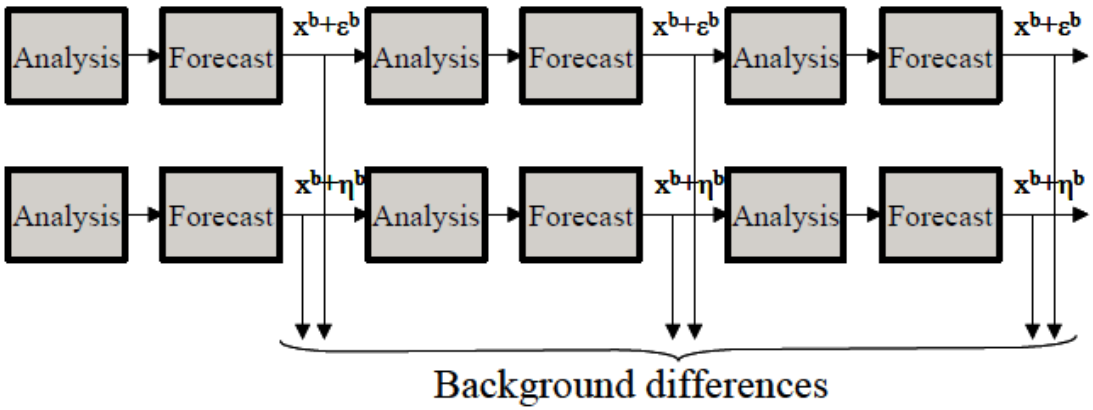
Improving REAN01 (towards REAN02)

Comparison of CDA when assimilating different instruments

- MLS and MIPAS
- N2O and CH4

Importance of

- B - background error covariance. Has been re-estimated



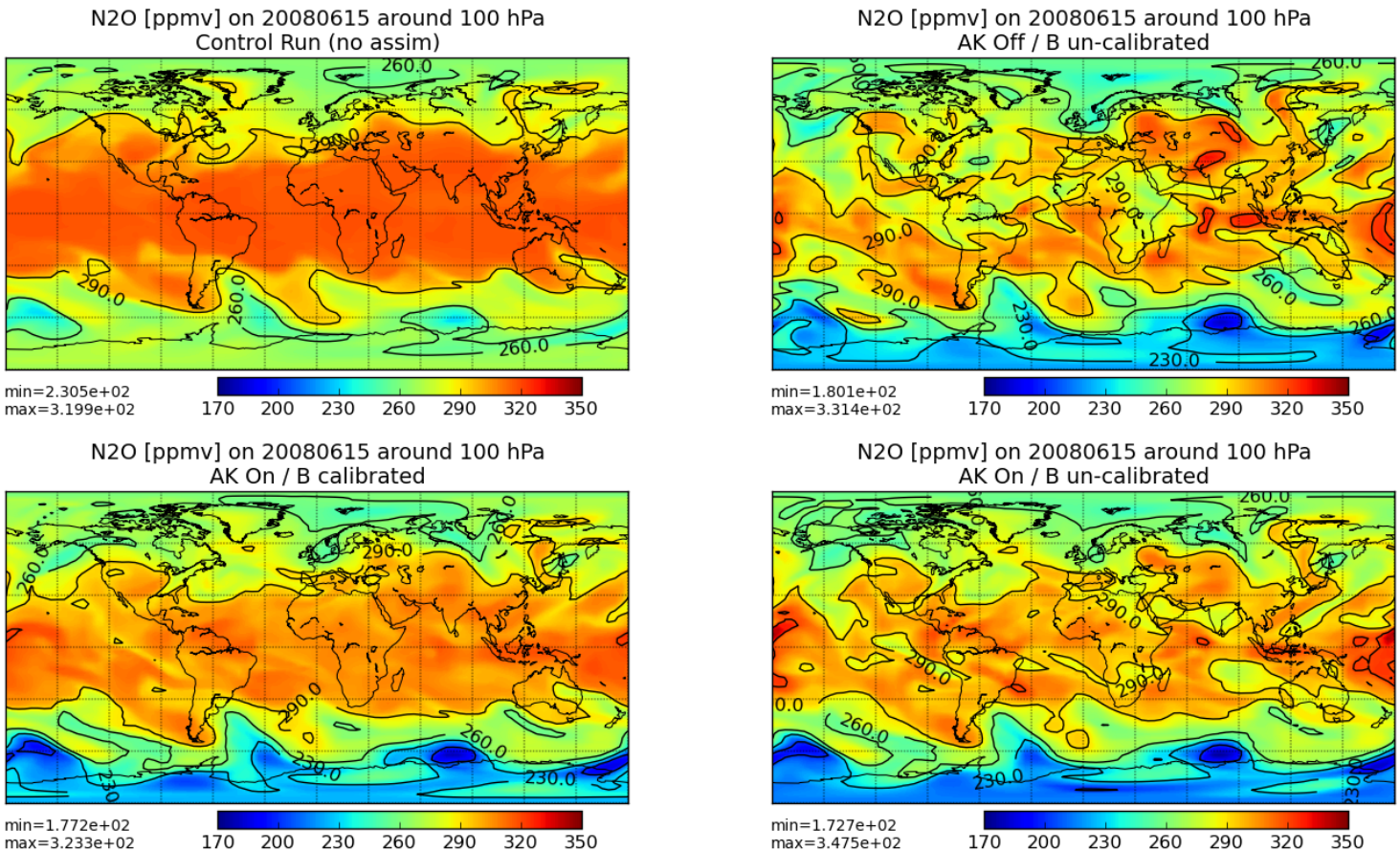
the background differences have the same correlation structure as B but twice the error variance

- Averaging kernels
- o Quality control

Impact of Averaging kernels and calibration of B : N_2O MIPAS

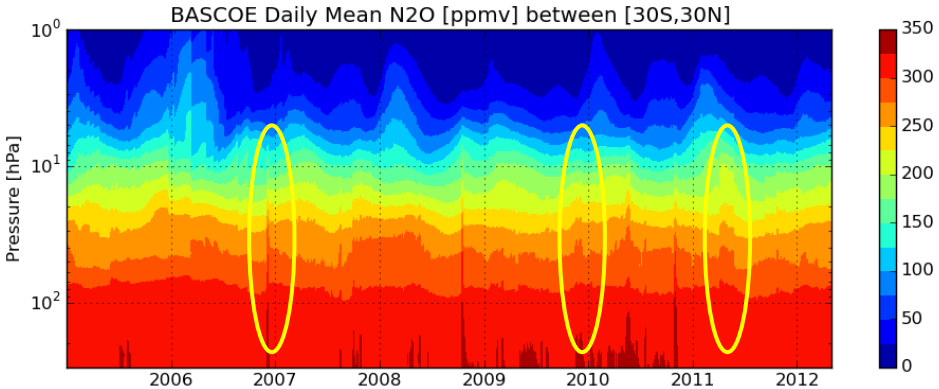
- N_2O analysis at 100 hPa for different config of BASCOE

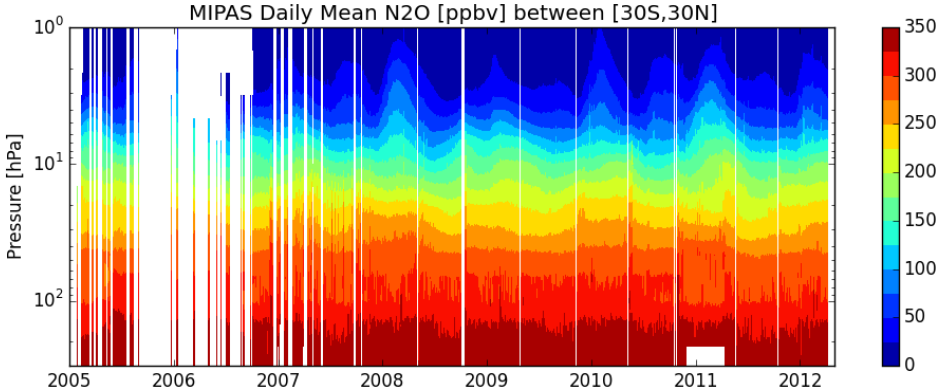
  => *AK and calibrated B are important*

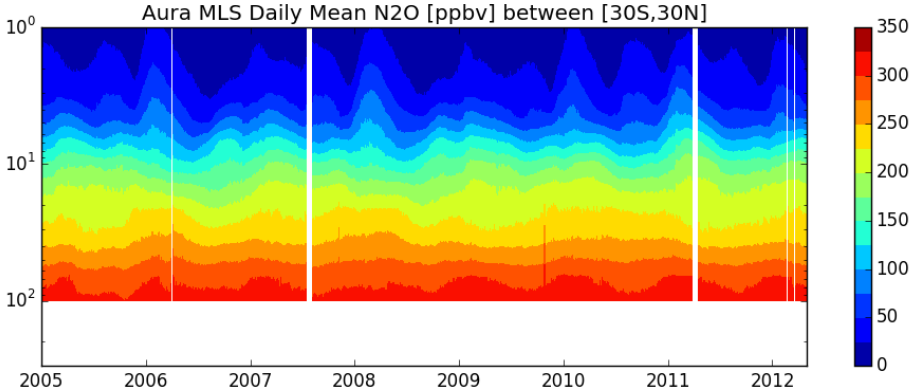


Time stability of reanalysis: Assim N_2O MIPAS vs Assim N_2O MLS

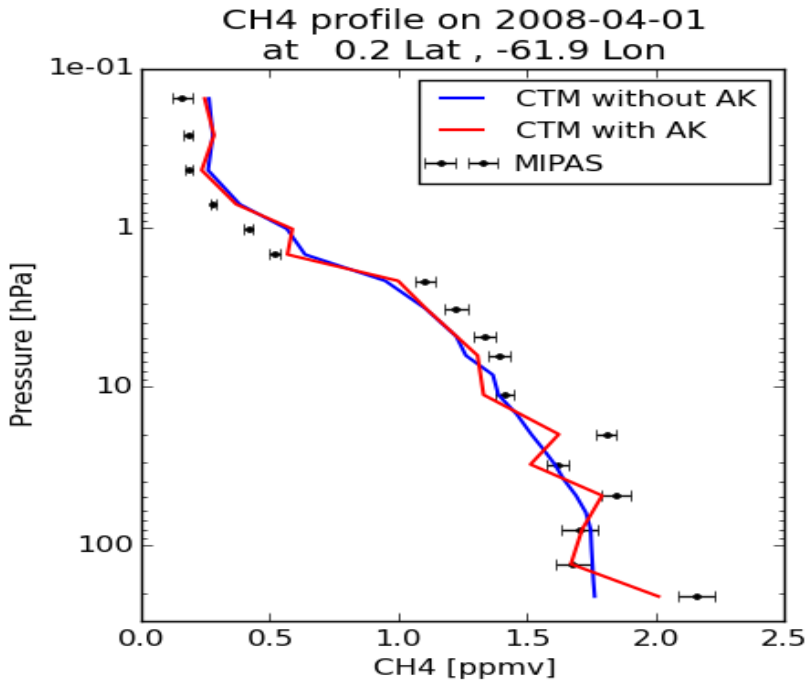
- Time series of reanalysis is “noisy” at some dates
- This noise is due to noisy MIPAS data
- Quality control of O-F still needed

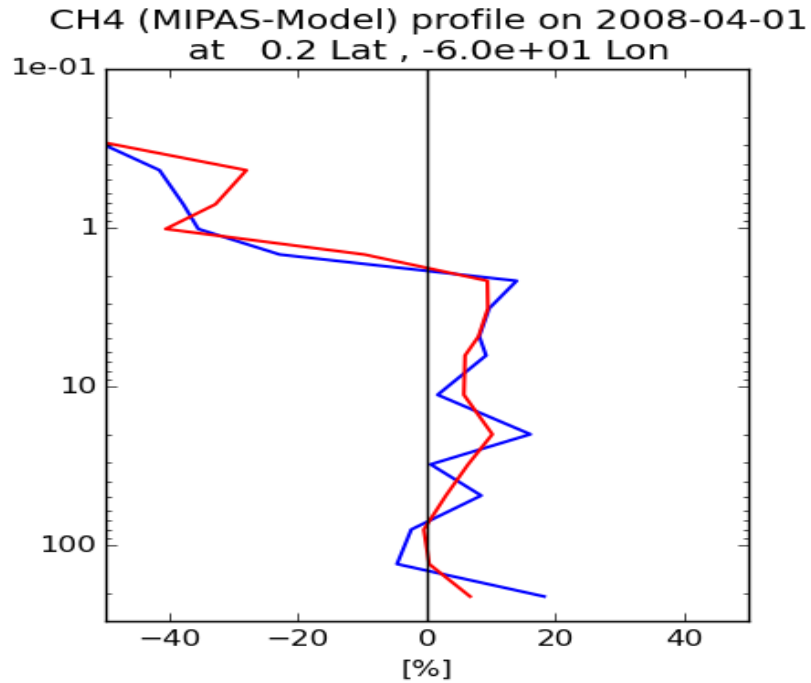


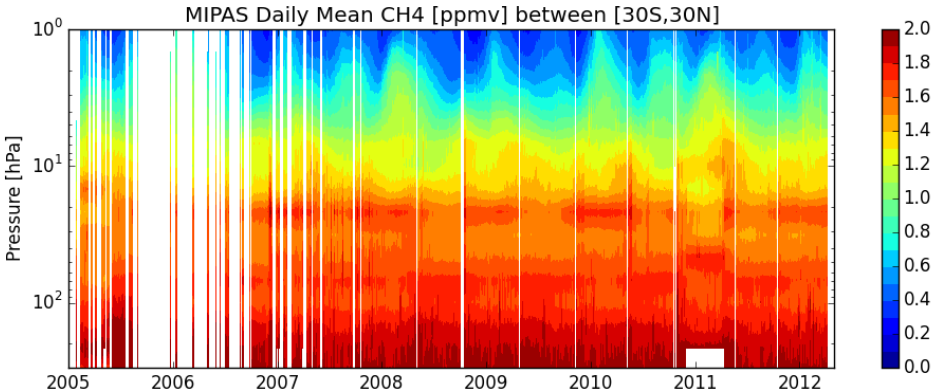


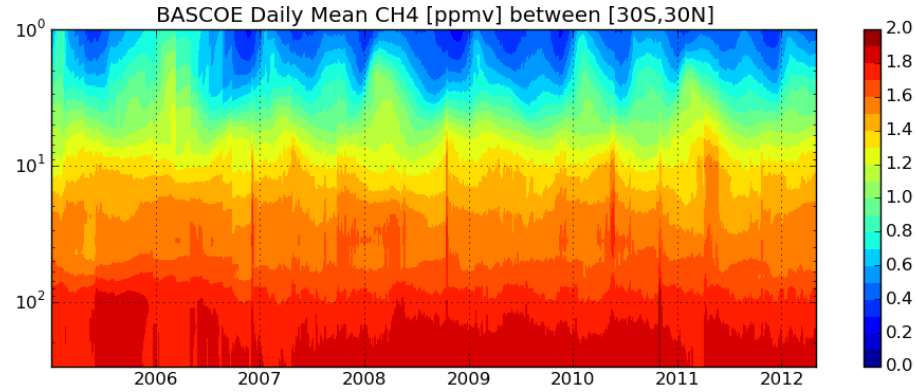


Impact of averaging kernels for CH_4 MIPAS



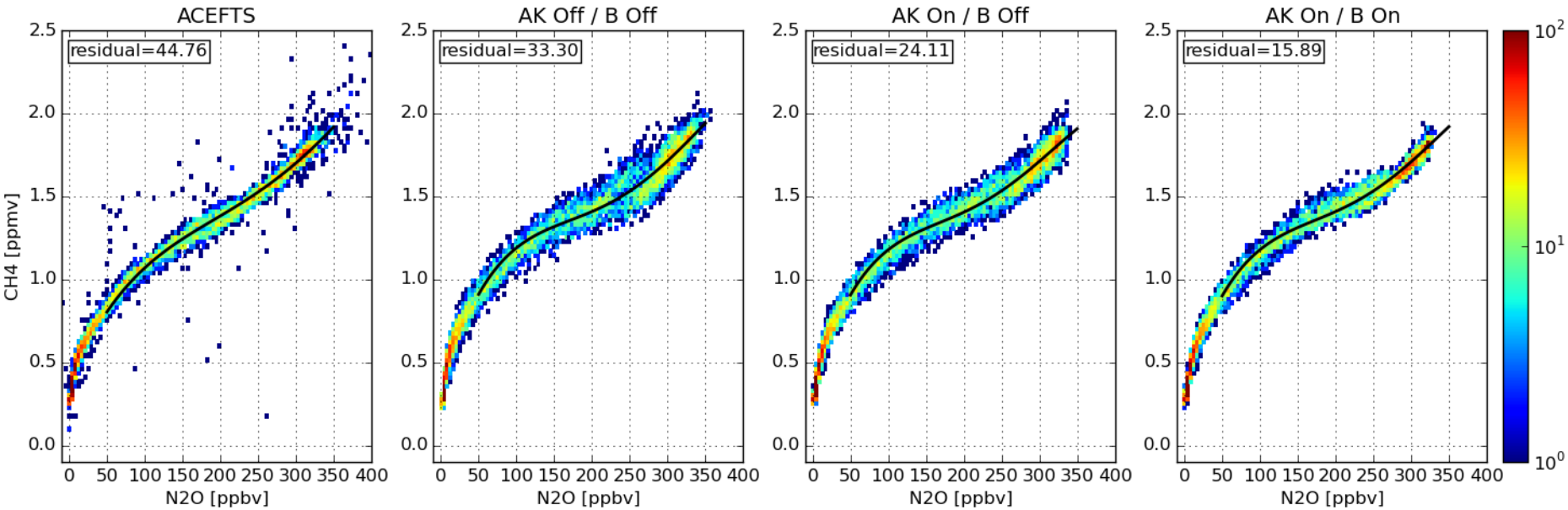






N_2O-CH_4 correlations in 2010 between 30°S-30°N

- Using AK and calibrated **B**, correlations are much compact, in particular in the lower stratosphere
- Better agreement with ACEFTS

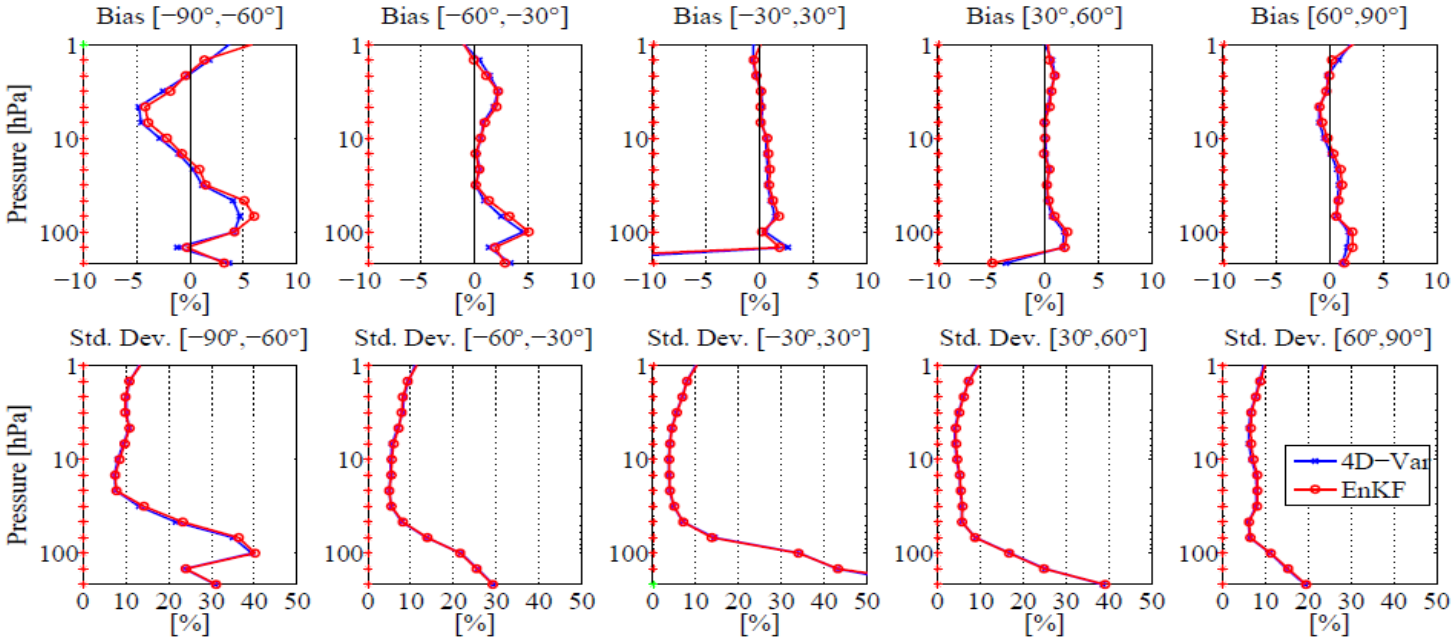


BASCOE – EnKF

EnKF

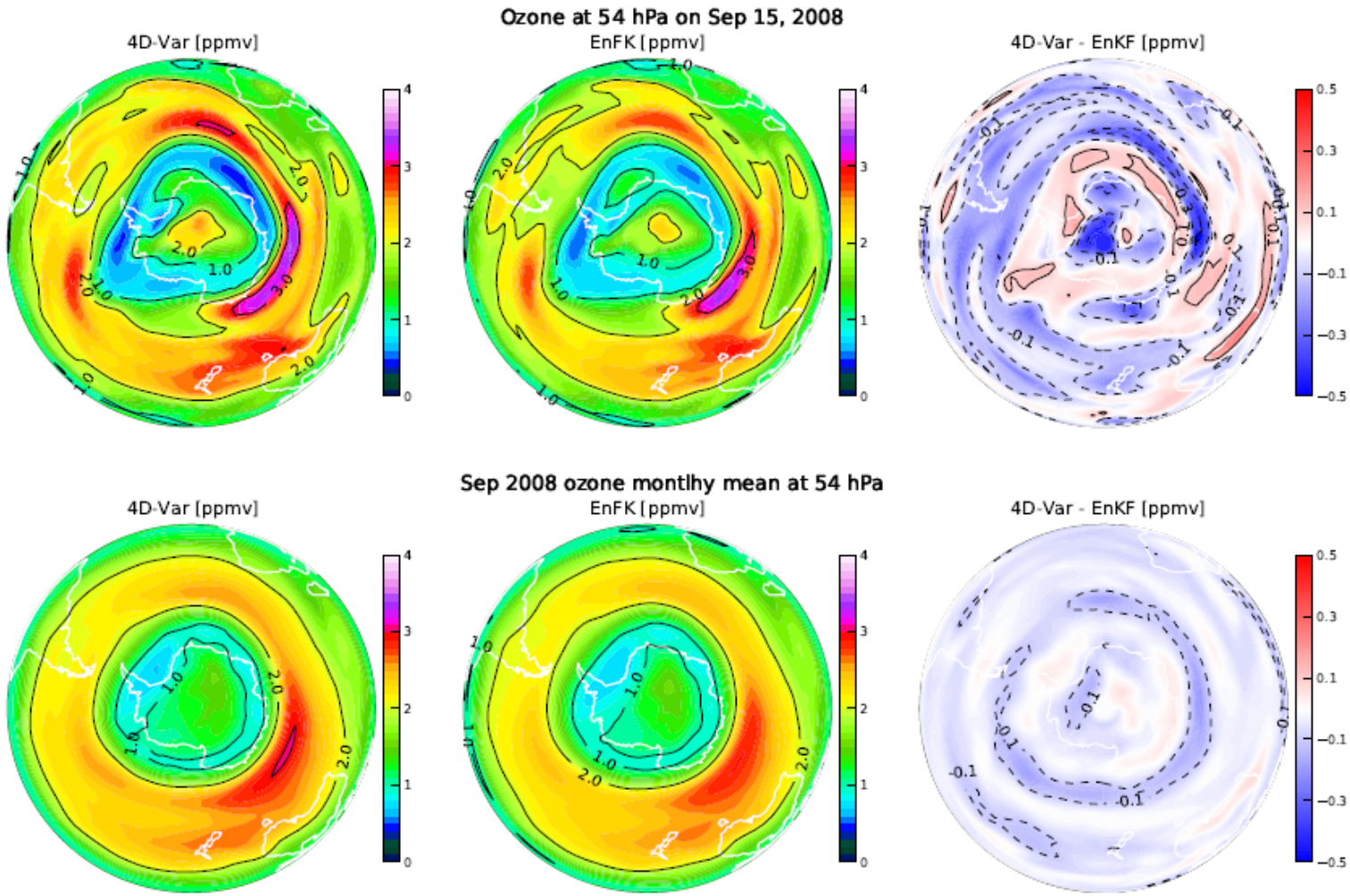
- Using same CTM and framework as BASCOE-4DVar
- Observation perturbation method (Houtekamer and Mitchell 2001) with additive model error

Comparison EnKF-4DVar tracer (O3 assimilation)



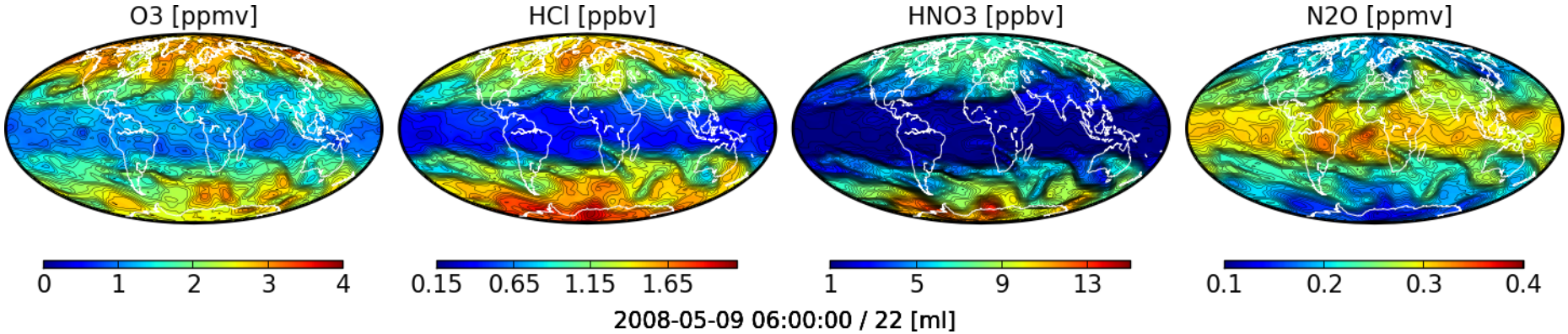
The OmF are computed for September-October 2008

Skachko et al (2014) GMD

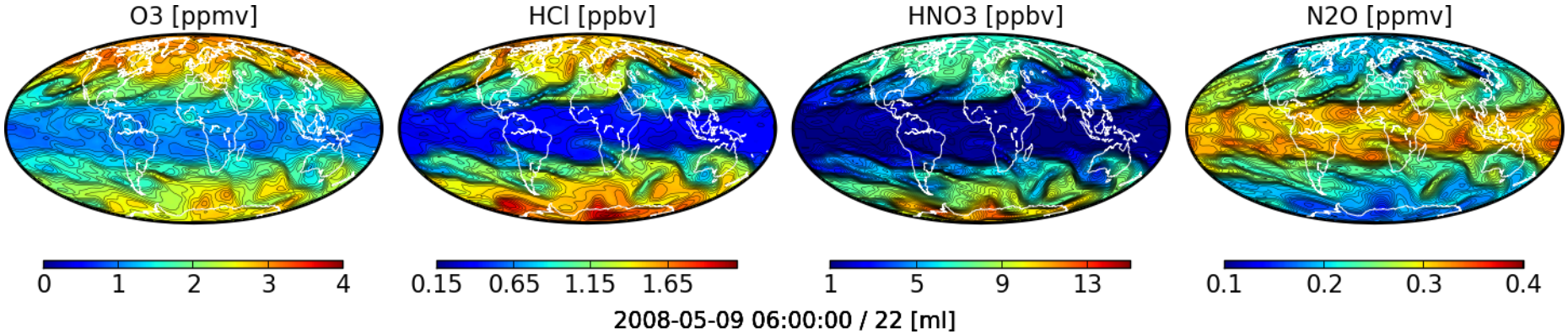


Assimilation of ozone as passive tracer transport, using the same input errors and with model error the EnKF and 4D-Var solutions gives nearly identical O-P zonal statistics, but the EnKF analyses are somewhat smoother than the 4D-Var analyses

BASCOE - EnKF

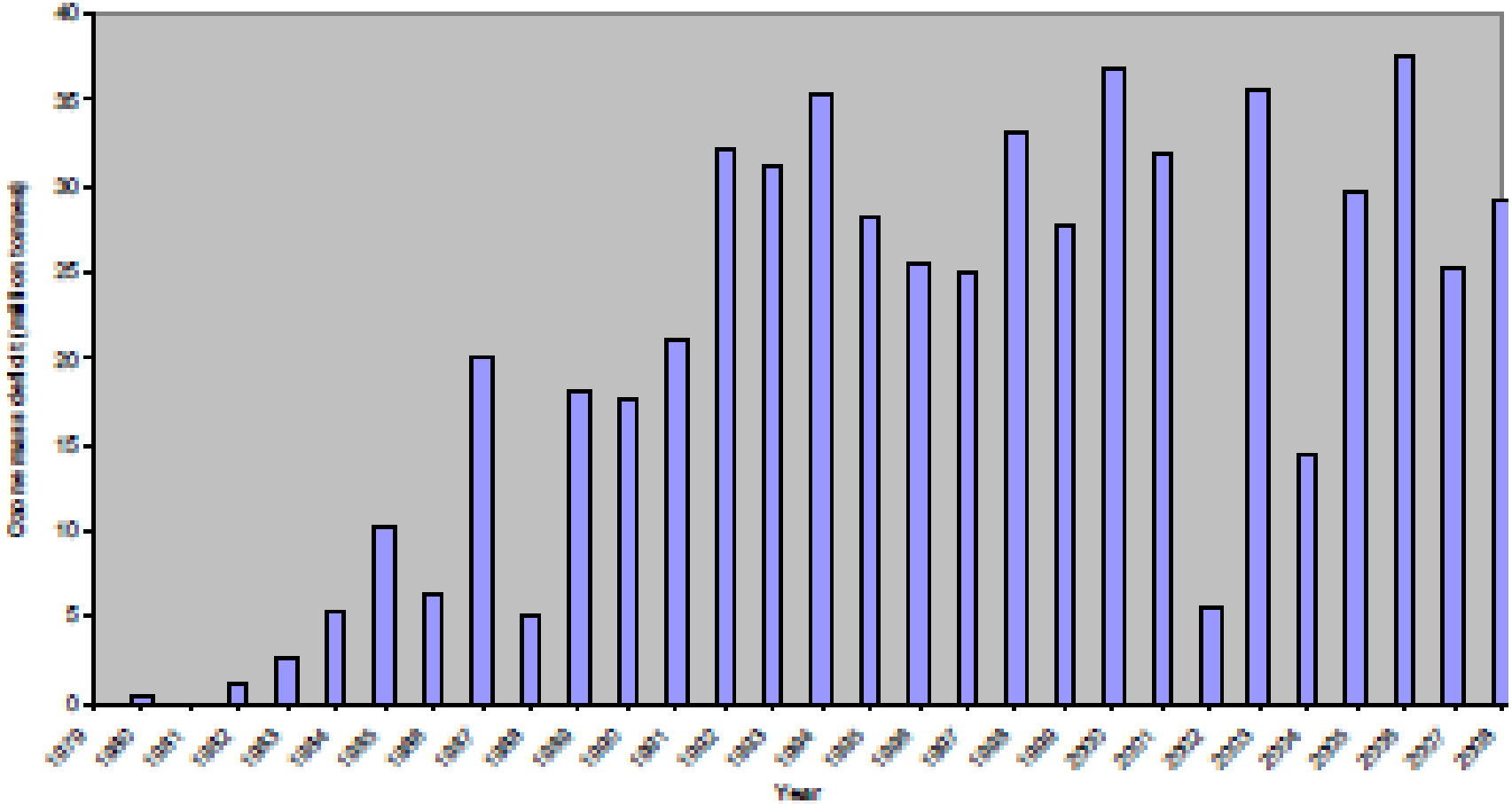


BASCOE – 4D-Var



Assimilation of nadir observations : Ozone deficit (< 220 DU)

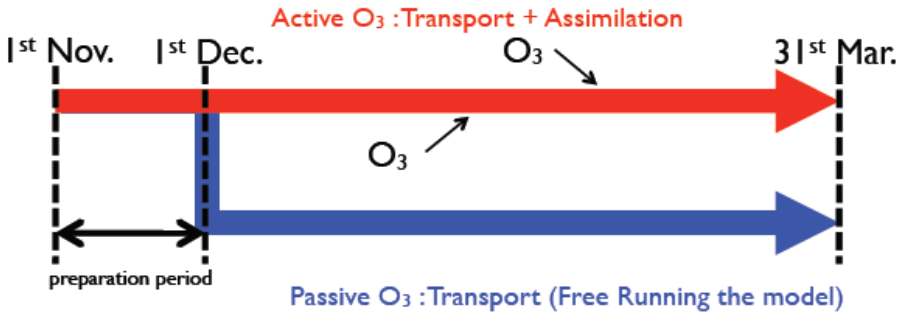
30 year reanalysis. van der A (ACP) 2010



Emerging new methodology using limb sounding measurements

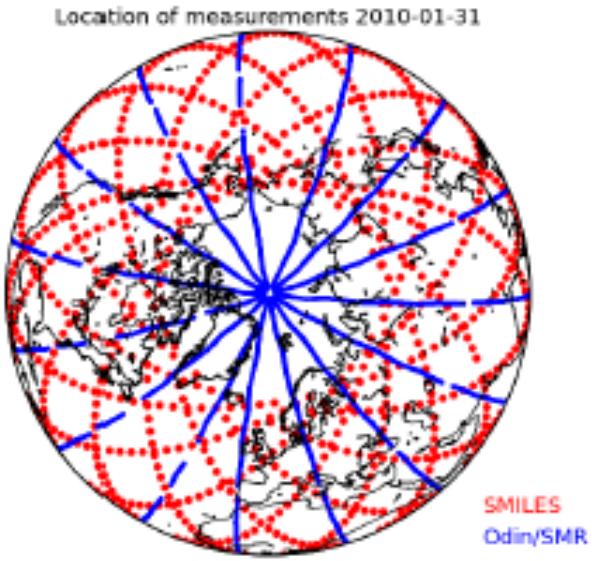
(Rosevall et al. 2007, Sagi et al., ACP 2014)

To separate ozone variation into "transport" and "chemical" processes



$$O_{3loss} = O_{3active} - O_{3passive}$$

ODIN SMR limb measurements



Using an accurate transport model

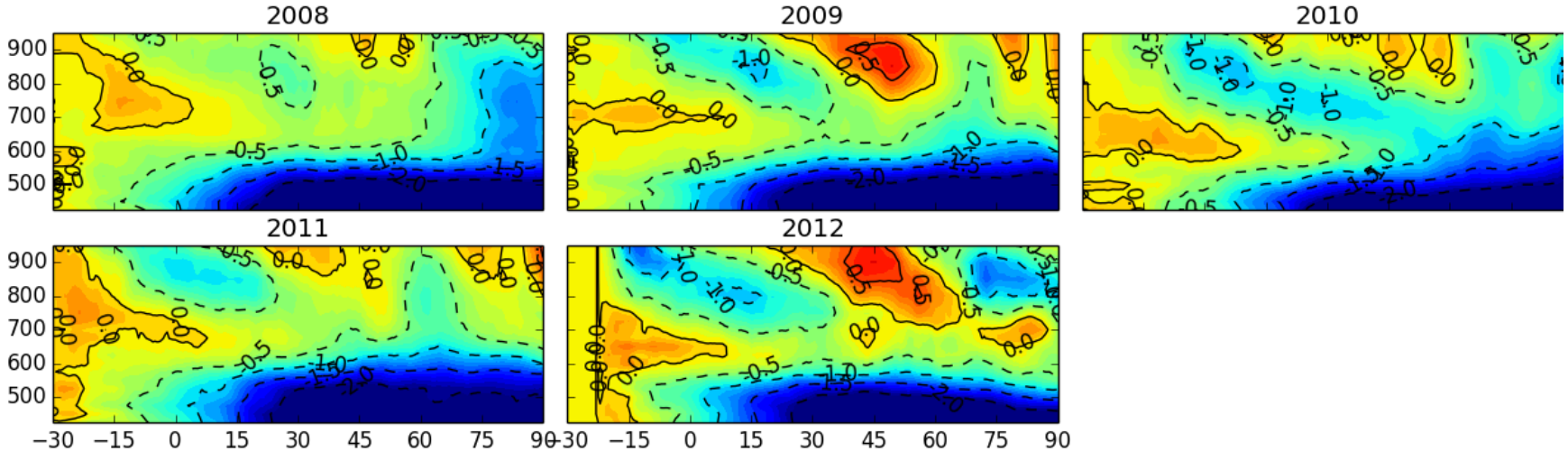
- Prather 2D isentropic
- Vertical upwind scheme driven by diabatic heating

Estimation method

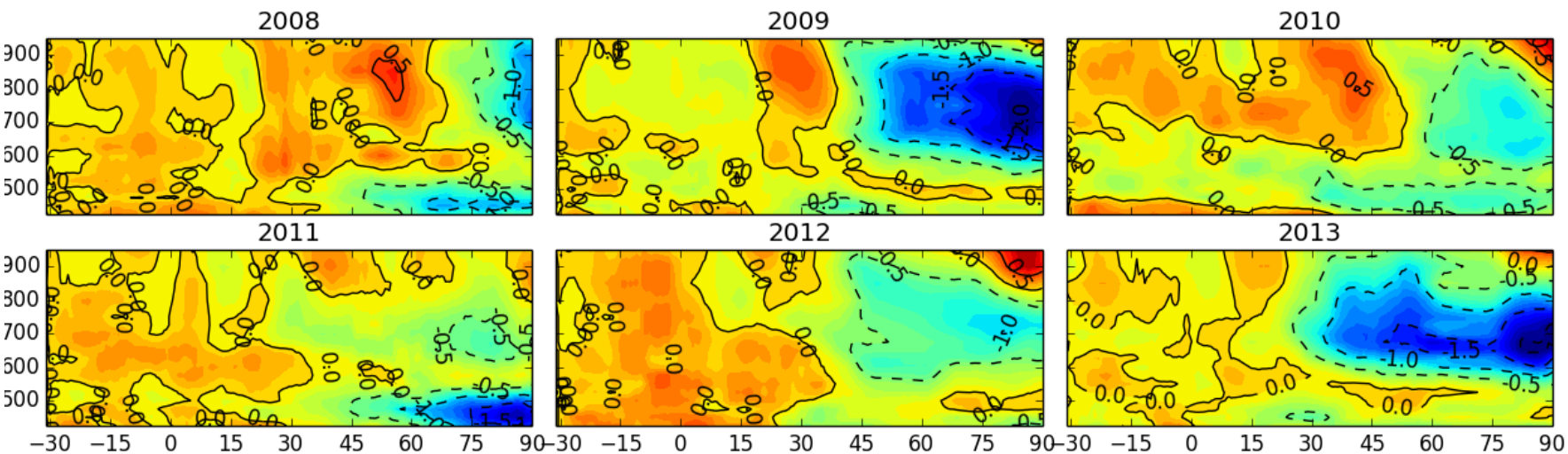
- Estimates of the **chemical** ozone loss

Chemical ozone loss - vortex mean average (70- 90 equivalent latitude s)

Antarctic ozone loss - from December 1st

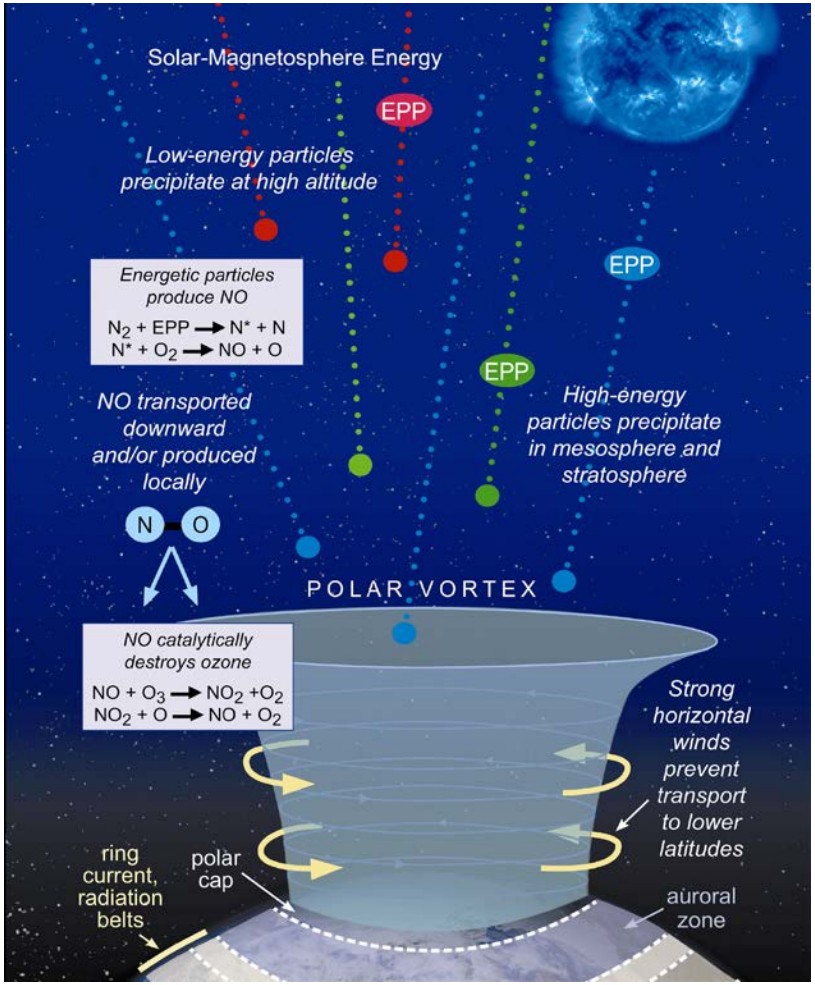


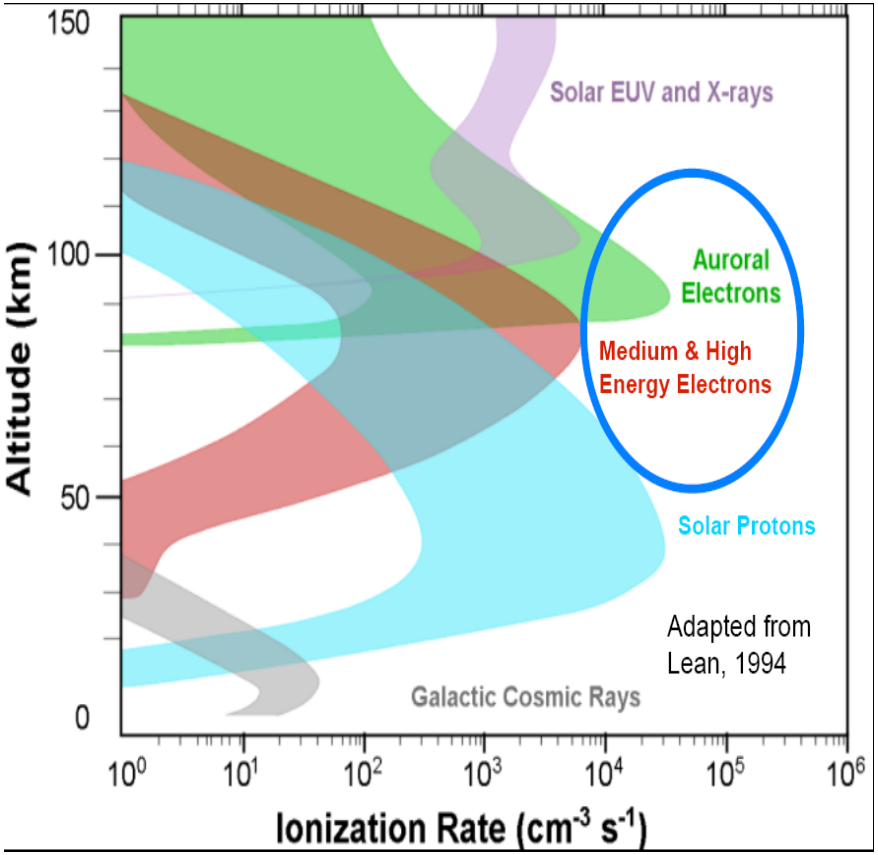
Arctic ozone loss - from August 1st



Another method based on analysis increments (and thus does not requires accurate long-range transport is under development

Energetic particle precipitation impact on the middle atmosphere



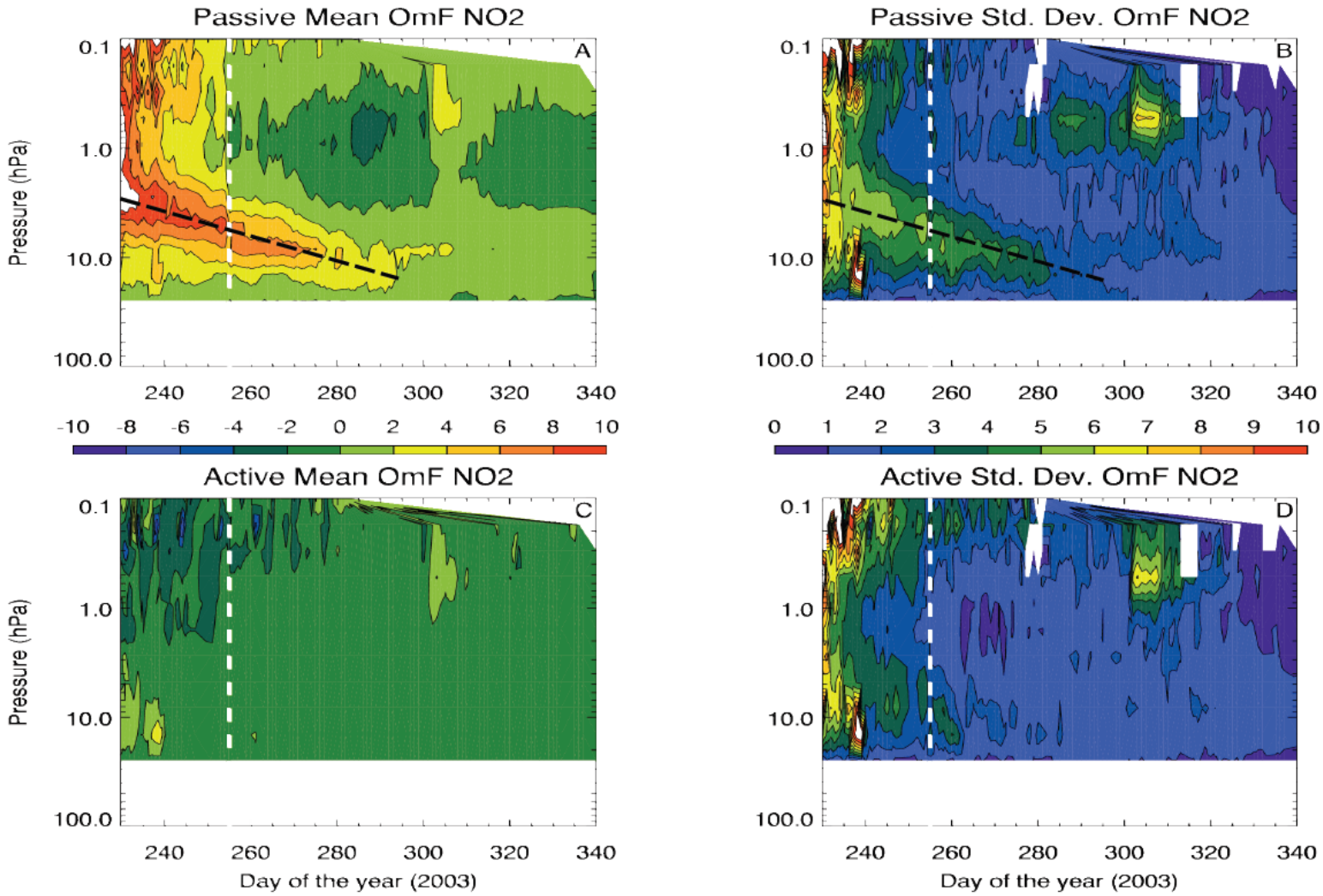


EPP produces NO_x continually, but transport downwards into stratosphere involves interplay with dynamics

- **EPP contribute up to 10% of the stratospheric budget (40% polar regions)**
- **Not well modeled by comprehensive models**
- **EPP-NOx interfere with catalytic cycles involving O_3**
- **Changes in O_3 can lead to changes in temperature and predictability**

Can we assimilate when there is model error bias

Robichaud and Ménard (ACP, 2010) $\bar{\varepsilon}^a_\infty = -\bar{q} \quad ; \quad \overline{(A-F)_\infty} = \frac{k\bar{q}}{1-k} = \left(\frac{\sigma_f^2}{\sigma_0^2}\right)\bar{q}$

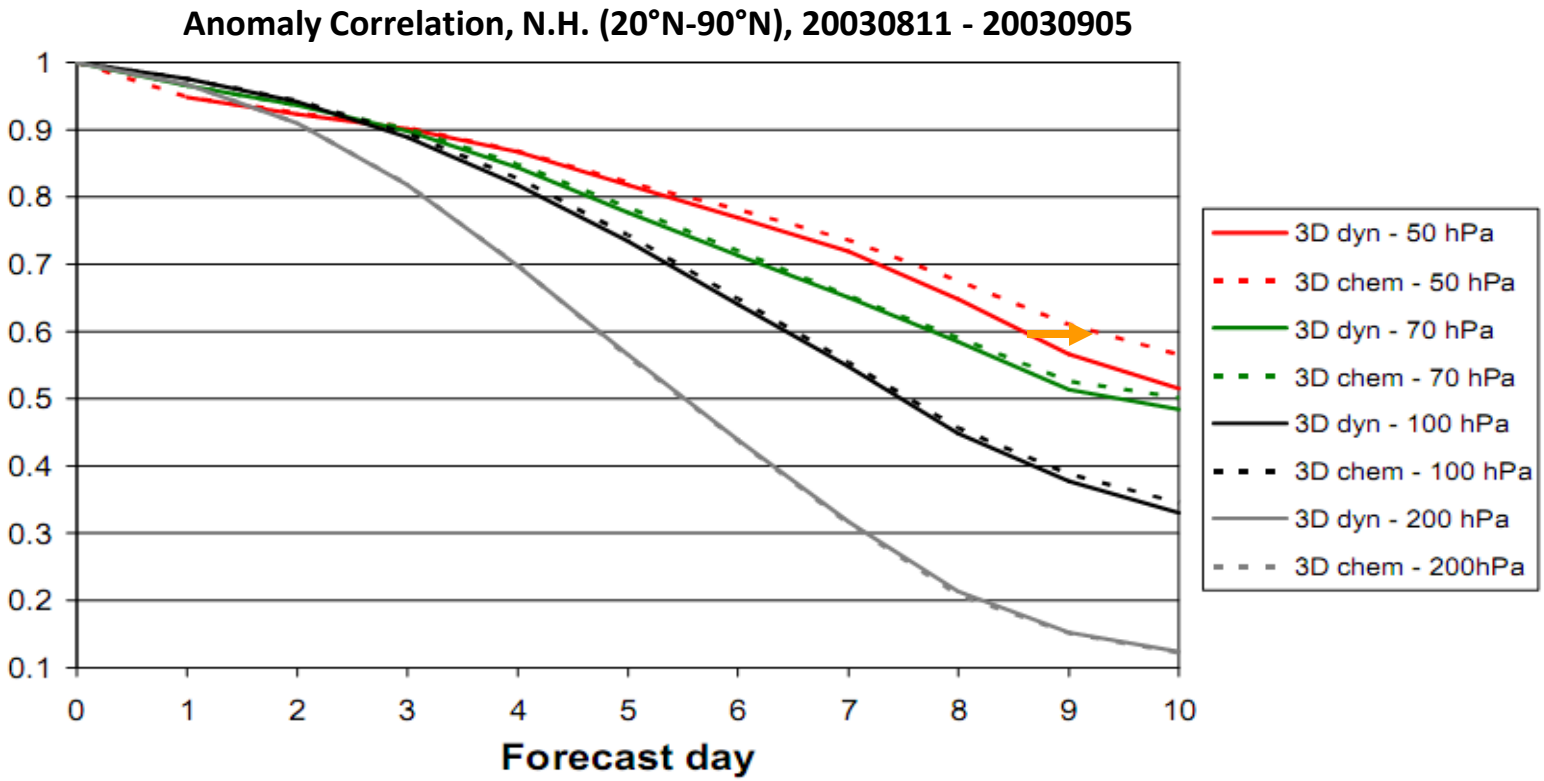


Works well for EPP-Indirect effect (slow time scale). EPP direct effect would require a bias estimation and correction scheme.

de Grandpré *et al.*, Mon. Wea. Rev., 2009 :

- MIPAS assimilation of ozone

→ big improvement of *T* forecast skill in lower strato:



Forecast verification against analyses

BIRA: Comprehensive chemistry

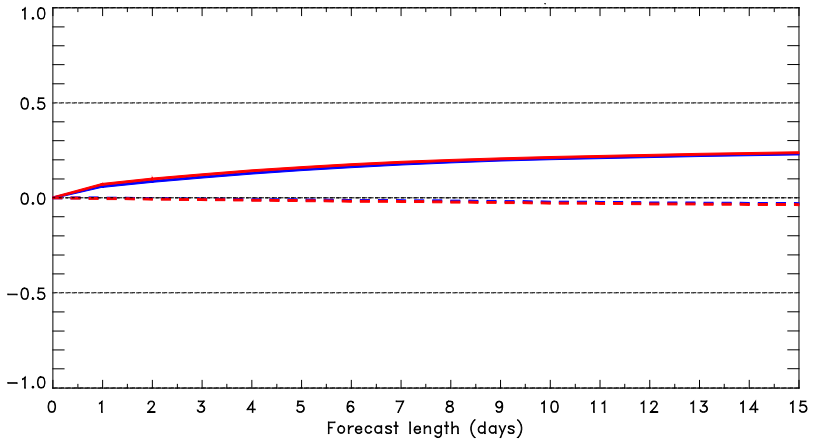
LINOZ: Linearized chemistry

FK : Ozone zonal monthly climatology

—— **RMSE**

----- **BIAS**

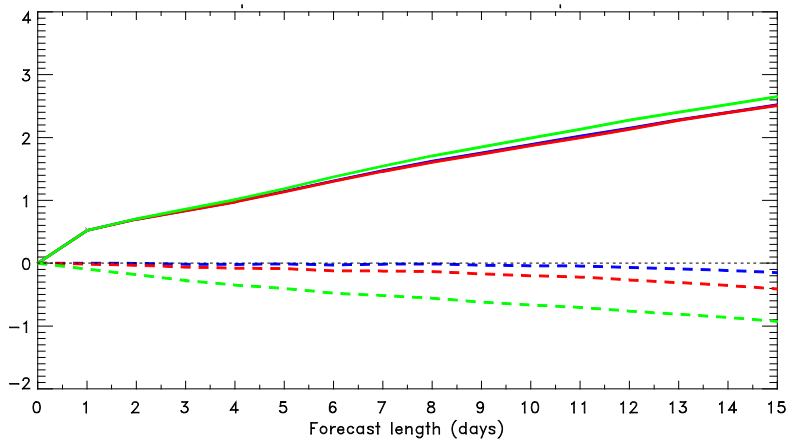
--- **BIRA** --- **LINOZ** ---- **FK**



Ozone (ppmv)

50 hPa

(NH)



Temperature (K)

50 hPa

(NH)

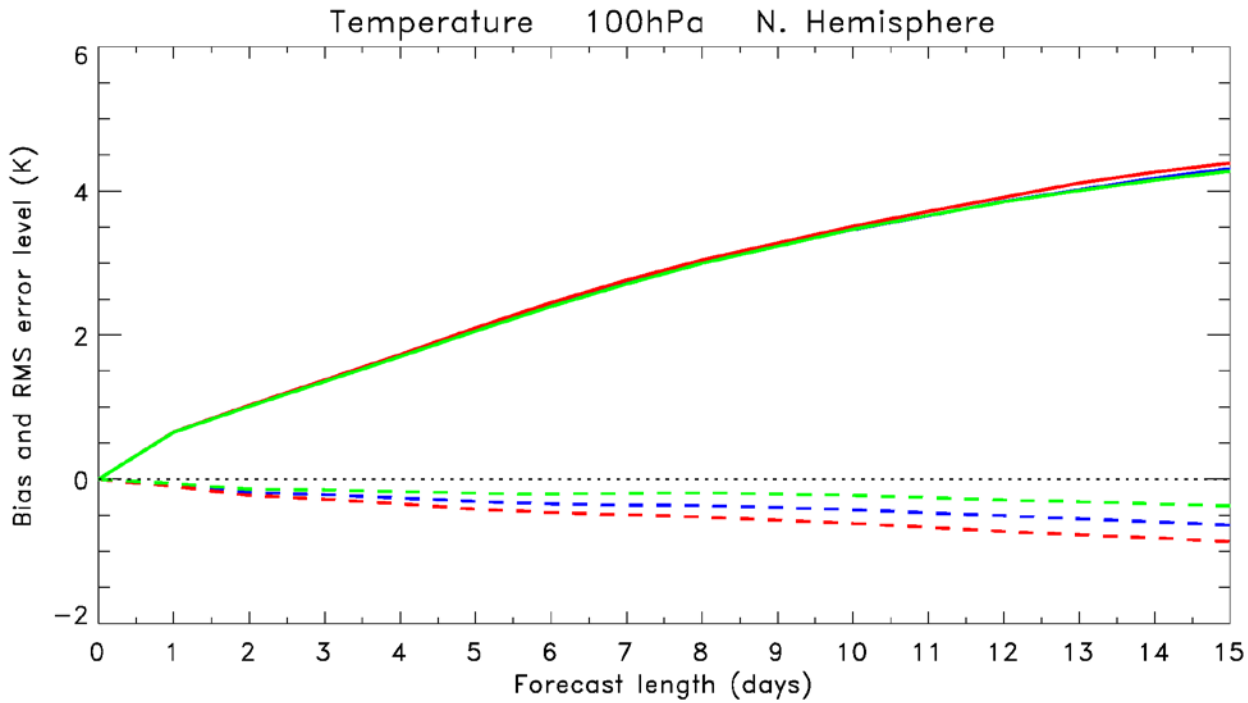
Forecast verification against analyses

BIRA: Comprehensive chemistry

LINOZ: Linearized chemistry

FK : Ozone zonal monthly climatology

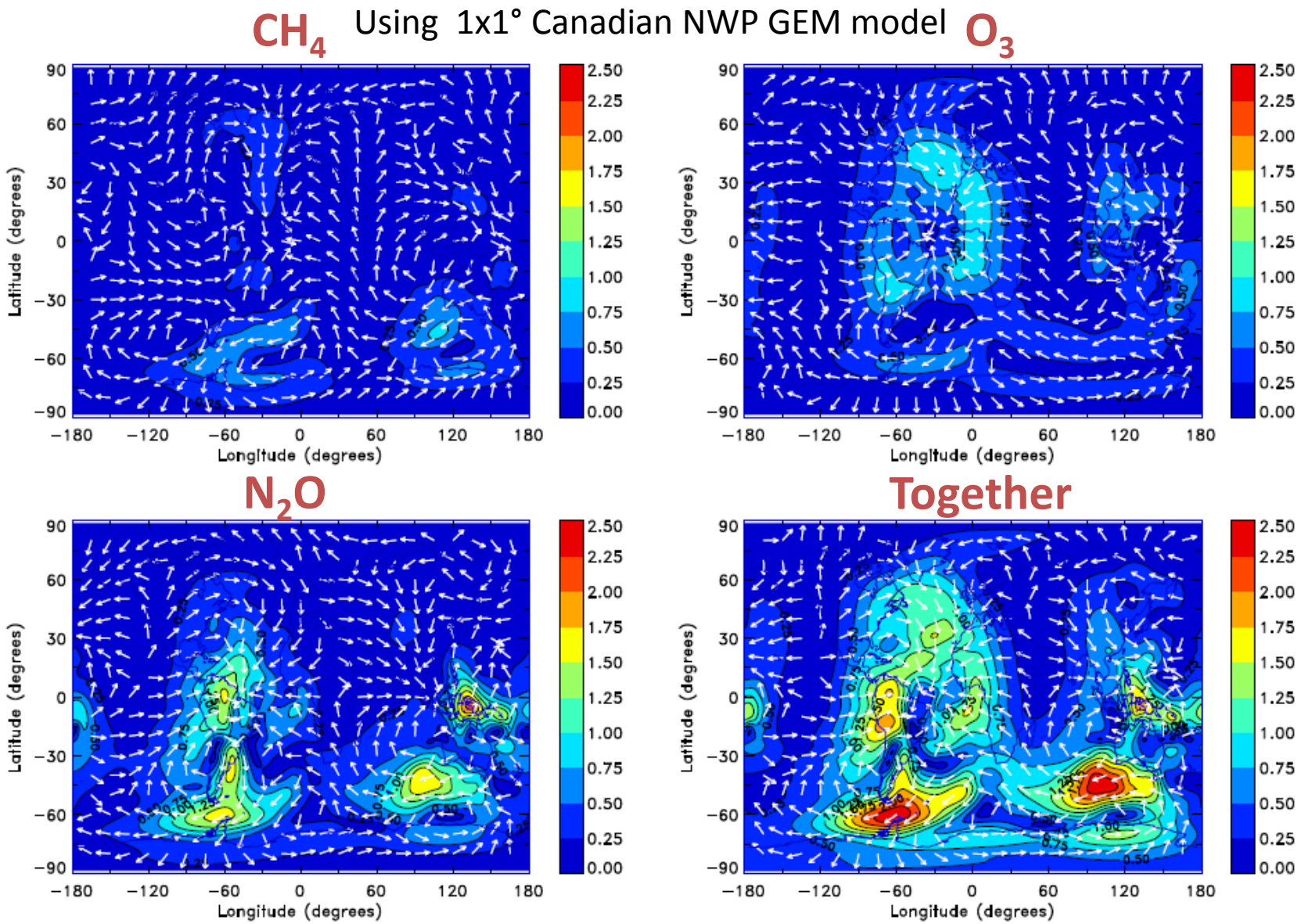
We have improvement 50 hPa and higher up. But lower down at 100 hPa - the reverse is observed



No clear why.? MIPAS observations at 100 hPa.
Other radiative processes cancellation of errors

Tracer-Wind using 4DVar: increment from different species

Using 1x1° Canadian NWP GEM model



Wind increments from TOVS and chemical species are of comparable magnitude

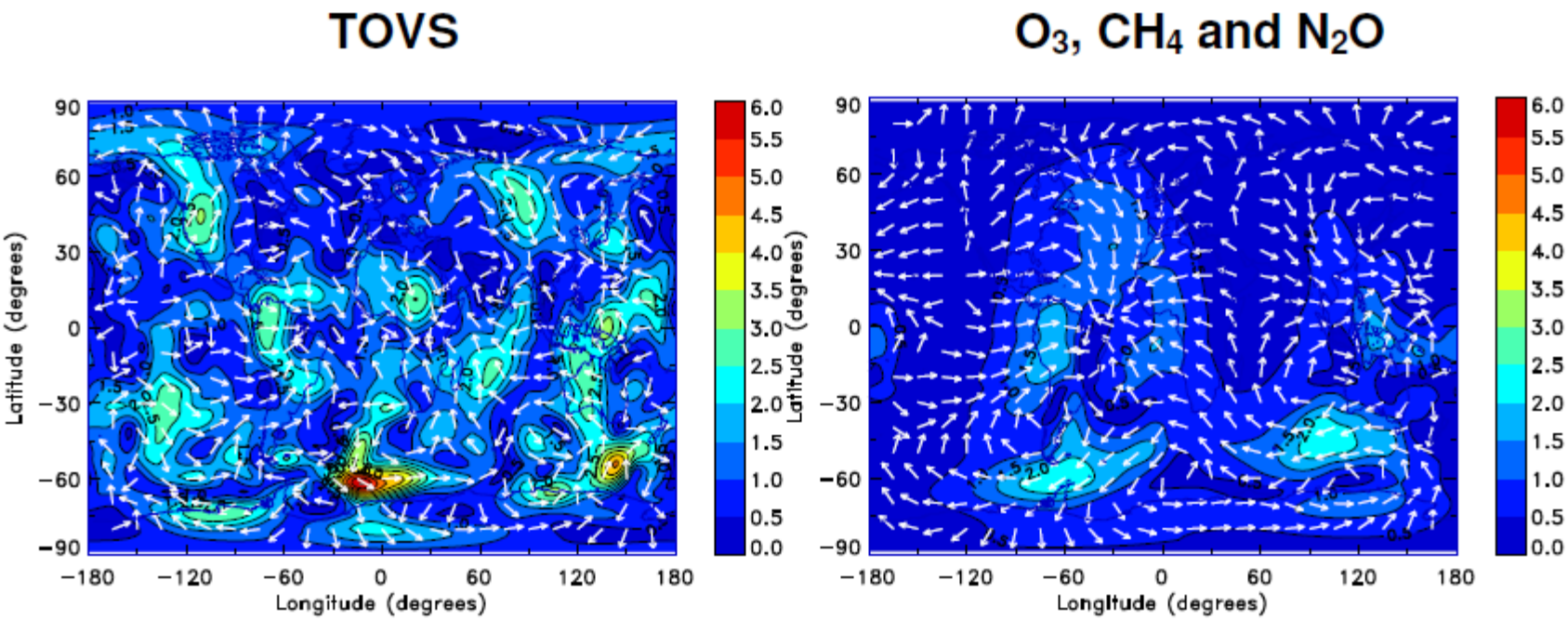
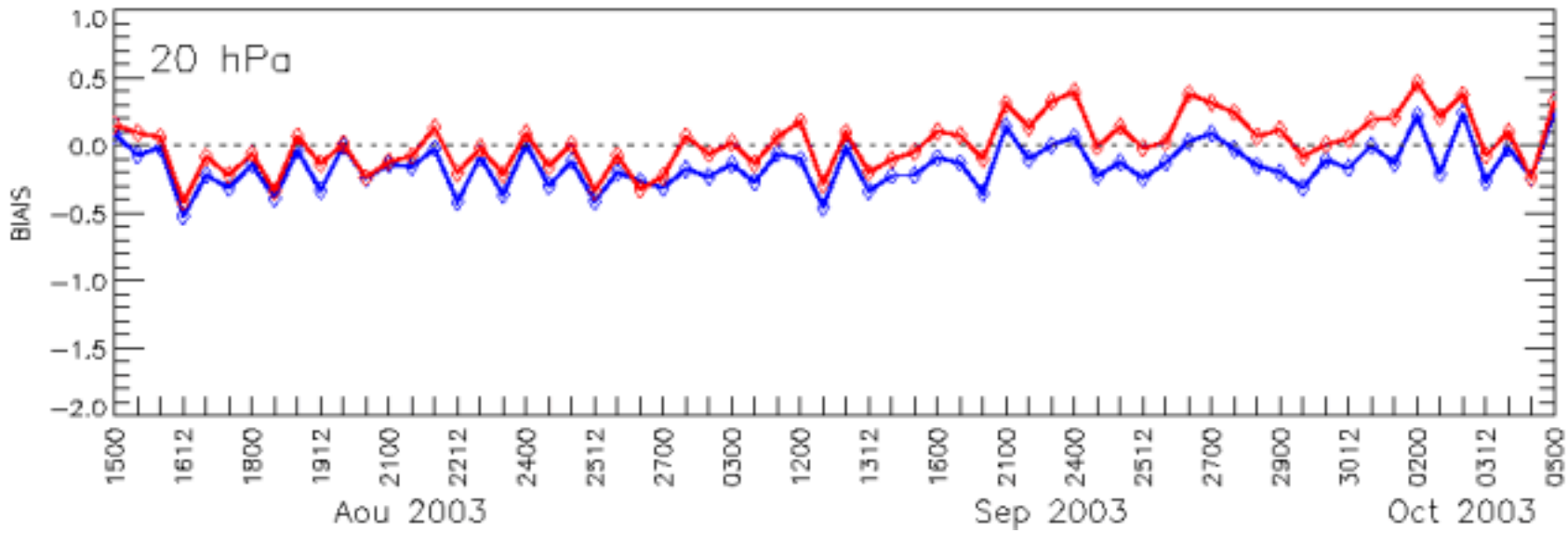


Figure 14.14 Wind increments at 10 hPa obtained from TOVS and chemical species when simultaneously assimilated in 4D-Var.



O-P temperature time series between RAOBS and the 3D-Var (blue) and 4D-var (red) assimilation cycles at 20 hPa in the North Hemisphere.

The strong coupling DA between chemistry-tracer and meteorology has introduced a temperature bias that increases in time

Summary and outlook

- The CDA methodology is improving. A more effective use of observations can be achieved by improving error covariances, adding retrieval consistency in the observation operator, and quality control, we are thus moving towards an effective multi-species multi-instruments integration that can be useful to address science question
- Methodologies based on CDA are being developed to estimate missing processes (e.g. ozone loss).
- Coupling with NWP
  - Ozone –radiation interaction have been shown to have an impact on lower stratospheric temperatures on the meteorology with a linearized chemistry scheme. However the improvement is not seen in LS/UT region so further work need to be conducted to improve medium-range NWP
  - Tracer-wind. Analysis increment on winds are consistent and significant (compared with increments due to temperature observations). However, temperature biases develops over time.

Papers in preparation

- Added-value of stratospheric chemical data assimilation. An overview. BAMS ?. Menard et al.

- Reanalysis of stratospheric chemical composition based on MIPAS N2O and CH4. ACP. Errera et. al.

- The long-term study of polar ozone loss observed by Odin/SMR. ACP. Sagi et al.

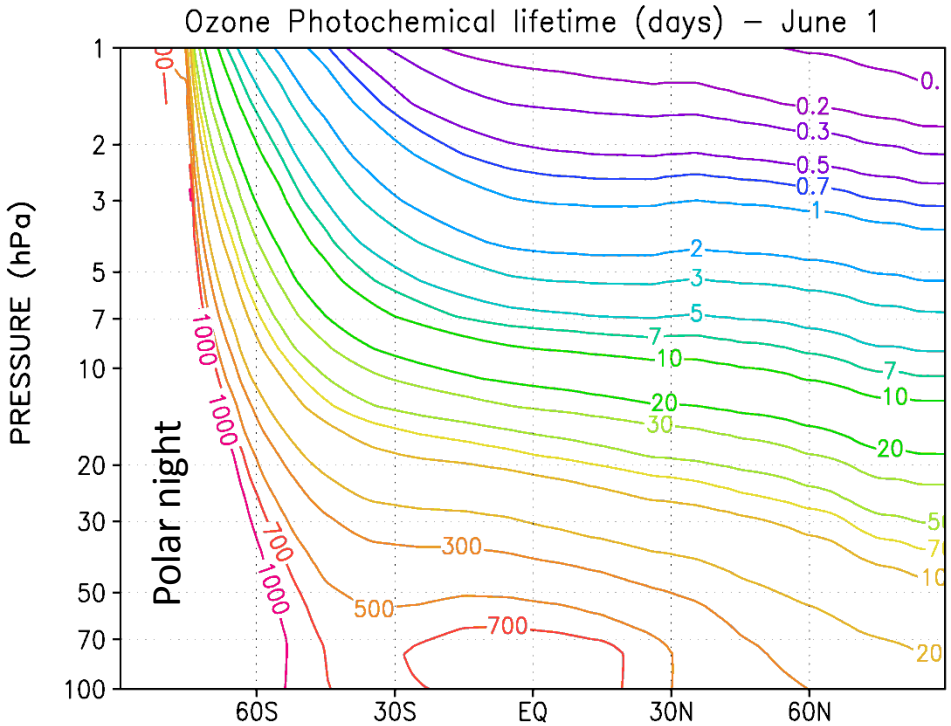
- Evaluation of modelled ozone in the upper stratosphere and lower mesosphere with a state-of-art chemistry transport model. ACP. Skachko et al.

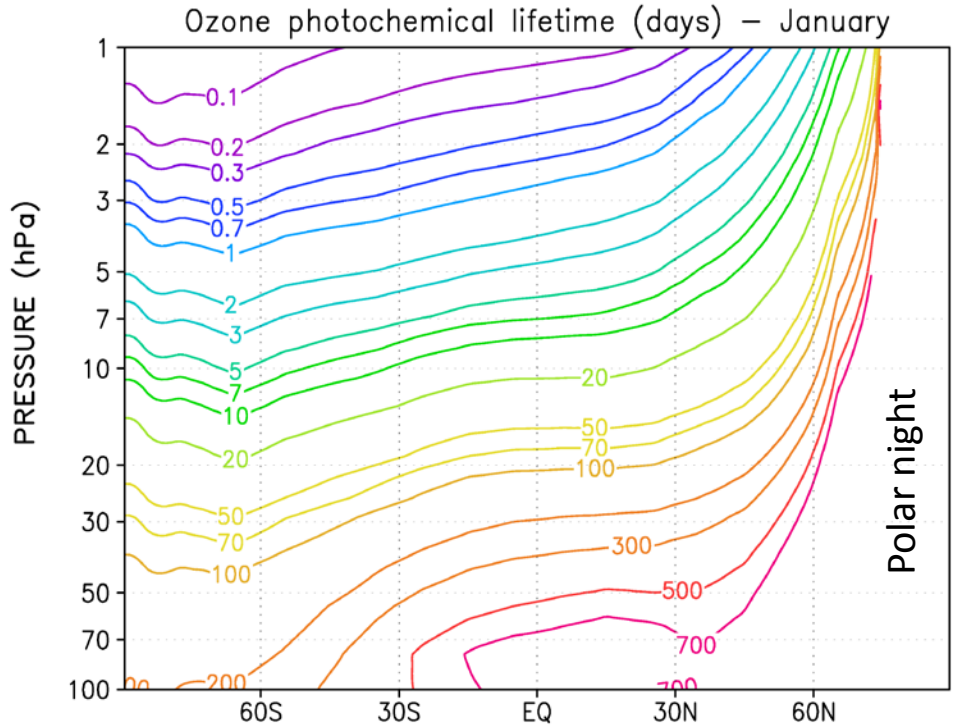
- Comparison of EnKF and 4D-Var data assimilation systems of multi-species chemistry transport model. GMD. Skachko et al.

- Ozone predictability in a numerical weather prediction model. De Grandpré et al.

Extra slides

Ozone chemical life-time



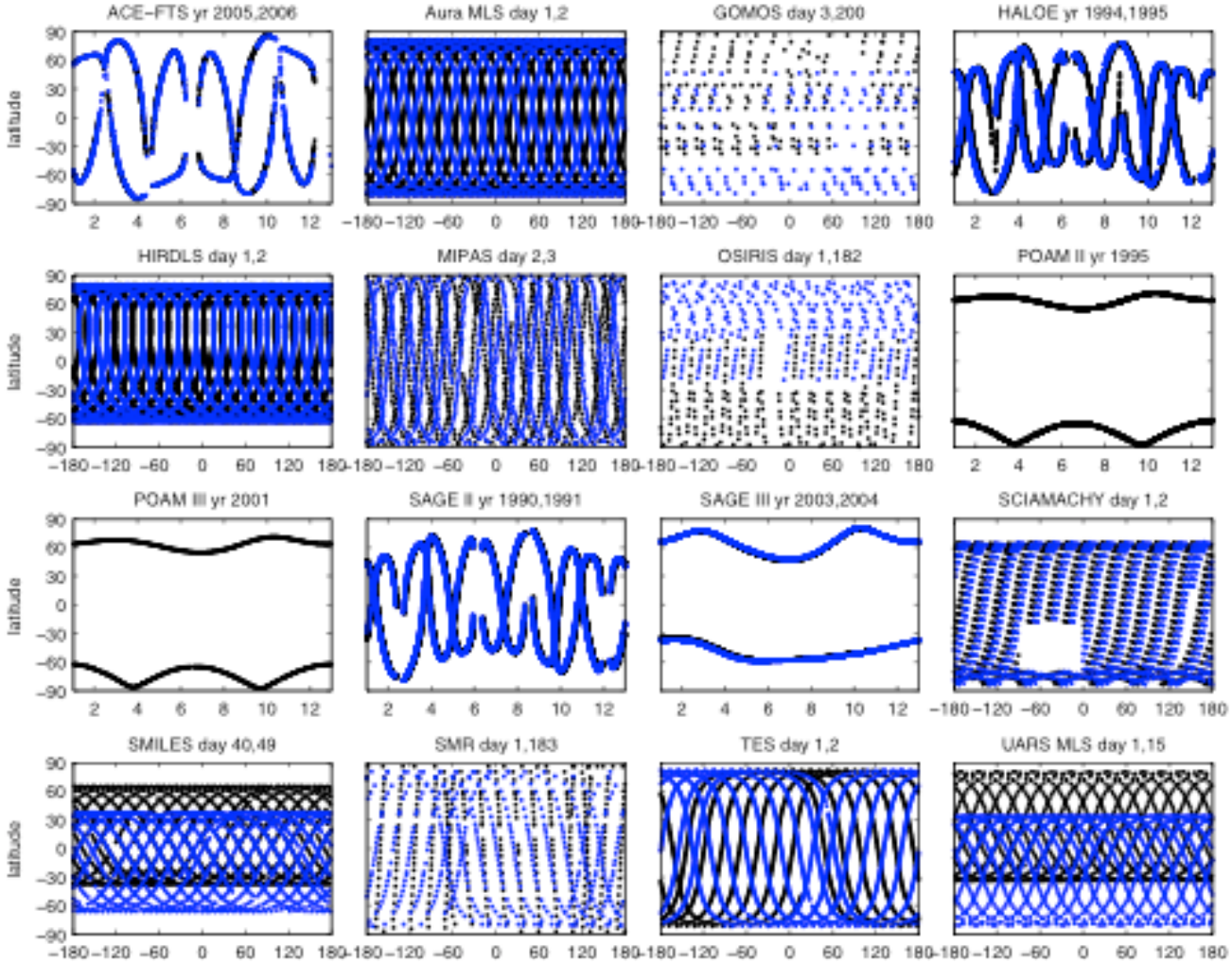


(figures from Jean de Grandpré)

- τ is more than one week , below 10 hPa
- τ > one day , below 4 hPa

for mid and lower stratosphere we can treat ozone as a tracer

Diagnostics – multiple sensor



Errera and Ménard (2012) ACP

ISSI: - Analysis of short-lived species to validate CCMI models

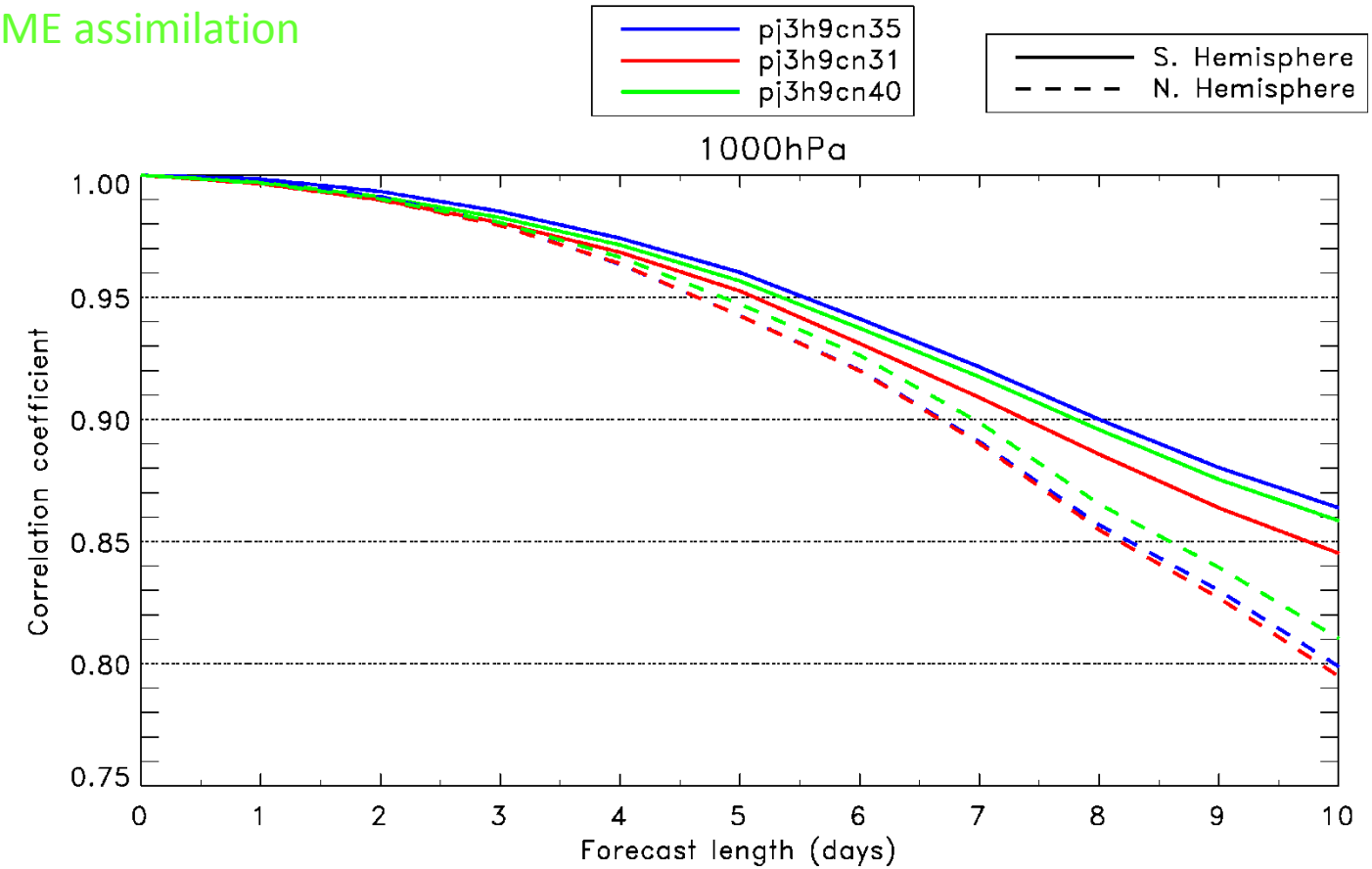
- Assimilation as a transfer standard for comparison between data-sparse instruments

Ozone forecast predictability

No assimilation

MLS assimilation

GOME assimilation



Column ozone