Ozone – do we need to simulate it ?

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Vincent Huijnen (KNMI), Beatriz Monge-Sanz and Paul Berrisford.

How do we model ozone chemistry in atmospheric models and how does it interact with NWP – in particular at ECMWF?

Modelling atmospheric composition

$$\frac{\partial c_i}{\partial t} + \mathbf{V}_h . \nabla_h c_i + \frac{\partial}{\partial z} w_c c_i - \frac{\partial}{\partial z} K_Z \frac{\partial c_i}{\partial z} = E + R - D$$

Transport

Source and Sinks

c_i concentration of species i

$E_i \neq f(c_i)$ ... Emission

$R_i = f(c_i, c_j, c_k, c_{m,} ...)$ ... Chemical conversion

$D_i = l_{Dep} c_i$ ... Deposition

ECMWF

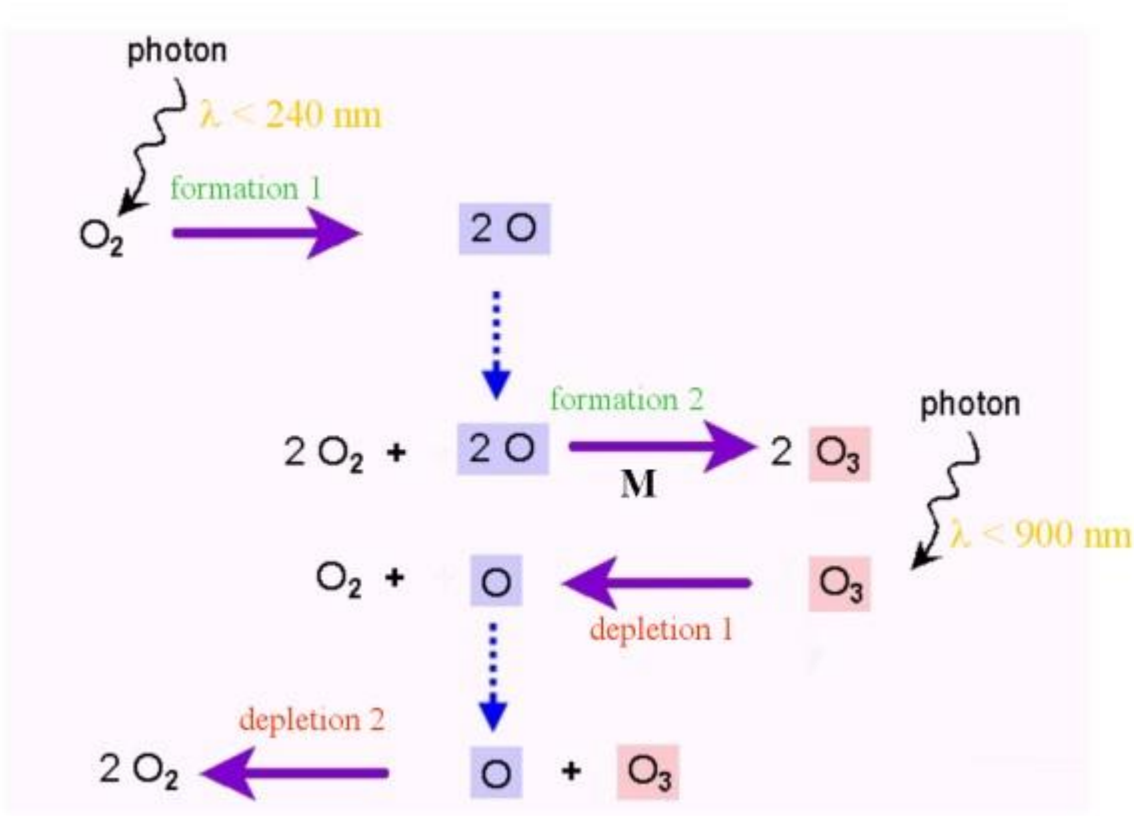
Modelling ozone chemistry I

- Parameterisation based on modelled climatologies (Cariolle and Deque, 1989)
  - Uses relaxation to modelled ozone, T and over head column (oc) ozone climatologies
  - $\Delta [O3] / \Delta t = A_1 + A_2 (O_3 - O_3^{clim}) + A_3(T - T^{clim}) + A_4(ocO_3 - ocO_3^{clim})$
  - Extend to deal with heterogeneous ozone loss (Cariolle and Teyssedre, 2007)
  - Similar approaches by McLinden et al. 2000, McCormack et al. 2006, Monge-Sanz et al. 2011
  - Works well for stratospheric ozone but not for tropospheric ozone
  - Problematic for larger deviations from linearization point O_3^{clim} *and* T^{clim}

Modelling ozone chemistry II

- Chemical Mechanism to simulate chemical reactions
  - Set of species (50-150) and set of reaction (100-300)
    - A + B -> C, C -> D + E , …
  - Set of reaction rates k to calculate reaction speed:
    - - d[A]/dt = - d[B]/dt = d[C]/dt = **k [A] [B],** k = f (T)
  - Solve coupled system of stiff ordinary differential equations
  - Tropospheric, stratospheric and atmospheric schemes
  - High computational cost (factor 3-10 of IFS NWP forecasts at T159-T511 resolution)

Ozone cycle in Stratosphere (Chapman, 1930)



a) $O_2 + h\nu(240\,nm) \xrightarrow{j_2} O + O$

b) $O + O_2 + M \xrightarrow{k_b} O_3 + M$

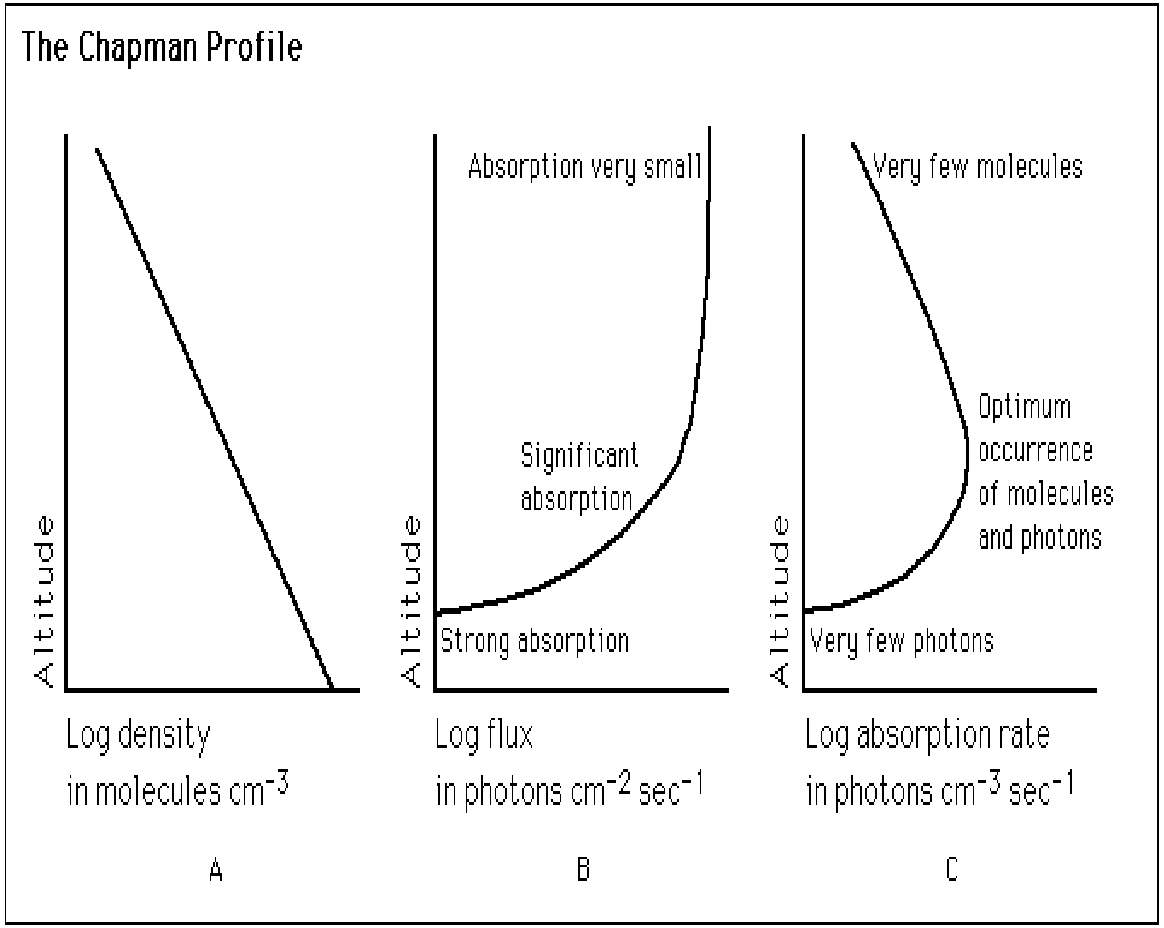
c) $O_3 + h\nu(900\,nm) \xrightarrow{j_3} O_2 + O$

d) $O_3 + O \xrightarrow{k_d} 2O_2$

A simple chemical mechanism to explain the existence of the ozone layer

Ozone profile predicted with Chapman Cycle and observations

$O_2 + O + M \rightarrow O_3 + M$ $O_2 + h\nu \rightarrow 2\,O$ O_3 profile



Catalytic reactions with NOx, HOx, ClOx, BrOx & Transport

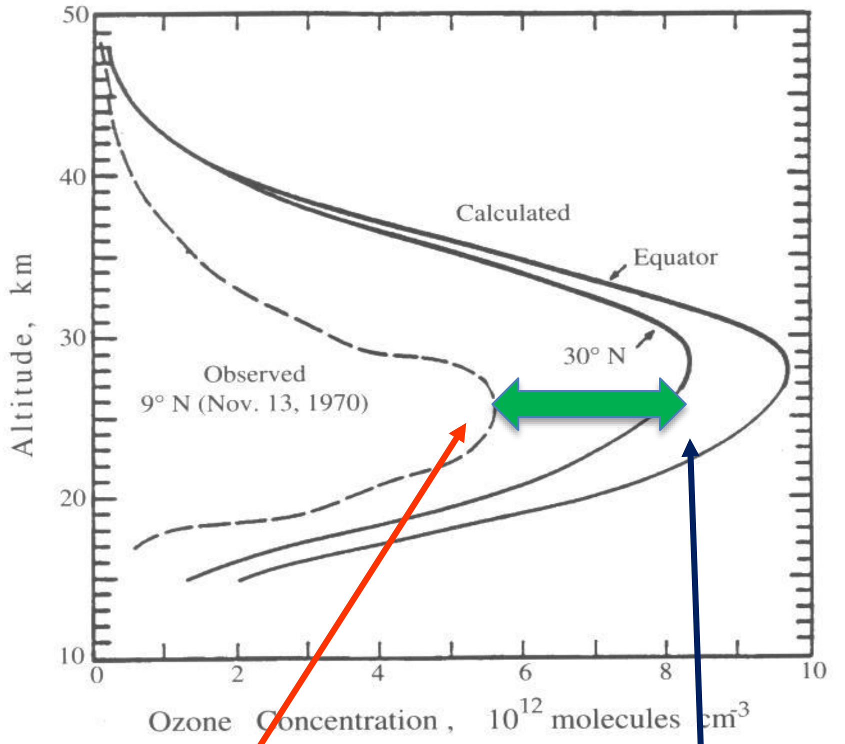
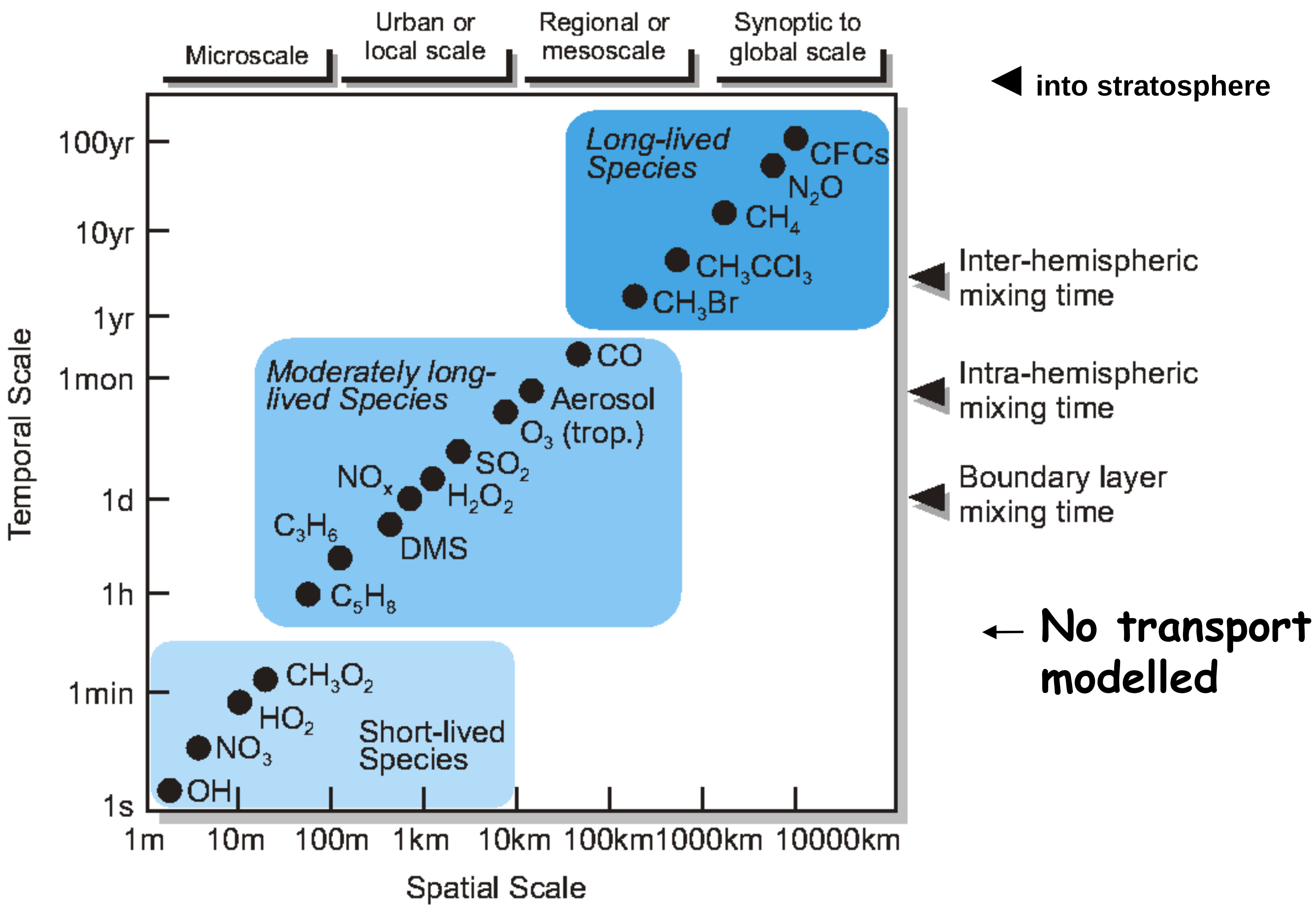


FIGURE 4.6 Comparison of stratospheric ozone concentrations as a function of altitude as predicted by the Chapman mechanism and as observed over Panama (9° N) on November 13, 1970.

observed   Pre 1979

Chapman theory

Chemical Life Time vs Spatial scale



After Seinfeld and Pandis [1998]

Atmospheric chemistry needs to consider
a wide range of species at different temporal scales (life time)

The chemical life time control the scope of the atmospheric transport processes

Ozone in the Atmosphere

- Ozone layer in stratosphere
  - Absorption of UV => heating => temperature increase that constitutes the stratosphere
  - Climate change: stratospheric ozone has small negative radiative forcing
- Tropospheric ozone
  - Influx from stratosphere and photochemical production
  - Air quality and tropospheric chemistry
  - Important green house gas (after H_20, CO_2, CH_4)

Heating and cooling due to trace gases

Brasseur G. and Solomon S.,
Aeronomy of the Middle Atmosphere
1984

0.01

0.1
1

10
100

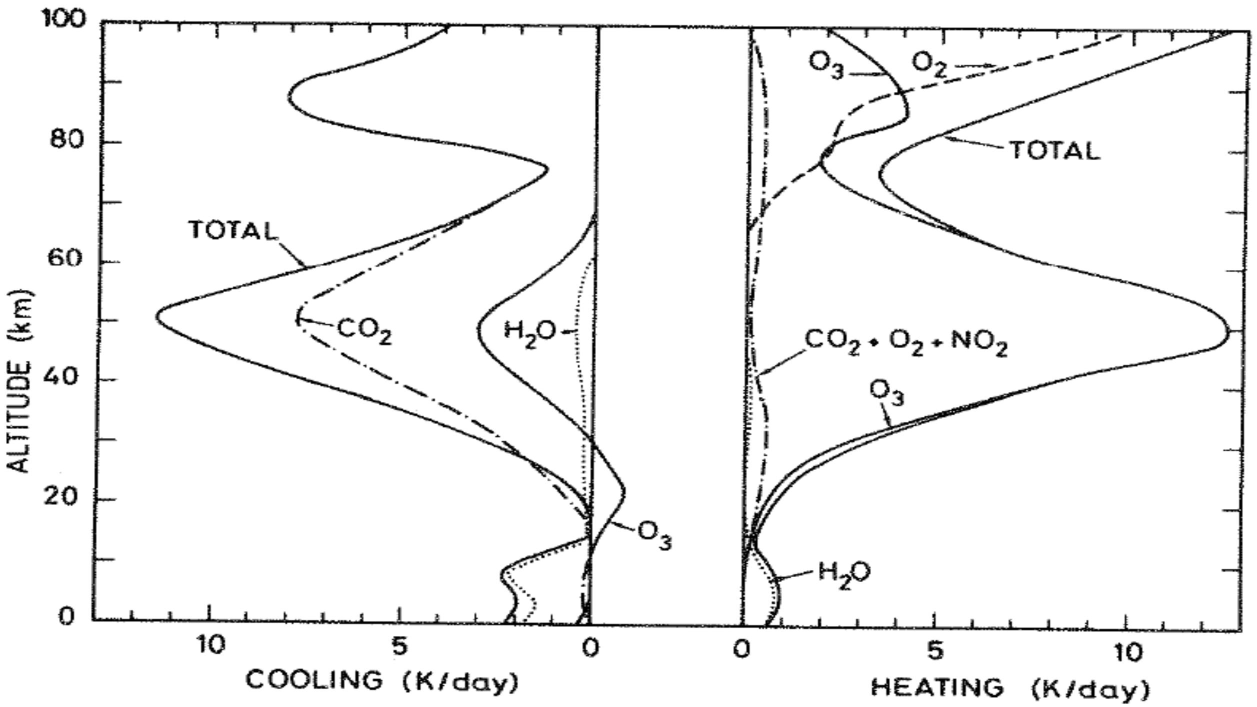
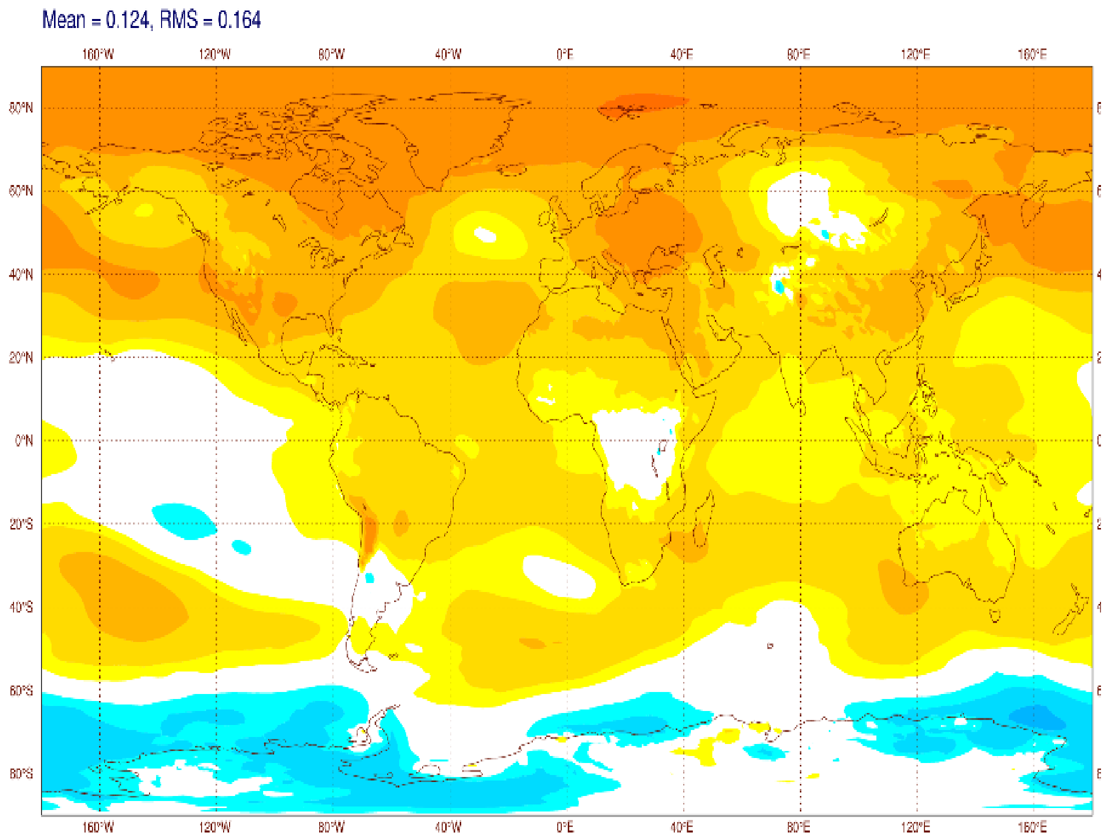


Fig. 4.19b. Vertical distribution of solar short wave heating rates by O_3, O_2, NO_2, H_2O, CO_2, and of terrestrial long wave cooling rates by CO_2, O_3, and H_2O. From London (1980).

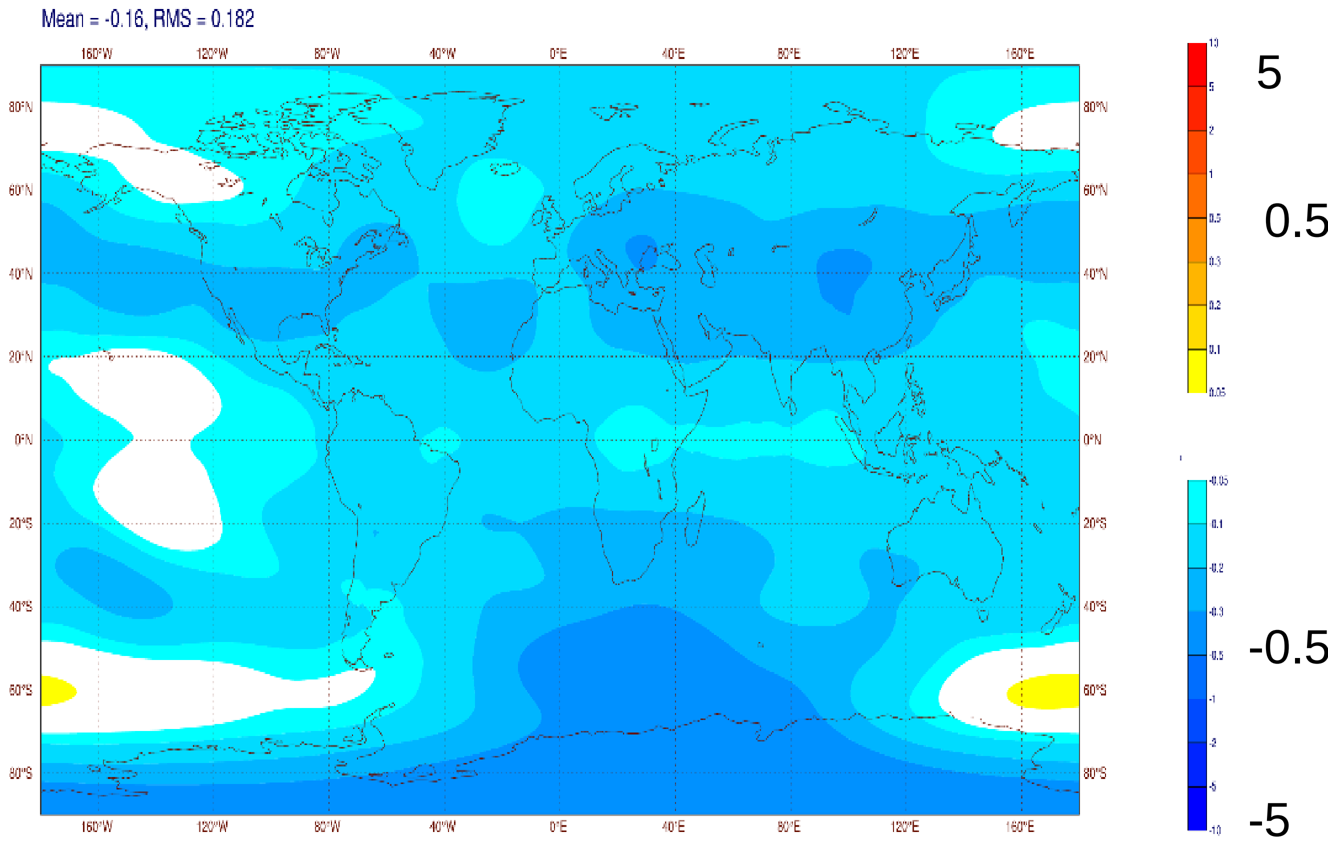
Most important:
Stratosphere:
CO_2,(LW), O_3 (SW)
Troposphere: $H_2$0

Temperature Trend 1979-2015 (K/10yr) Era-Interim

TLT Troposphere



TLT Lower Stratosphere

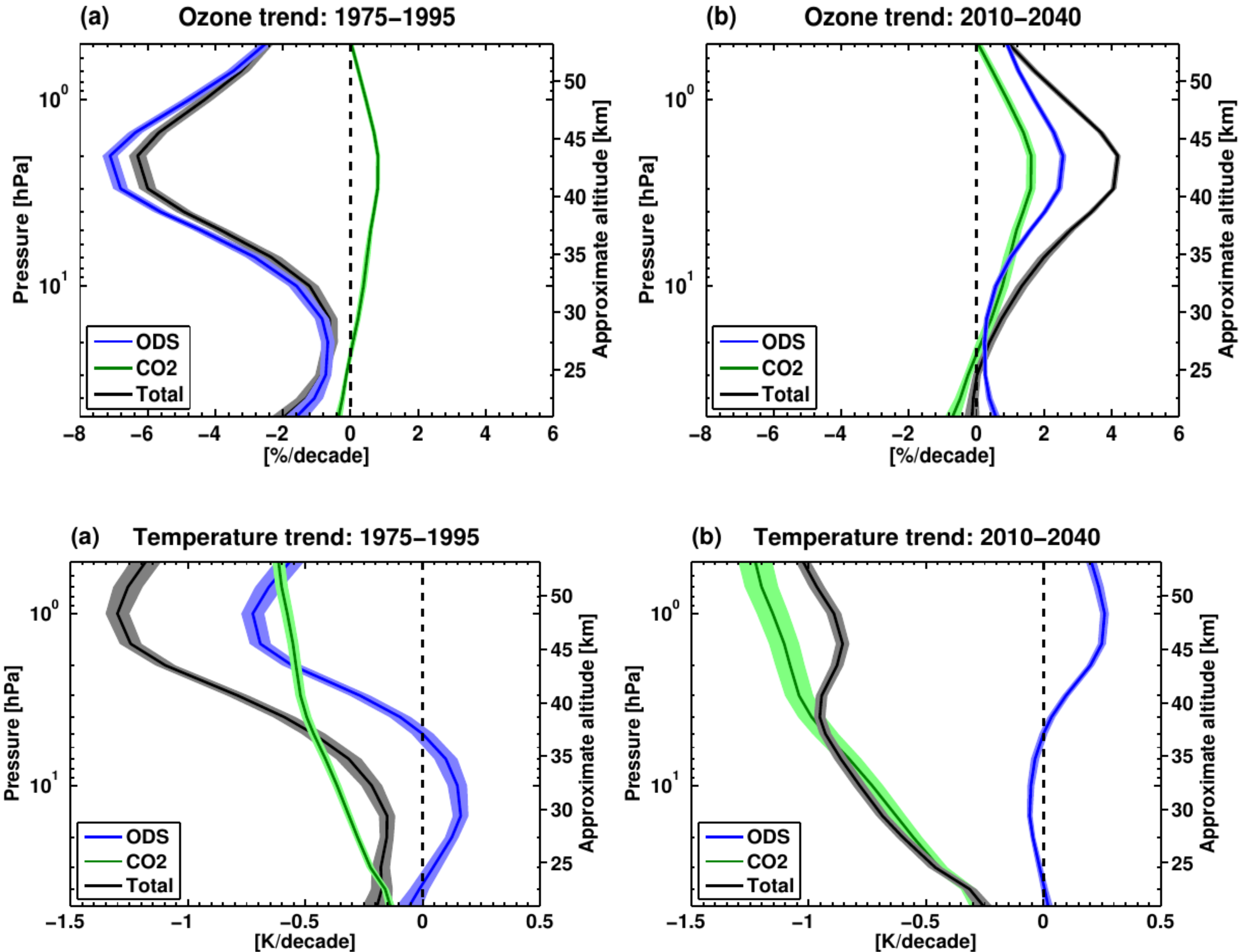


Colling because of ozone loss and $C0_2$

ECMWF

Paul Berrisford

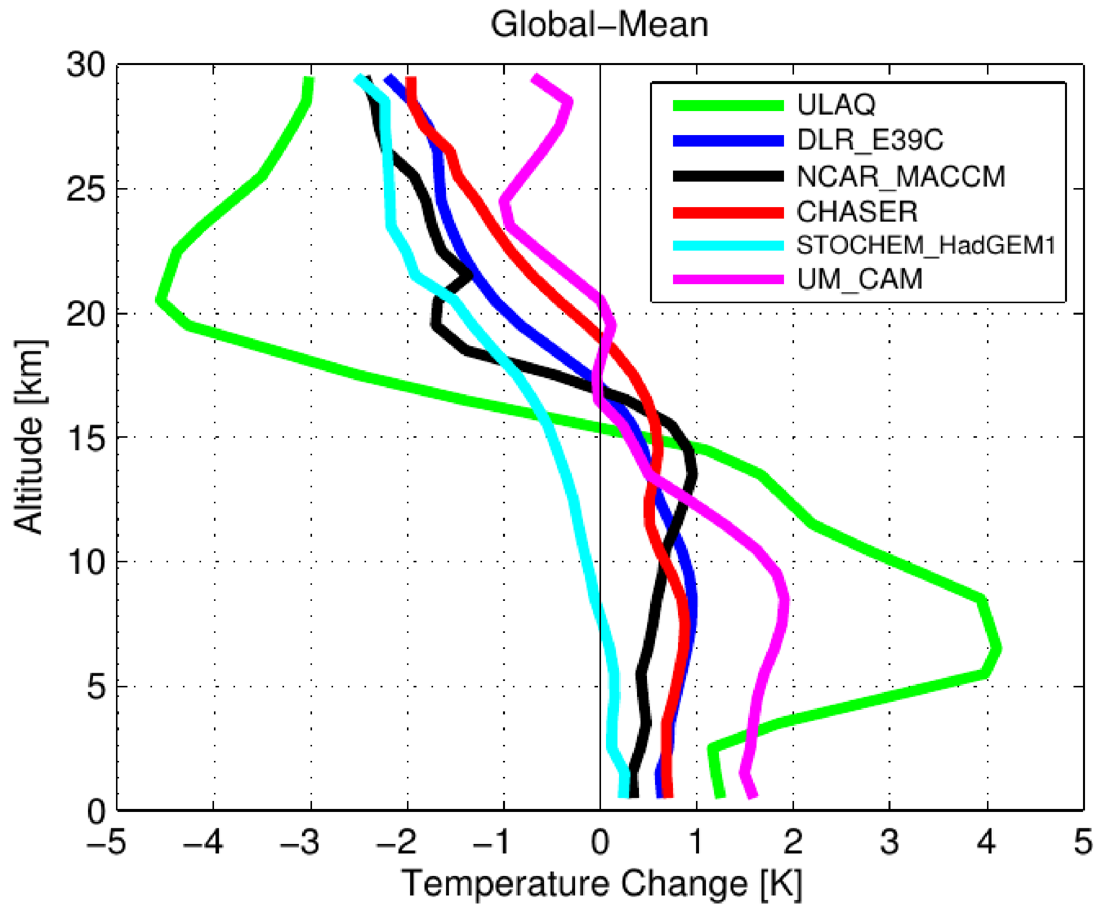
Ozone and Stratospheric Temperature Trends



- Stratosphere is cooled by increased CO2
- Ozone cools or warms depending on ozone trend
- Ozone trends because of Ozone Depleting Substances (ODS) but also by T itself

Shepherd and Jonsson, 2008

Ozone and Tropospheric Temperature Trends



ECMWF

ACCENT
Coupled chemistry climate models with stratospheric and tropospheric chemistry, Gauss et al. 2006

Fig. 4. Annually and globally averaged zonal-mean temperature change (K) between 1850 and 2000 as represented by the difference “2 minus 1”. For UM CAM “2 minus 1d” is shown.

Climate	OSD	O3 precursors
1: 1850	1850	1850
2: 2000	2000	2000

Ozone is an important tropospheric greenhouse gas especially in upper troposphere

Ozone in the ECMWF model

I. IFS (NWP/ERA): Stratospheric Ozone using the Cariolle Parameterisations
II. C-IFS (CAMS): Atmospheric ozone using different chemical mechanism as well as Cariolle scheme
III. Ozone climatology for radiation scheme

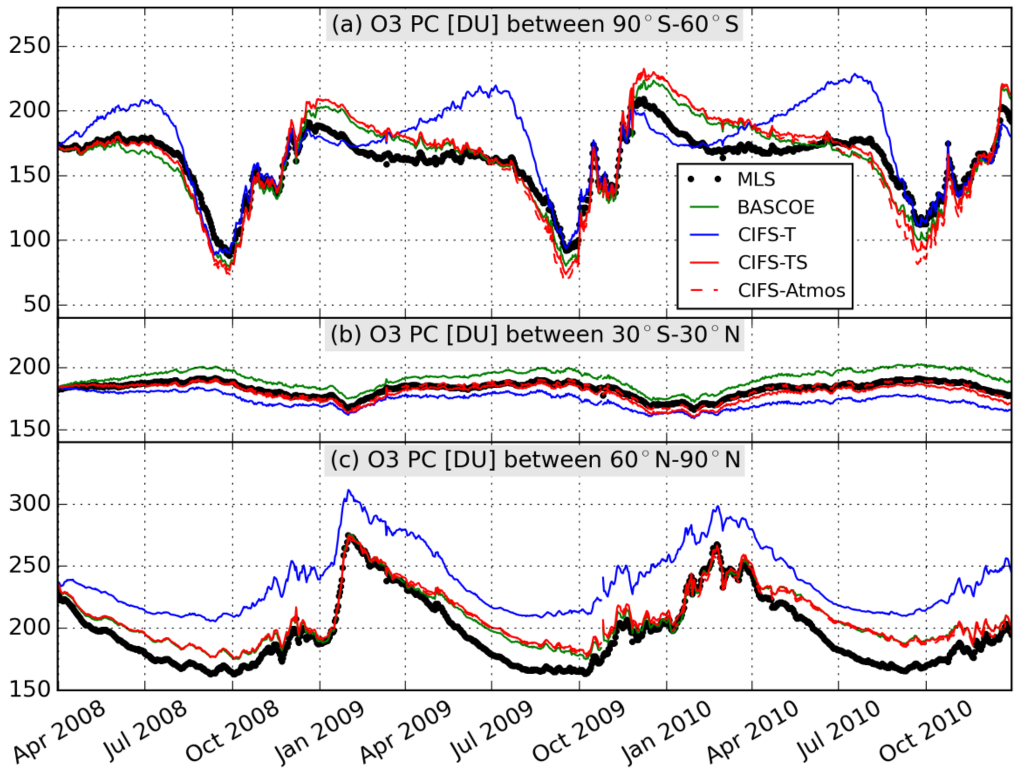
Ozone (I and II) was introduced to use 4D-VAR assimilation system to assimilate ozone !

Ozone simulation and assimilation in the Copernicus Atmosphere Service at ECMWF

- CAMS objective is to make operational forecast and assimilation of atmospheric composition, i.e. for tropospheric and stratospheric ozone
- Global CAMS system (operational since 2015) was developed in EU research projects (GEMS, MACC) since 2004
  – Extend ECMWF model (C-IFS) to with modules to simulate reactive gases, aerosols and greenhouse gases
  – Assimilation of atmospheric composition retrievals for NRT forecast and analysis of global atmospheric composition

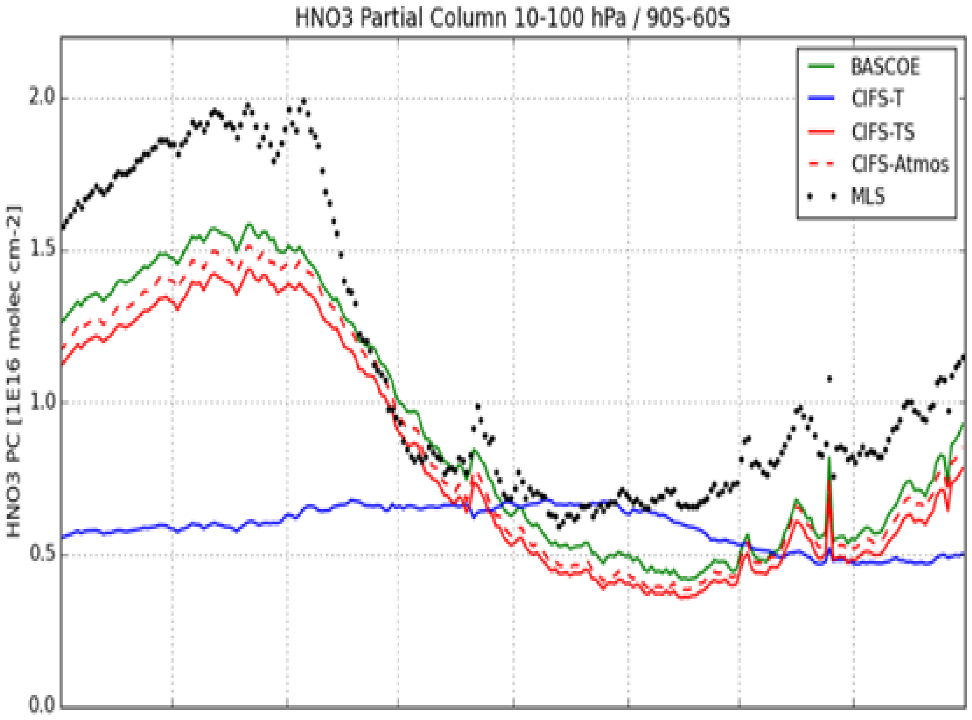
Chemical mechanism vs - *vs.* Cariolle Parameterisation

Ozone



. Daily averages of O3 partial columns (10-100hPa) for the Arctic (60°N-90°N), Tropics (30°S-30°N) and Antarctic (60°N-90°N) over the period April 2008 – December 2010. Datasets are averaged in 5-day bins and model output is interpolated to the location and time of Aura MLS v3 retrievals (black dots). Blue line: C-IFS-T; green line: BASCOE-CTM; red dashed line: C-IFS-Atmos; red solid line: C-IFS-TS.

HNO_3



C-IFS T: T: CB05 S: Cariolle

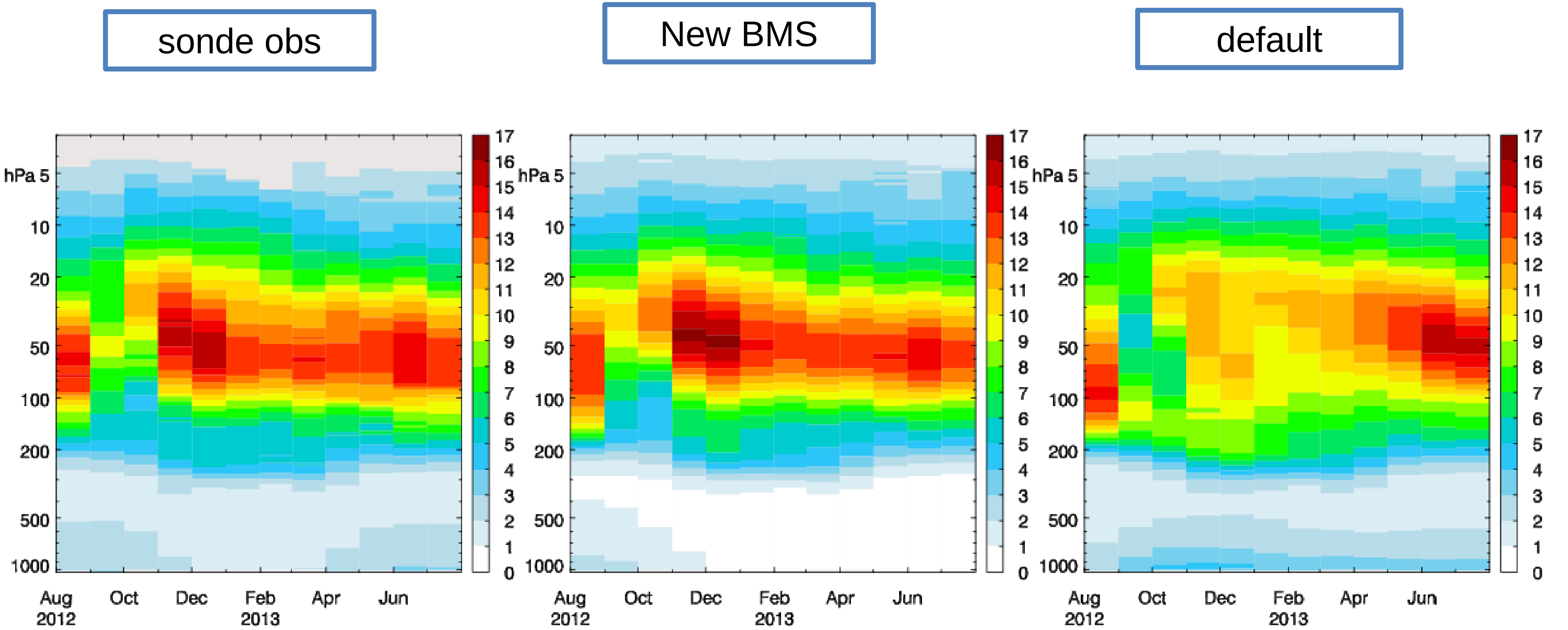
C-IFS TS T: CB05 S: BASCOE

Observations

Huijnen et al.2016

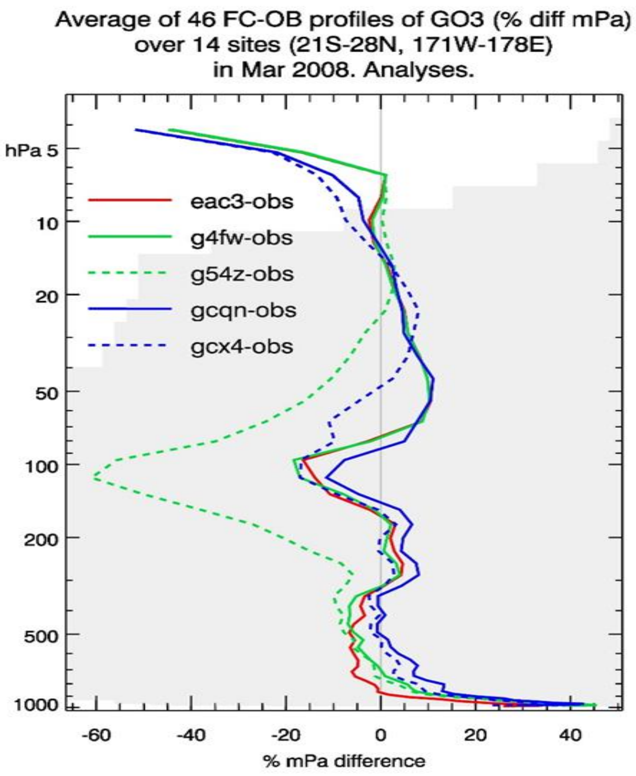
B. Monge-Sanz scheme vs Cariolle scheme

Antarctic O_3 (1000-3hPa)



Impact of simulation approach in assimilation – ozone profiles Tropics

C-IFS CB05 CAR vs CB05 – BASCOE)

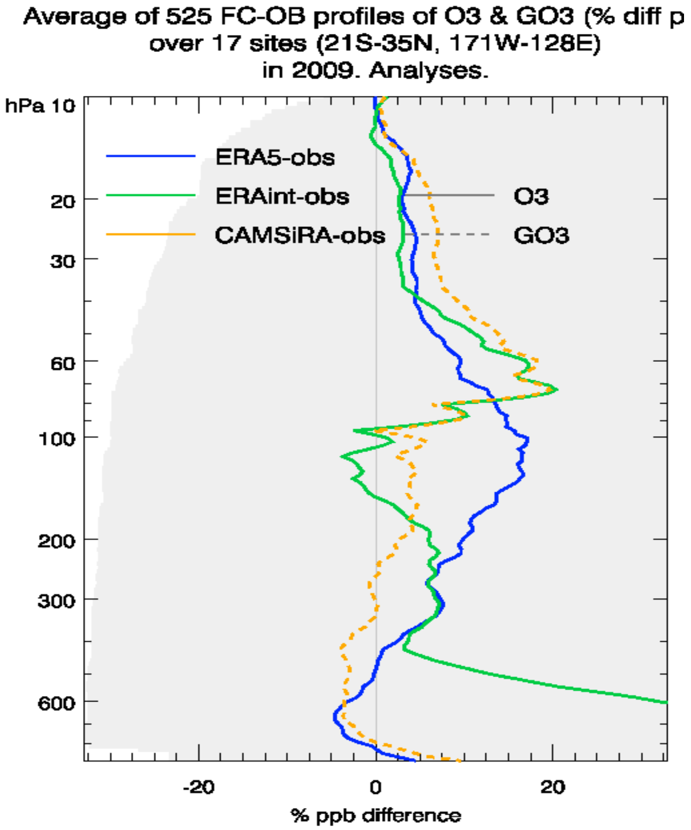


Assimilation
Reduces greatly the differences between the model approaches

C-IFS CB05 BASCOE
CIFS CB05 CAR
Interim rean

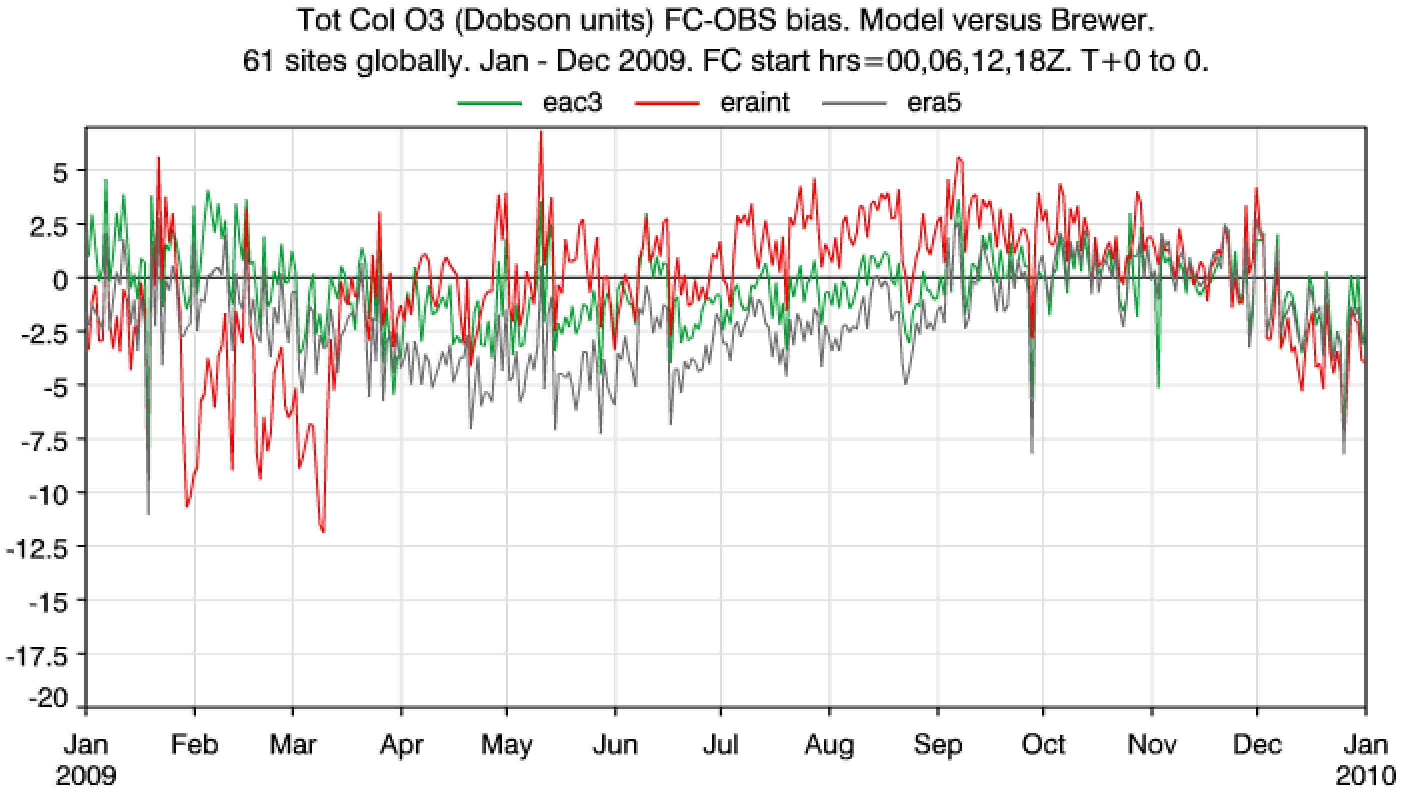
Assim:
Ctrl:

CAMSiRA vs ERAinteri vs ERA5



Assimilation Profiles of C-IFS with full chemistry
Tend to be better in troposphere

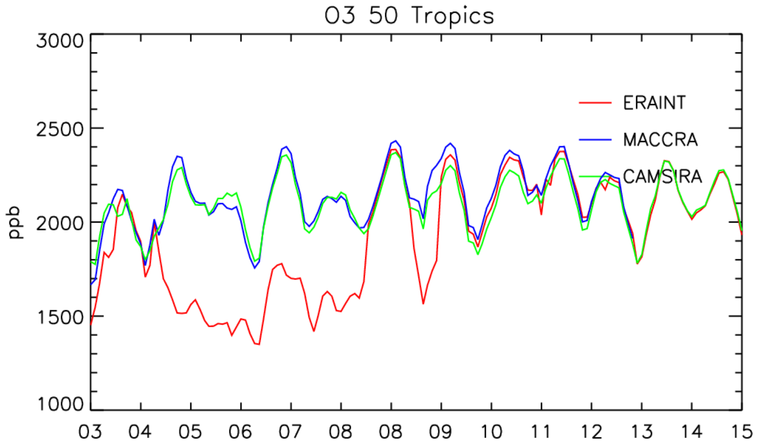
Impact of simulation approach in assimilation: TC

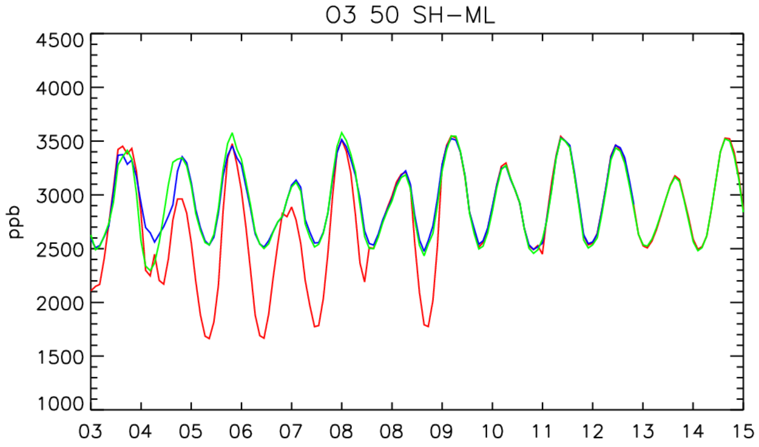


CAMSiRA
ERAINT
ERA5

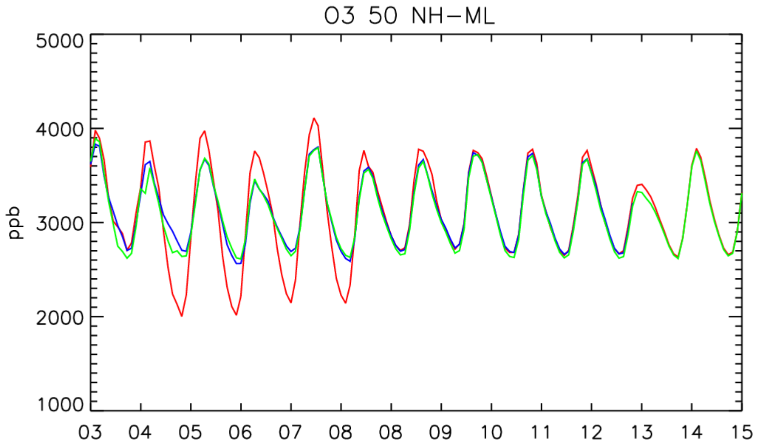
Total Columns are well constrained by assimilated retrievals

Temporal consistency of ozone re-analyses Ozone at 50 hPa





ERA interim
has artificial jumps



Atmospheric Composition re-analyses (MACCRA) are
Accompanied with a control run w/o DA of AC.
The control run helps to understand the impact of the assimilated data

Little impact of ozone assimilation at surface

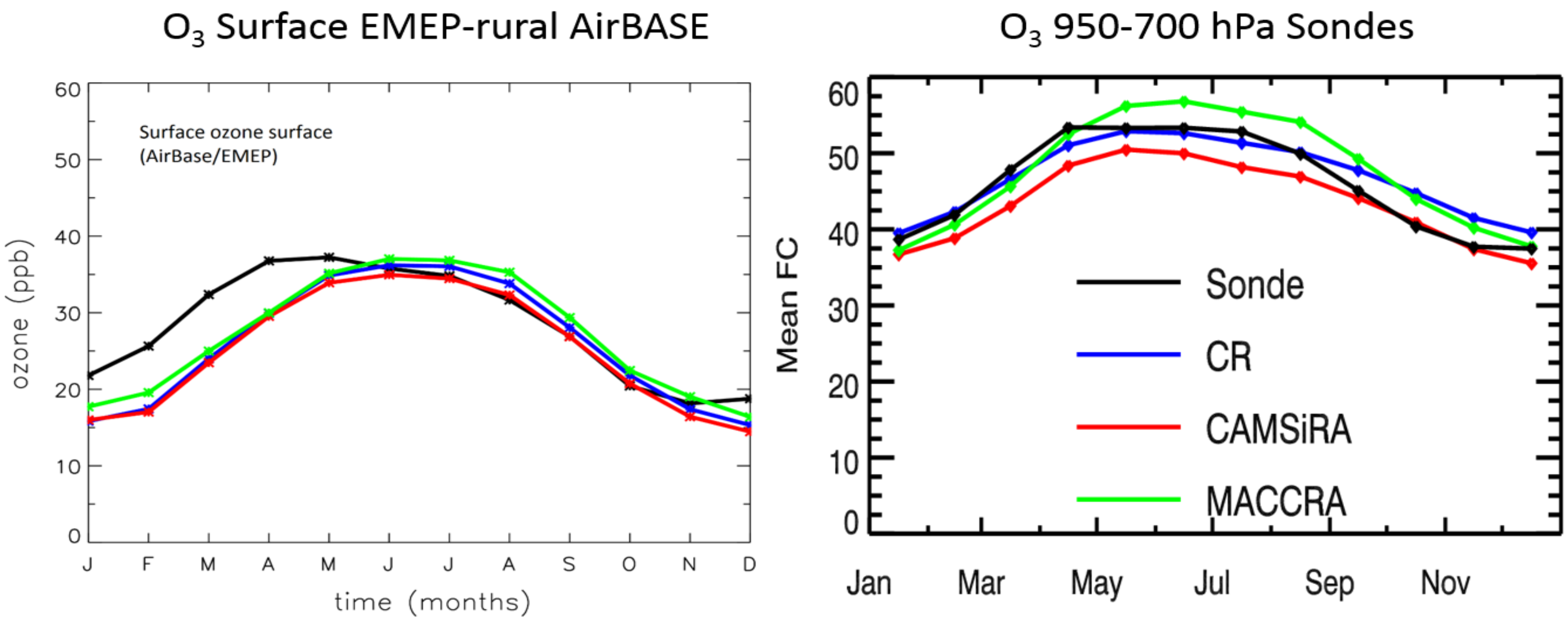


Figure 24 Average seasonal cycle of surface ozone at EMEP-AirBase stations (left) and at European ozone sonde sites in the pressure range (950–700 hPa) for CAMSiRA (red), CR (blue) and MACCRA (green).

Flemming et al. 2016

Summary : parameterisations vs. full scheme

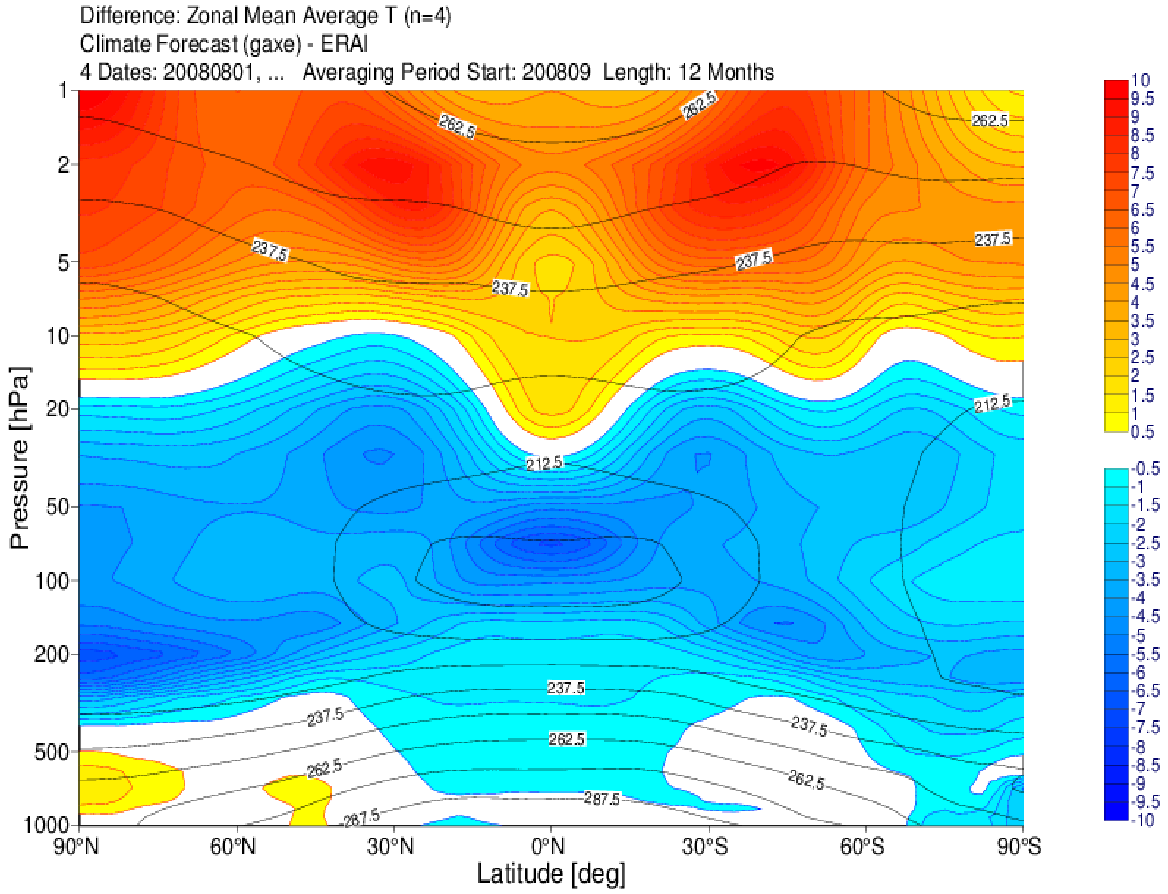
- Parametrisation scheme are more robust and computationally much cheaper
- Stratospheric ozone in chemical mechanism schemes is often better than in parameterisations - but only just
- Chemical mechanism schemes have more potential for understanding processes and the assimilation of other species (other than ozone)
- Tropospheric chemistry can not be dealt well with parameterisations
- Assimilation/re-analysis:
  - Ozone in the stratosphere (TC and profile) is well constrained by observations and the underlying model approach is less important
  - Modelling approach is important in upper stratosphere/mesosphere and troposphere

Impacts of Ozone in ECMWF model

I. Ozone in radiation scheme – impact on Temperature
II. Synergies of ozone assimilation within NWP assimilation

IFS temperature bias in 1yr forecast

IFS Temperature bias (EraInt)



"climate run" with 4 ensemble members

Can it be cured with mitigated with ozone in radiation scheme ?

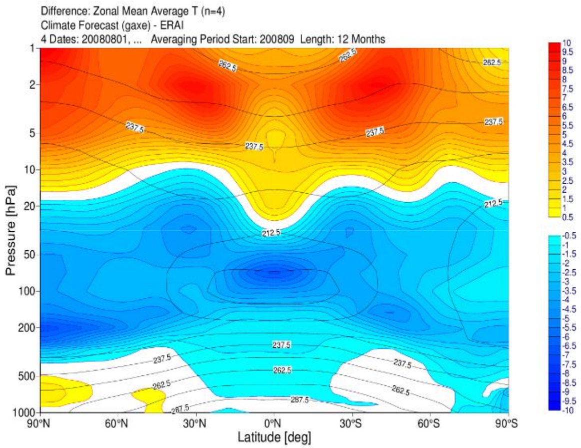
Testing different ozone representations in radiation scheme of ECMWF model (IFS)

- Ozone representations at ECWMF:
  - Monthly Climatology of MACC re-analysis (BASE)
  - MACC re-analysis 6 h (MACC6h)
  - Cariolle ozone parameterisation CAR
  - Monge-Sanz ozone parameterisation (as Cariolle but 3D model base) BMS
  - CB05 & BASCOE chemistry scheme C-IFS-B
  - CB05 & Cariolle chemistry scheme C-IFS-C
- 1-year “climate” runs (4 ensemble members) with interactive ozone

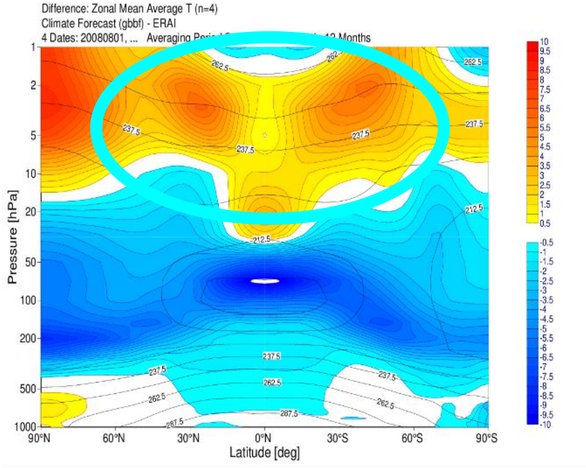
T bias w.r.t ERA interim in climate runs with different prognostic O_3 fields in radiation

IFS T bias Using MACC climatlogy

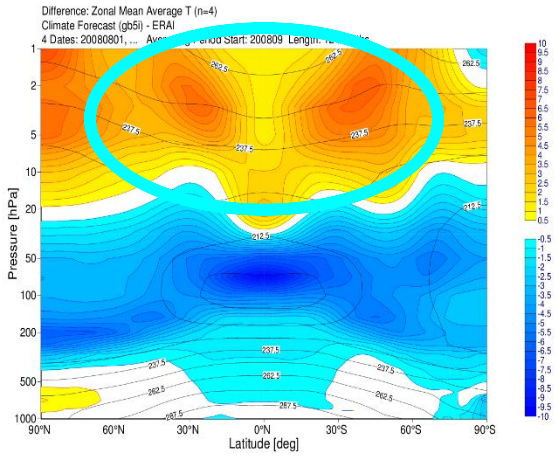
BASE

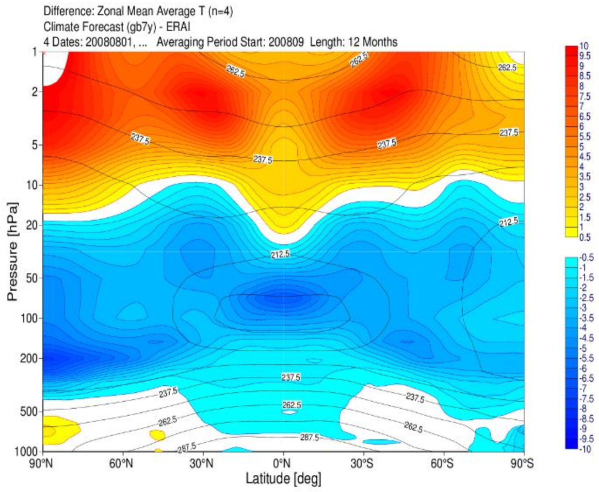


BMS

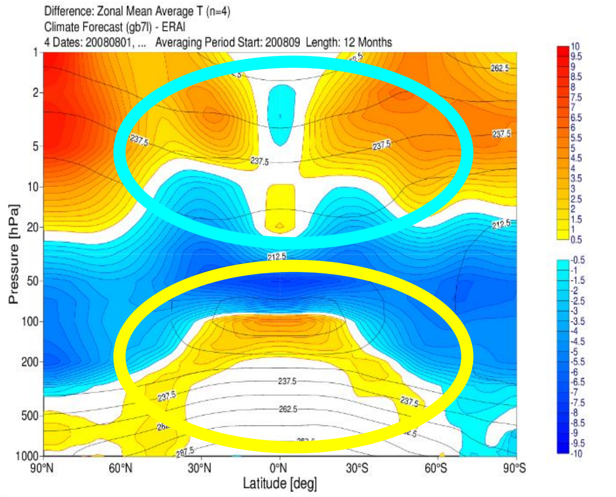


CAR

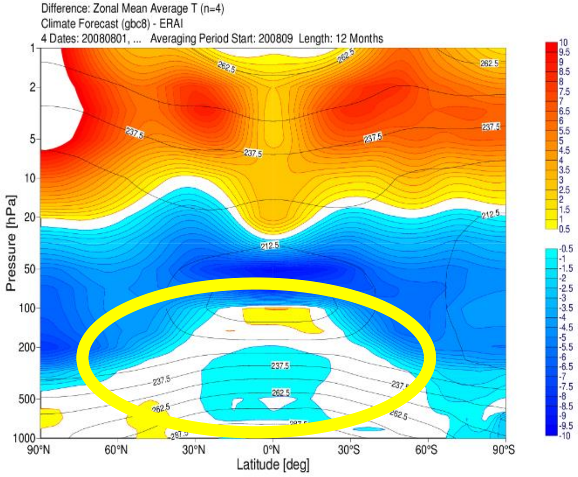




MACC-6hourly



C-IFS-CB05/Cariolle

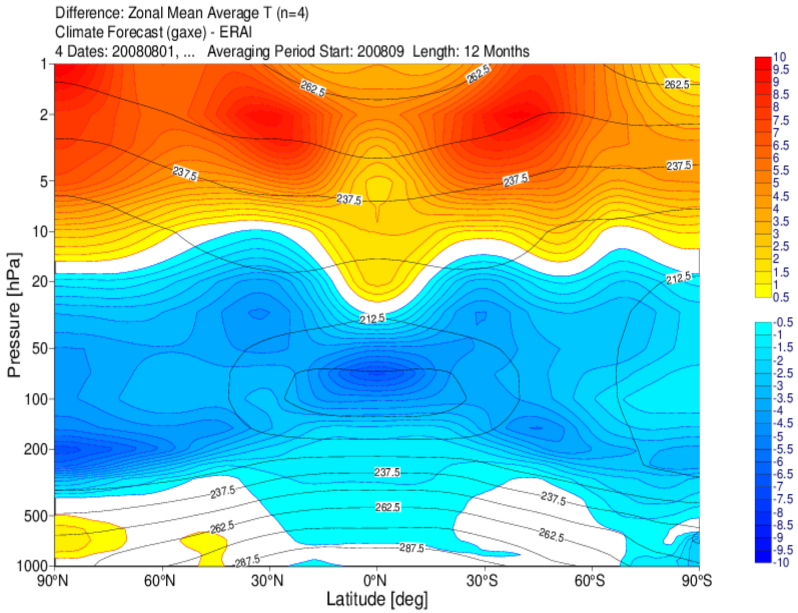


C-IFS-CB05/BASCOE

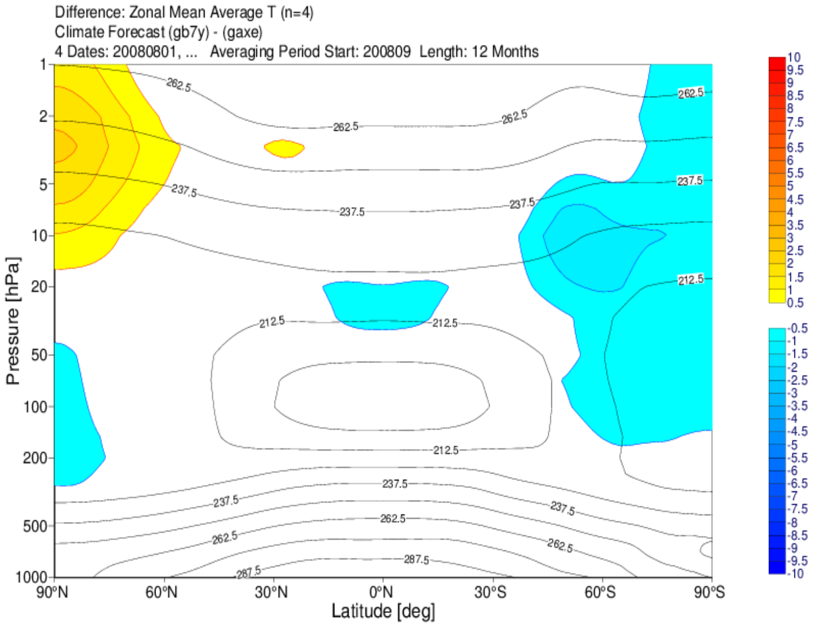
ECMWF

Monthly mean vs. 6 hourly MACC RA

T bias (12 month) of 1-year climate run (BASE) vs. ERA interim



T difference
Nudged (6h) O3 RA – base
(RA O3 MM)

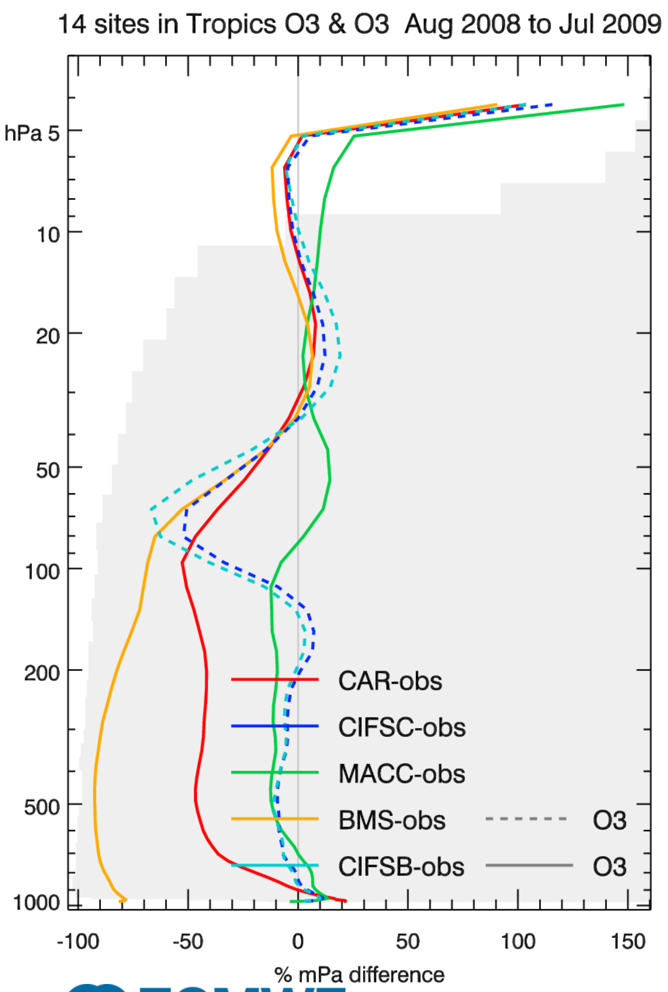


Change in “prognostic vs. climatological ozone is less important. T biases could be perhaps be cured already with better O3 climatology.

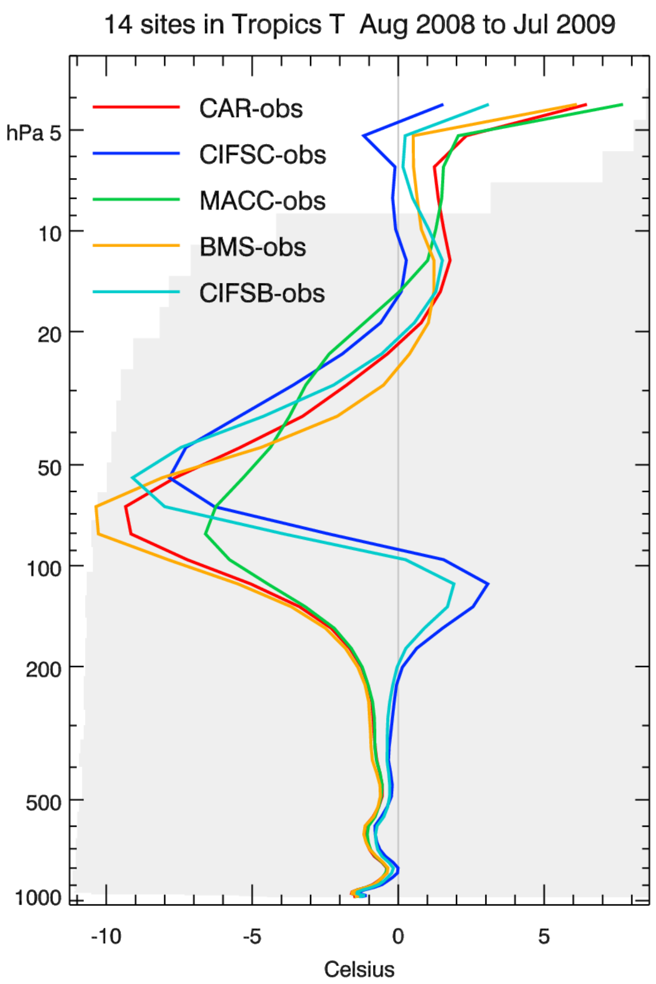
Note that 6 h MACCRA O_3 is not synoptically consistent with 1-year climate run

O_3 & T biases w.r.t v ozone sondes (Tropics: surface up to 5 hPa))

O3 bias %



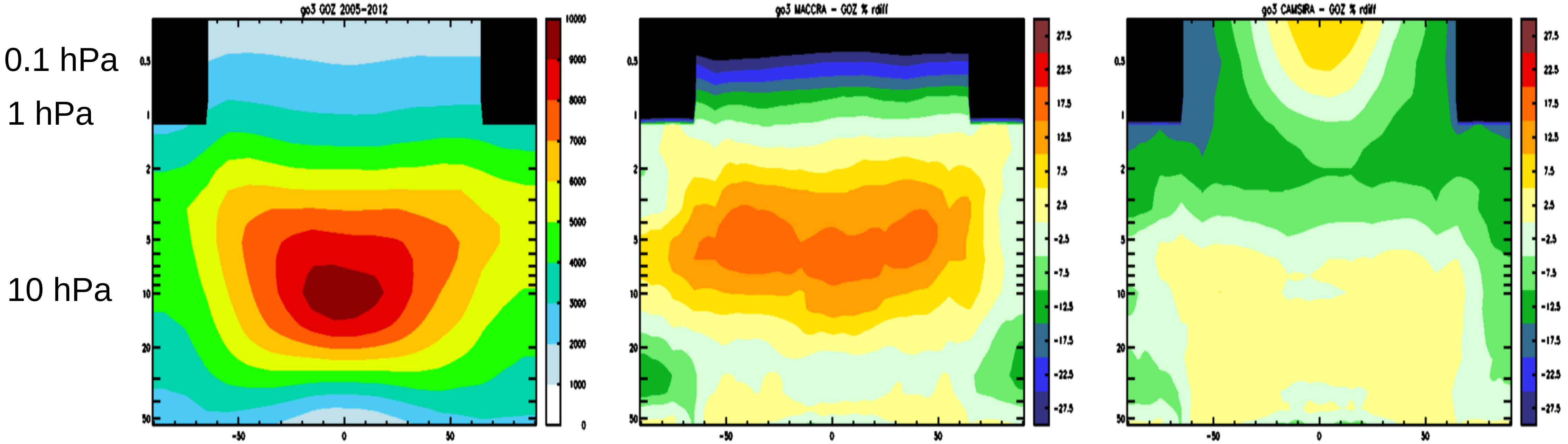
T bias K



Green has lowest Ozone bias against sondes but not lowest T bias if used interactively

Exception: Upper troposphere

Bias of MACC (IFS) and CAMS) O_3 climatology against GOZCARDS (ACE-FTS, MLS)

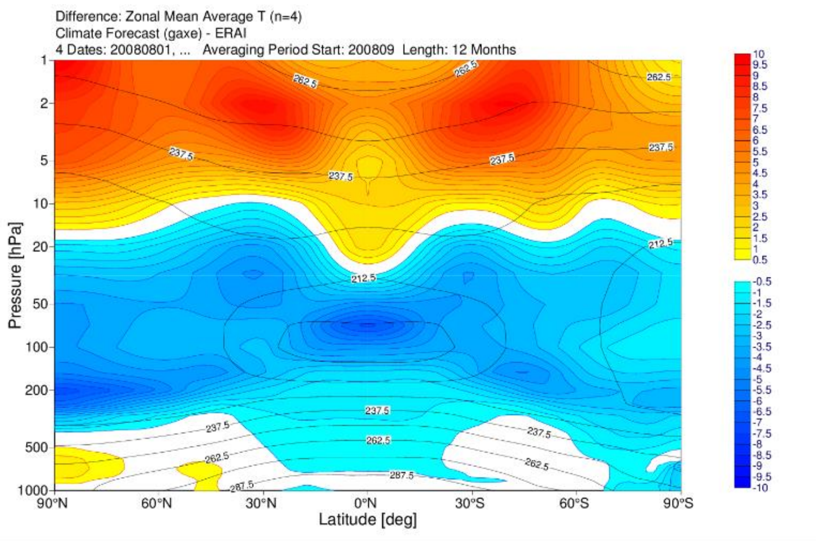


GOZCARDS

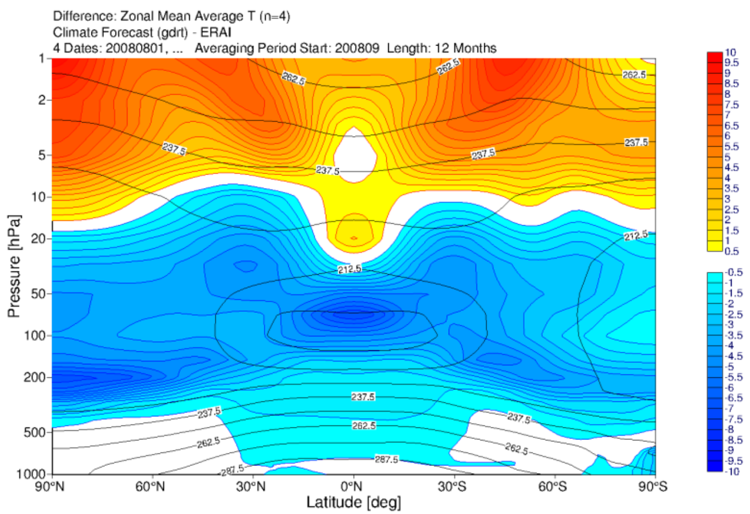
Relative Bias
MACC climatology
IFS operational

Relative Bias
CAMS climatology
IFS new operational

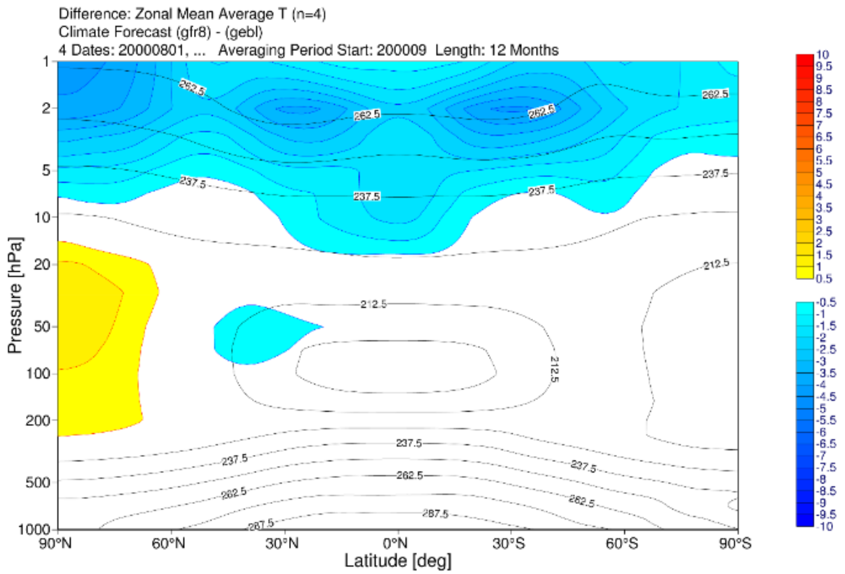
Impact of new ozone climatology in 1 yr. climate runs



MACC RA Clim



CAMS RA Clim

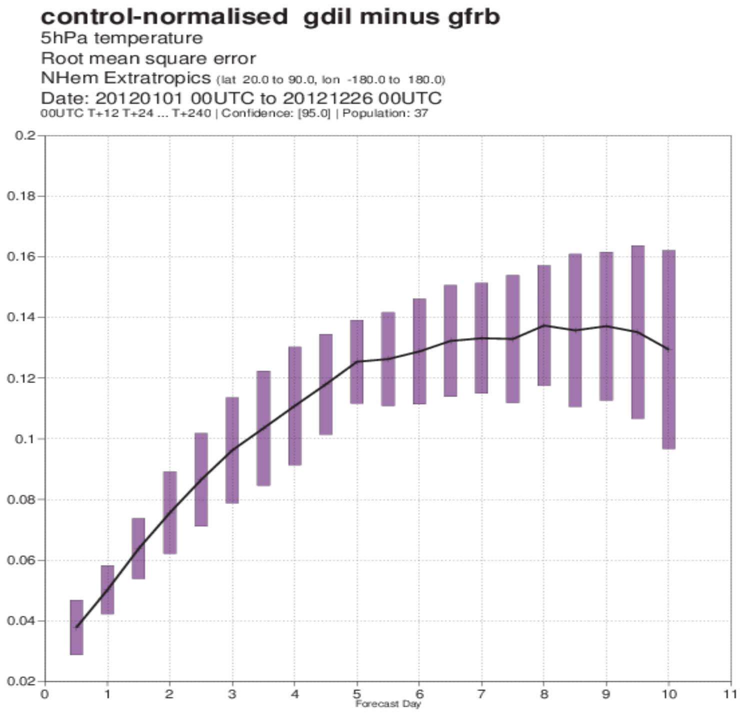


DIFFERENCE

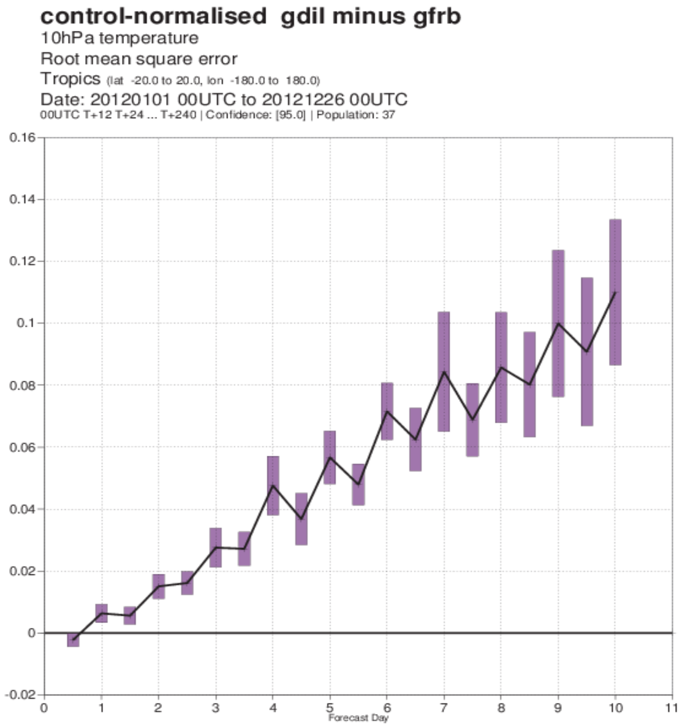
ECMWF

Reduced upper stratospheric biases in 10-day forecast with new climatology

RMSE change T 5 hPa NH ET
CNTR (MACC O3) vs NEW (CAMS O3)



RMSE change T 10 hPa Tropics
CNTR (MACC O3) vs NEW (CAMS O3)



ECMWF

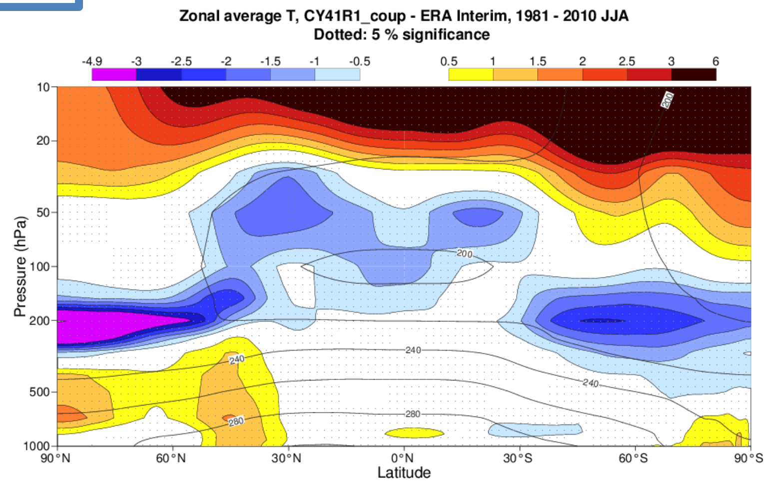
Next Steps … explore impact on UTLS Temperature bias by using CAMS prognostic O_3

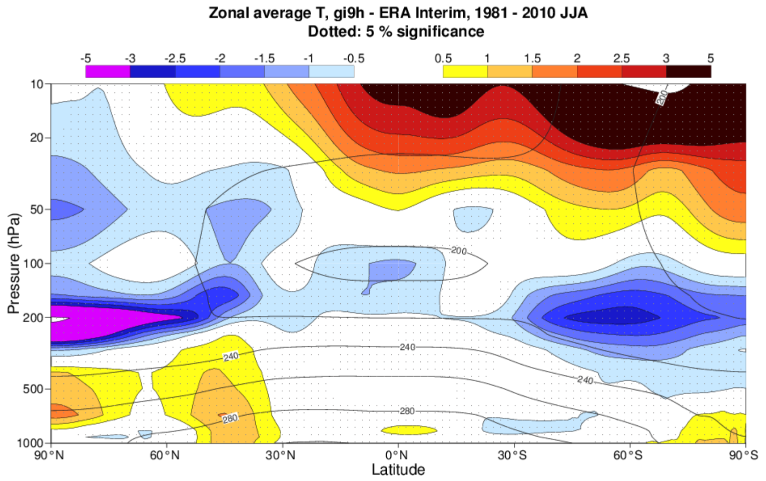
Improved Temperature Biases using BMS-ozone scheme in seasonal runs

JJA

Control – ERA Interim

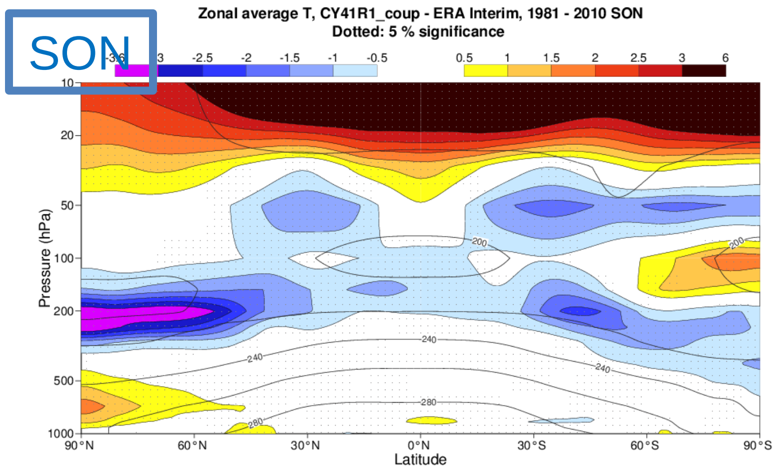
New BMS O_3– ERA Interim

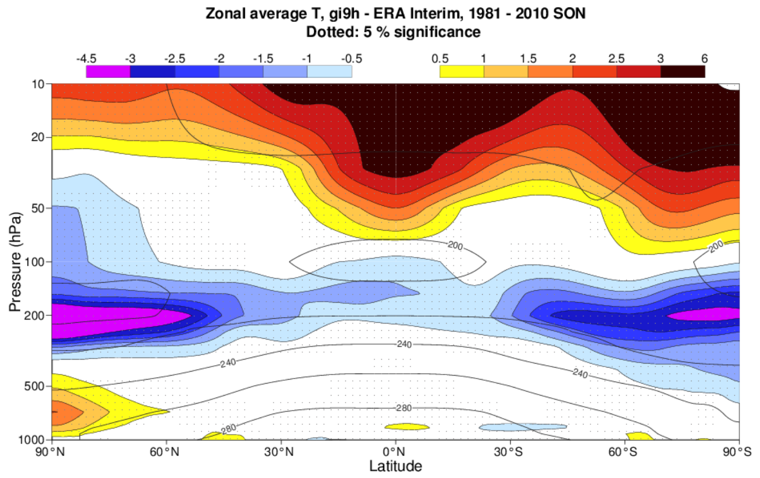




Control=
MACC RA
climatology

SON





ECMWF

Beatriz Monge-Sanz, Linus M.

Summary Ozone Temperature feedback

- Different ozone representations in radiation scheme lead to considerable temperature differences in 1-yr run in stratosphere and upper troposphere
- IFS temperature biases not curable with ozone alone
- The biases of the ozone representation are very important and less so the variability.
- Improved ozone climatology (CAMSiRA) gives improved T (and u &v) in climate runs **and** 10 day forecasts (Cy43R1) in upper stratosphere
- It is important to verify that any T improvement is due to improved ozone fields and not compensating errors
- Next step to explore prognostic tropospheric ozone from CAMS in radiation scheme in more detail

Impacts of Ozone in ECMWF model

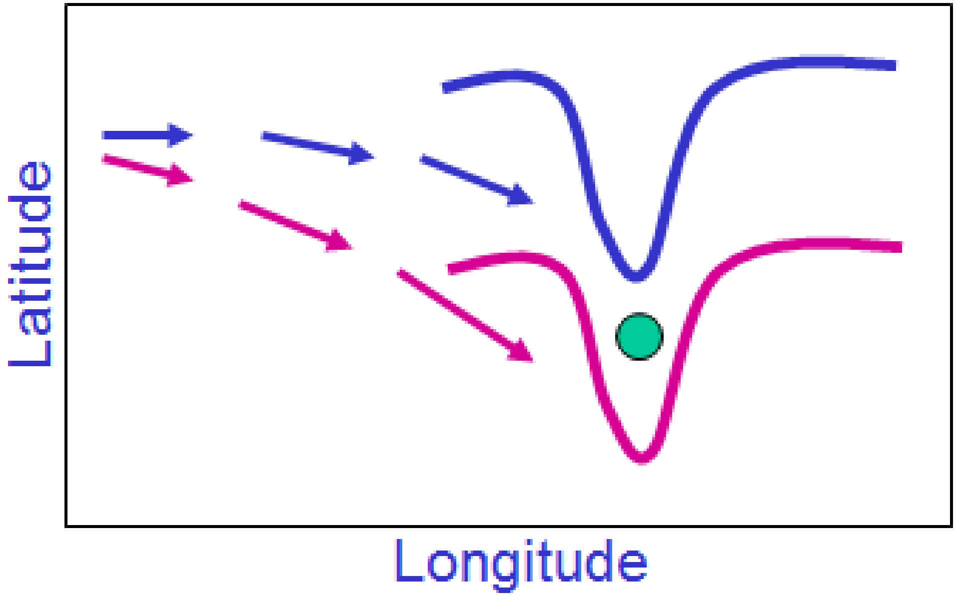
I. Ozone in radiation scheme – impact on Temperature

II. Synergies of ozone assimilation within NWP assimilation

   - Ozone assimilation to extract dynamical information
   - Ozone in NWP radiance retrievals (RTTOV)

Wind information from ozone assimilation in 4D-VAR

- Potential was demonstrated in early studies for H_2O (Thepaut 1992) and O_3 (Daley 1995; Riishojgaard 1996; Holm 1999; Peuch et al. 2000, Semane et al. 2009).
- Could compliment existing wind observations and help in areas where there is a lack of adequate global wind profile data



Coupling between tracer and wind field in 4D-Var: illustration using 1D advection model

Model equations

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2}$$

$$\frac{\partial q}{\partial t} + u\frac{\partial q}{\partial x} = 0$$

$u = u(x,t)$ = wind over periodic domain [0,L]
$q = q(x,t)$ = passive tracer
ν = diffusion coef.
$\delta u, \delta q$ = perturbations
$\delta' u, \delta' q$ = adjoint variables

Tangent linear equations:

$$\frac{\partial \delta u}{\partial t} + u\frac{\partial \delta u}{\partial x} + \delta u\frac{\partial u}{\partial x} = \nu\frac{\partial^2 \delta u}{\partial x^2}$$

$$\frac{\partial \delta q}{\partial t} + u\frac{\partial \delta q}{\partial x} + \delta u\frac{\partial q}{\partial x} = 0$$

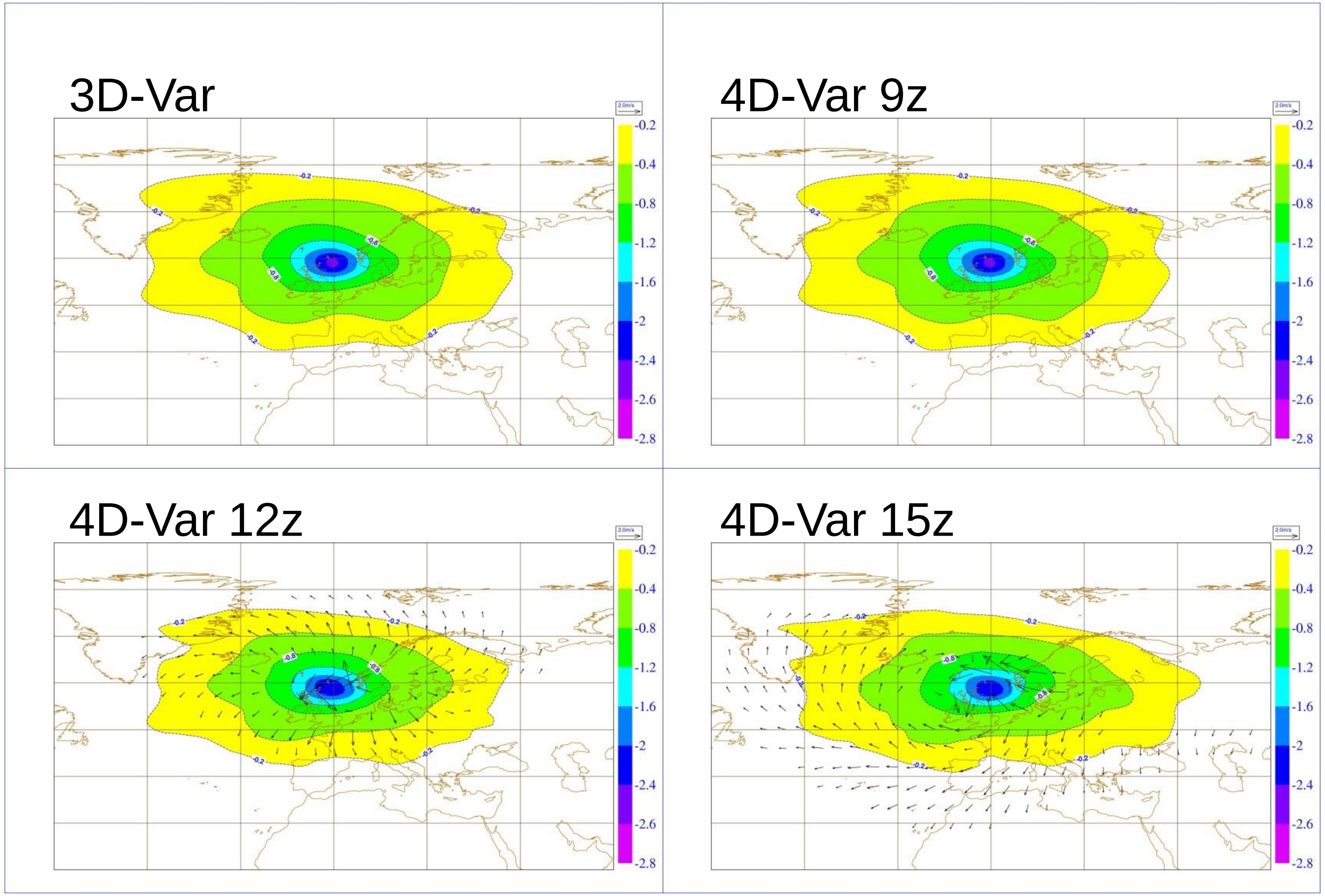
Adjoint equations:

$$-\frac{\partial \delta' u}{\partial t} - u\frac{\partial \delta' u}{\partial x} + \frac{\partial u}{\partial x}\delta' u - \nu\frac{\partial^2 \delta' u}{\partial x^2} + \delta' q\frac{\partial q}{\partial x} = 0$$

$$-\frac{\partial \delta' q}{\partial t} - \frac{\partial (u\delta' q)}{\partial x} = 0$$

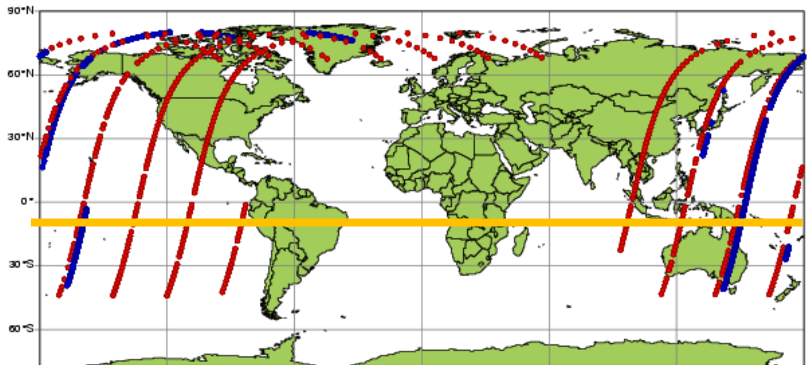
Single observation experiments - Ozone and wind increments

Antje Inness



Level 20,
≈ 30 hPa

Impact of ozone data in 4D-Var: Example from ERA-Interim



GOME 15-layer profiles (~15,000 per day)

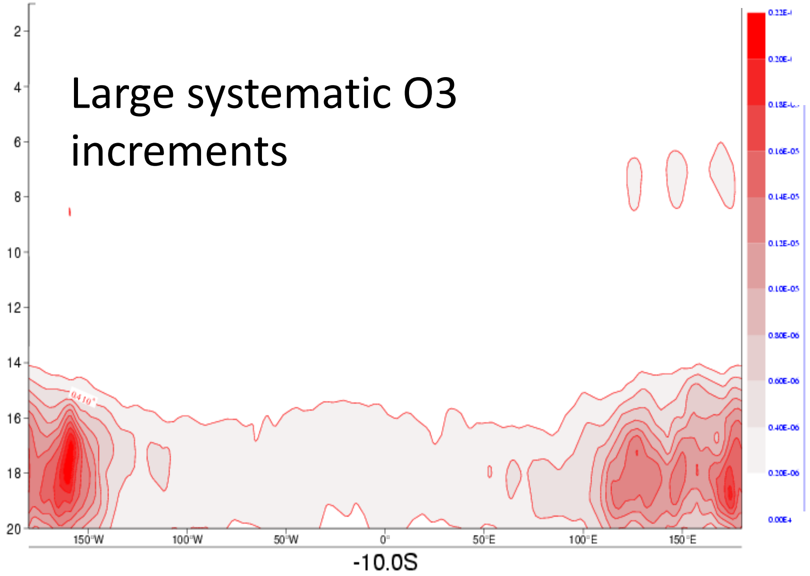
SBUV 6-layer profiles (~1,000 per day)

The stratosphere is not well constrained by observations:

- Ozone profile data generate large temperature increments
- 4D-Var adjusts the flow where it is least constrained, to improve the fit to observations

=> IFS O3 analysis is completely uncoupled now

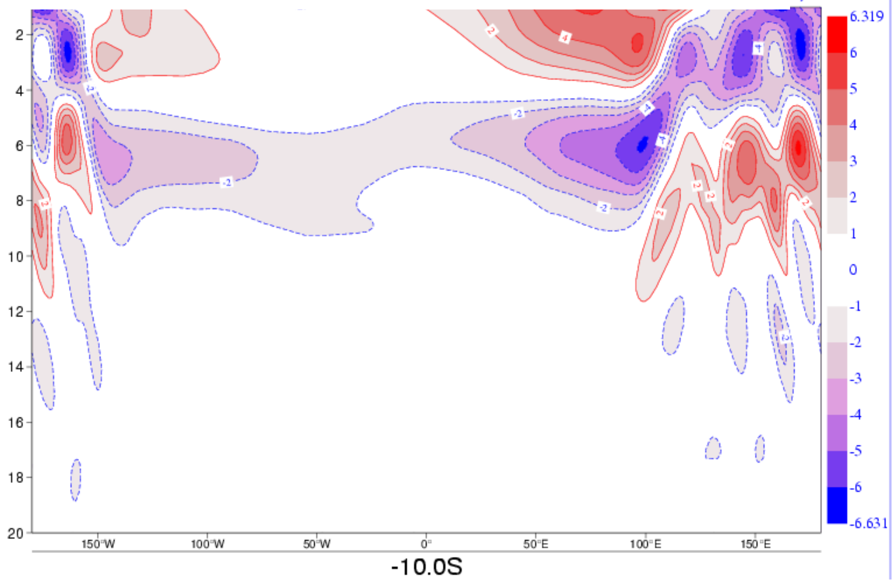
Ozone increments at 10S



1 hPa

20 hPa

Associated Temp increments

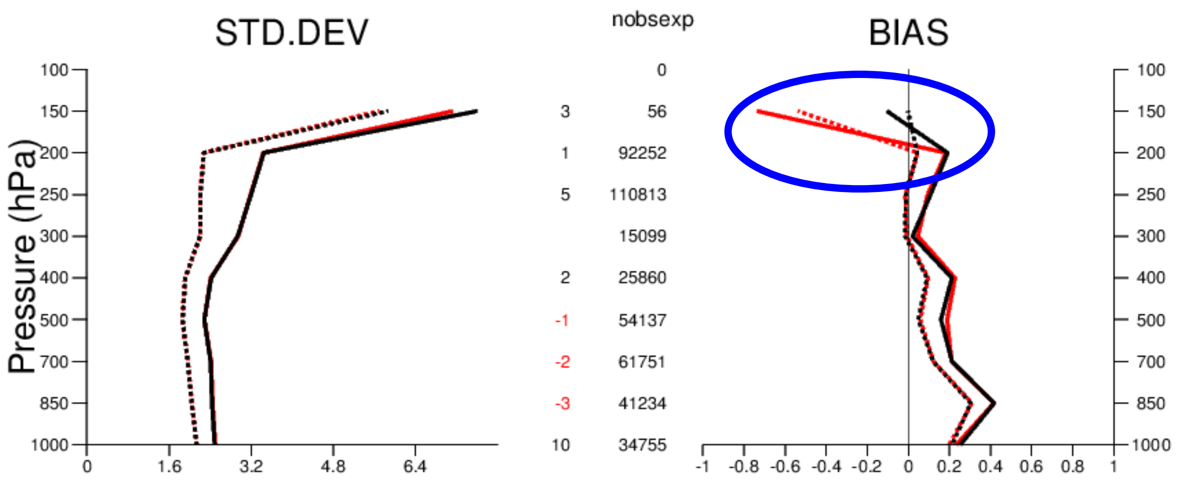


D. Dee

Link within 4D-Var - tracer

Rossana Dragani

Used AIREP-V wind (Tropics)



Some positive impact found in the upper troposphere (~ 150 hPa) in the tropics and in the summer extra-tropics – though small number of observations.

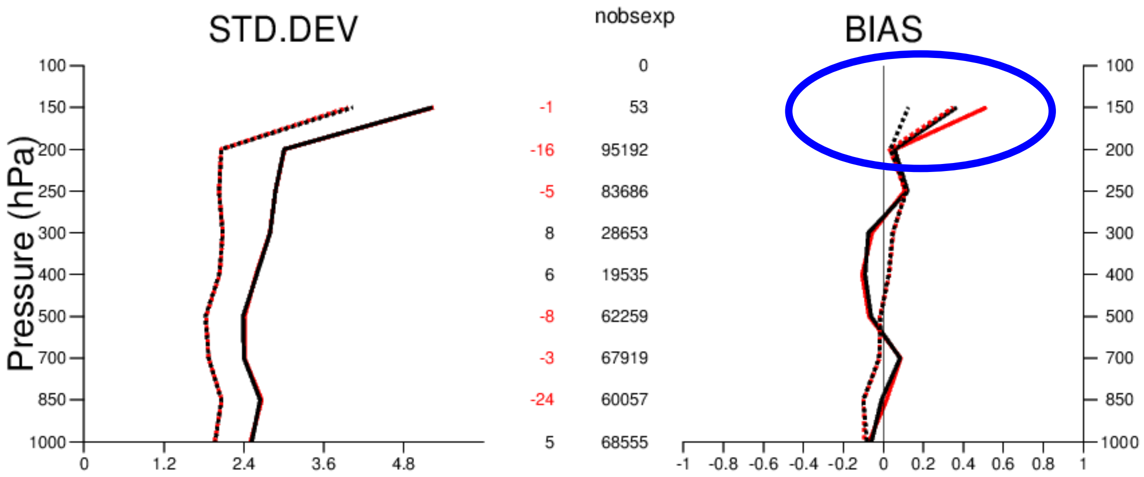
O-B (CTRL)

O-B (4D-Var ON)

O-A (CTRL)

O-A (4D-Var ON)

Used AIREP-V wind (SH)



Summary synergy wind ozone

- Successful idealised studies
- Mixed results with ECMWF model
  - ERA interim, more testing (A. Inness, pers. communication)
  - More encouraging more lately (R. Dragani)
- The success is depends
  - on the quality and number of available observations both for ozone and the T data
  - On quality on background error statistics
- IFS Kalman Filter (Hamrud and Bonavita, 2015) interesting new approach as missing covariance term (O3 DIV/VOR) is calculated from ensemble
  - Encouraging preliminary results for KF assimilation of CH_4 (S. Massart)

O_3 impact in NWP radiance assimilation:

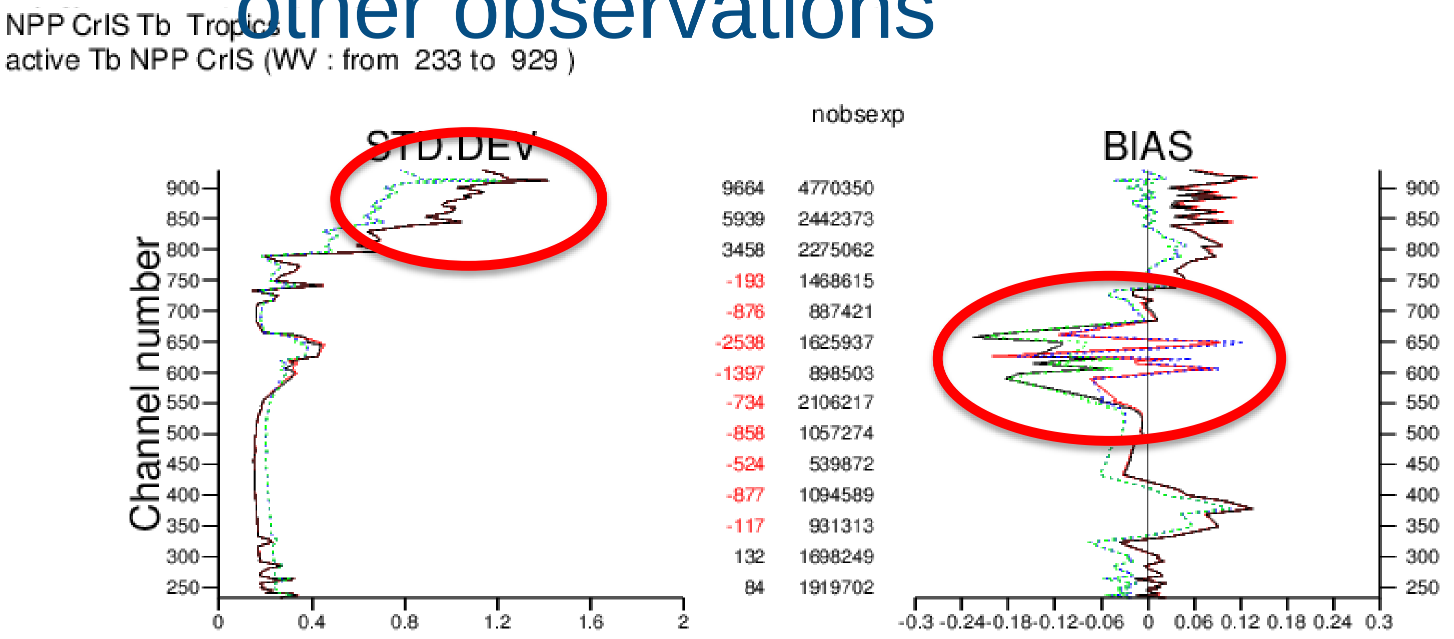
- Impact of using a prognostic O3 in RTTOV vs. use of an ozone climatology
  - Direct impact on satellite radiance assimilation, particularly in the tropics, e.g. on WV channels
  - (Most likely indirect) Impact on the lower troposphere humidity observations from conventional network
  - Synergy between ozone-sensitive channel assimilation and ozone retrievals lead to significant positive impact on forecast scores

PRELIMINARY RESULTS ARE PROMISING

(R.Dragani)

Impact of O3 assimilation on the assimilation of other observations

Satellite observations



O-B (CTRL)

O-B (NoO3_Assim)

O-A (CTRL)

O-A (NoO3_Assim)

Conventional observations

Use prognostic ozone in RTTOV
Satellite radiances

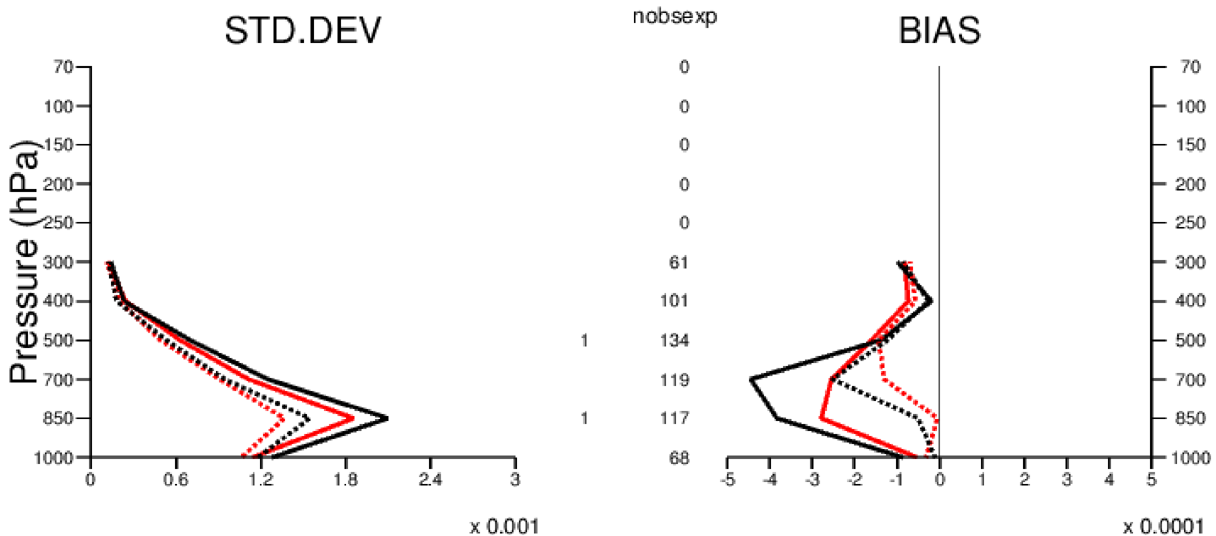
O-B (CTRL)

O-B (NoO3_Assim)

O-A (CTRL)

O-A (NoO3_Assim)

Used Drop-q (Tropics)

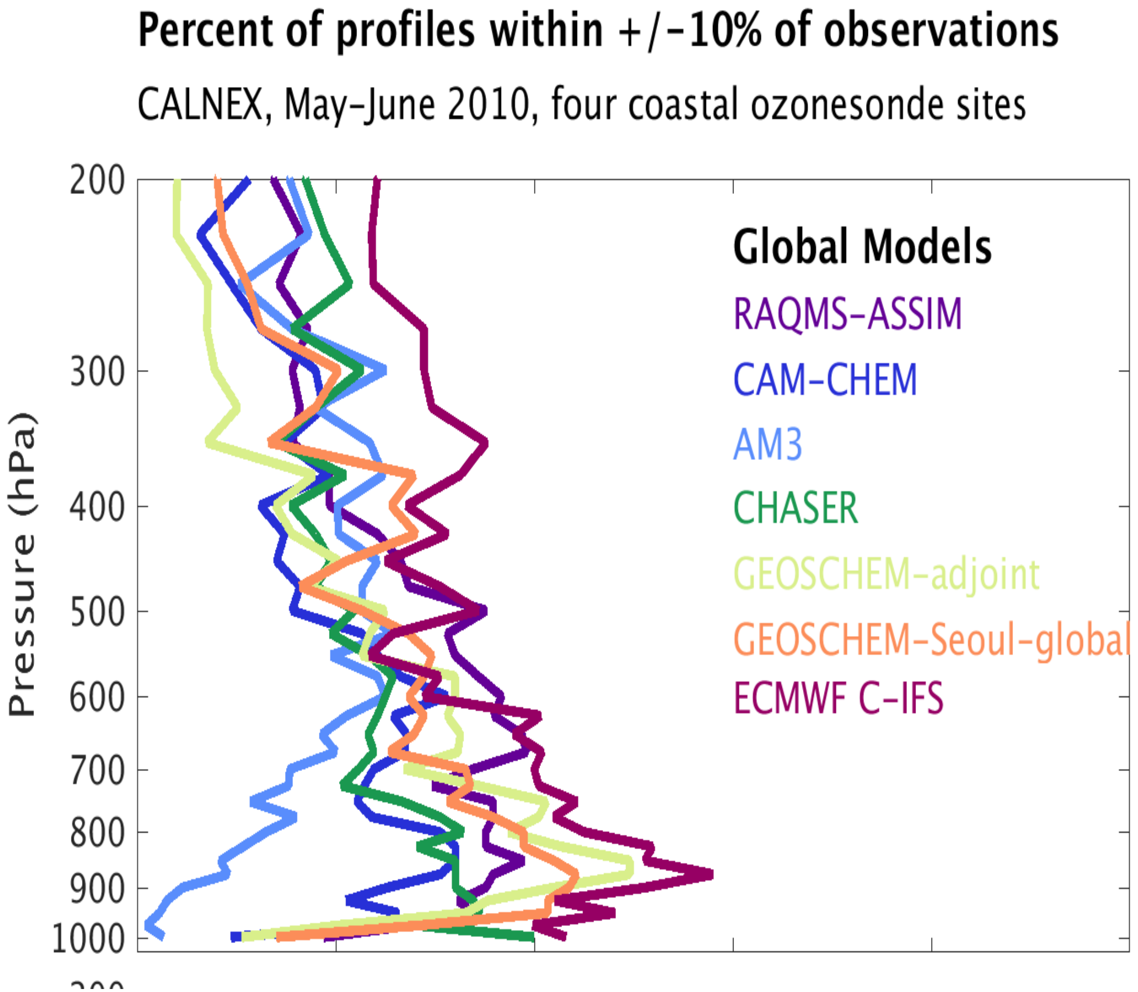


Is the IFS a good model to simulate ozone and atmospheric composition ?

- Yes !
  - Excellent meteorology
  - High computational efficiency
- But there are also issues:
  - No mass conservation of SL transport scheme – partially solved with global mass fixers
  - Stratospheric transport
- Resolving these issues may help NWP progress
- Tracer are good way to test transport on different scales

C-IFS tropospheric ozone simulation without data assimilation

<u>Model success rate:</u>
The frequency that a model is within +/- 10% of the co-sampled observations.

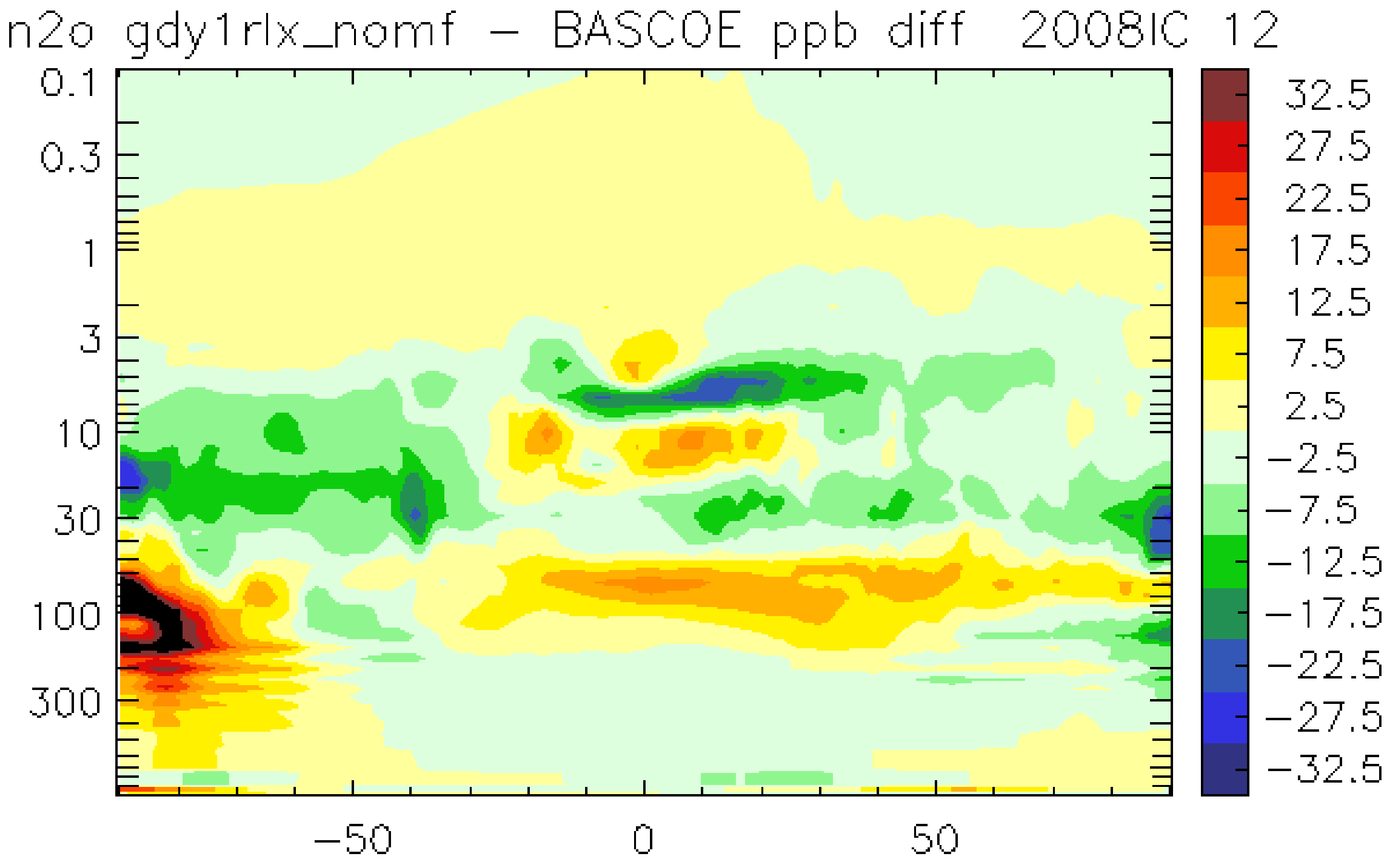


Inflow processes influencing air quality over
Western North America:
models vs.
observations

C-IFS benefits from IFS qualities
(also high computational efficiency that allows high resolution chemistry run T255)

Owen Cooper

Using long-lived tracer N_2O to diagnose stratospheric transport



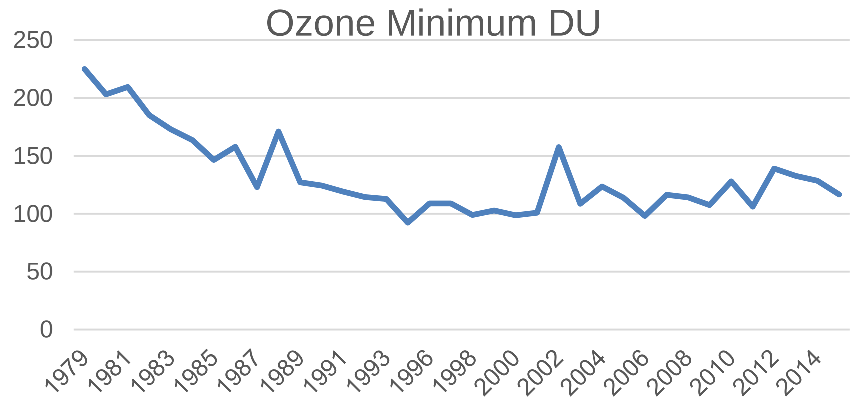
N_2O forecast bias after 4 month
Against MLS-BASCOE N_2O analysis

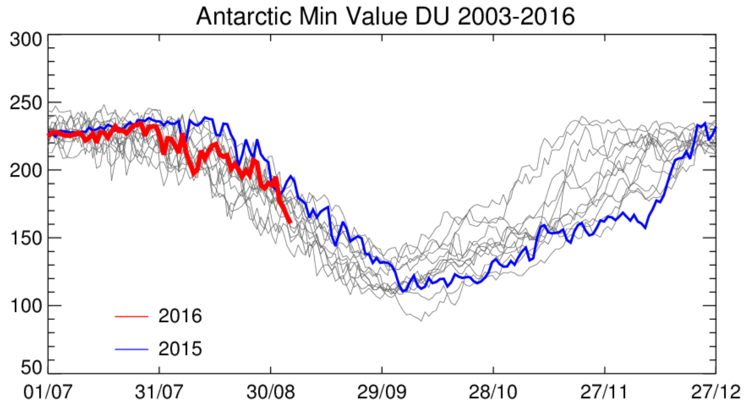
Initialised with MLS-BASCOW N_2O analysis

Ozone hole 2016

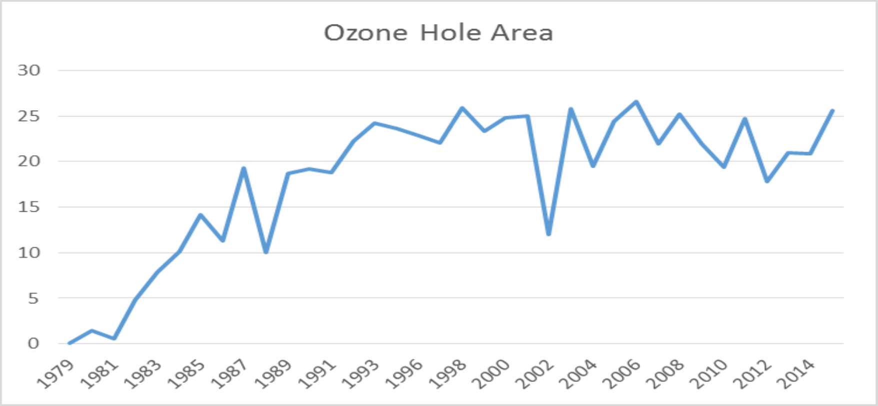
Ozone hole 1979-2015
NASA

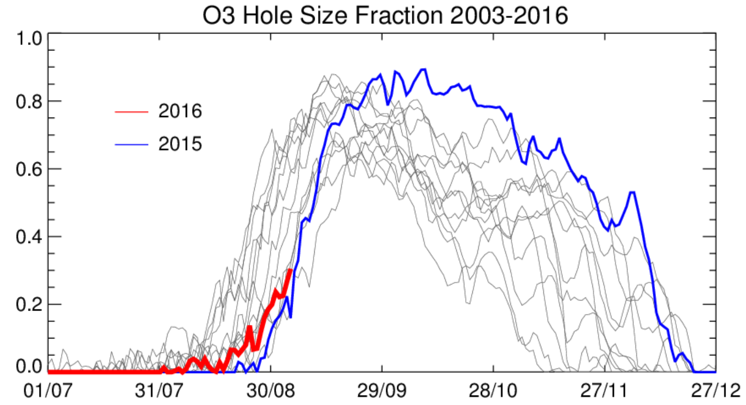
Ozone hole 2003-2016
CAMS – ECMWF (1.7-31.12)





Minimum





Area

NASA Record

Copernicus Atmosphere Service - ECMWF

Summary

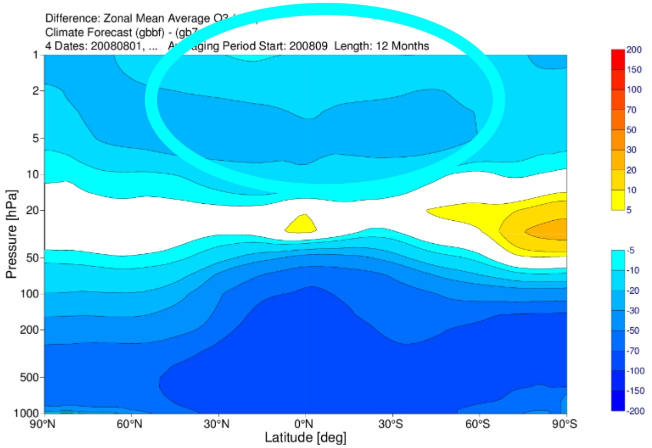
- ECMWF has two approaches to simulate ozone chemistry
  - NWP/RA ozone with focus on stratosphere (Cariolle scheme)
  - CAMS: operational composition forecast, which include stratospheric and tropospheric ozone (chemical mechanisms)
  - Assimilation of ozone retrieval with 4D-VAR system is the main objective at ECMWF for simulating ozone
- Ozone in NWP radiation scheme
  - Strong T response due to different ozone representations in 1yr runs
  - Improved ozone representation helped to improve upper stratospheric positive bias in 1yr runs **and** operational 10-day forecasts
  - *Investigate radiative impact tropospheric ozone with full chemistry*
  - *Benefit of prognostic ozone vs. improved climatology to be further studied for different time scales*
- Benefits of joint ozone and NWP assimilation
  - Improved representation in radiative transfer calculation
  - Extracting wind information with mixed results

Thank you !

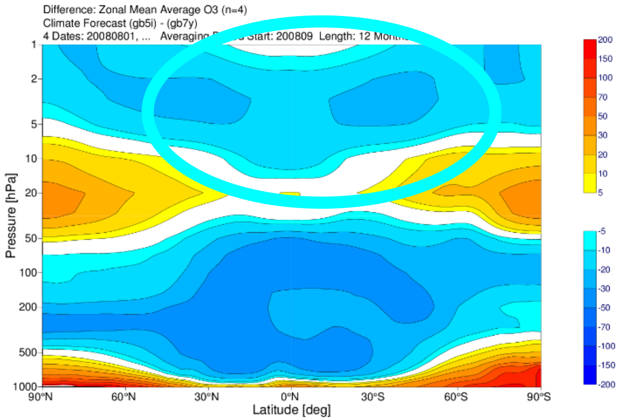
O_3 - O_3 MACC RA in %

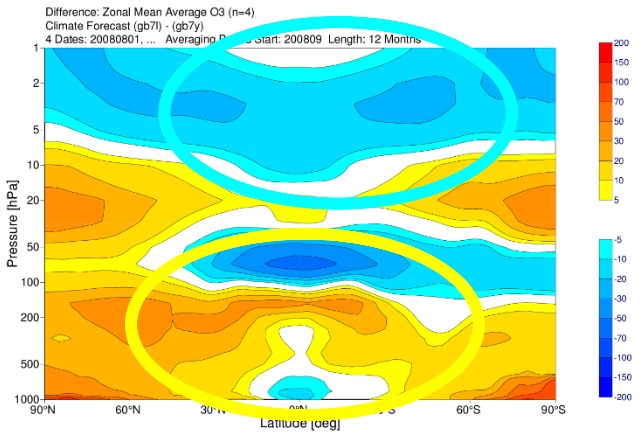
Base

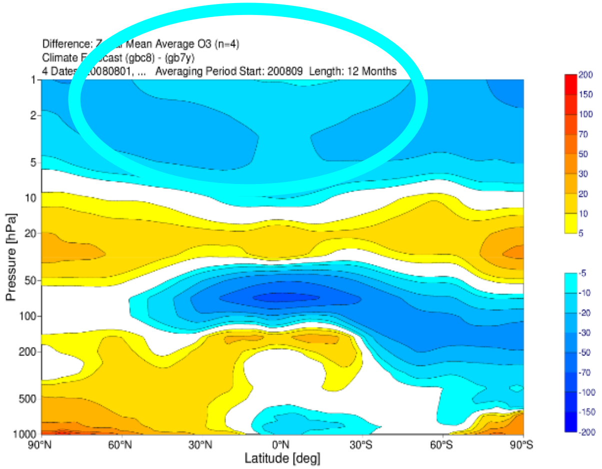
BMS



CAR







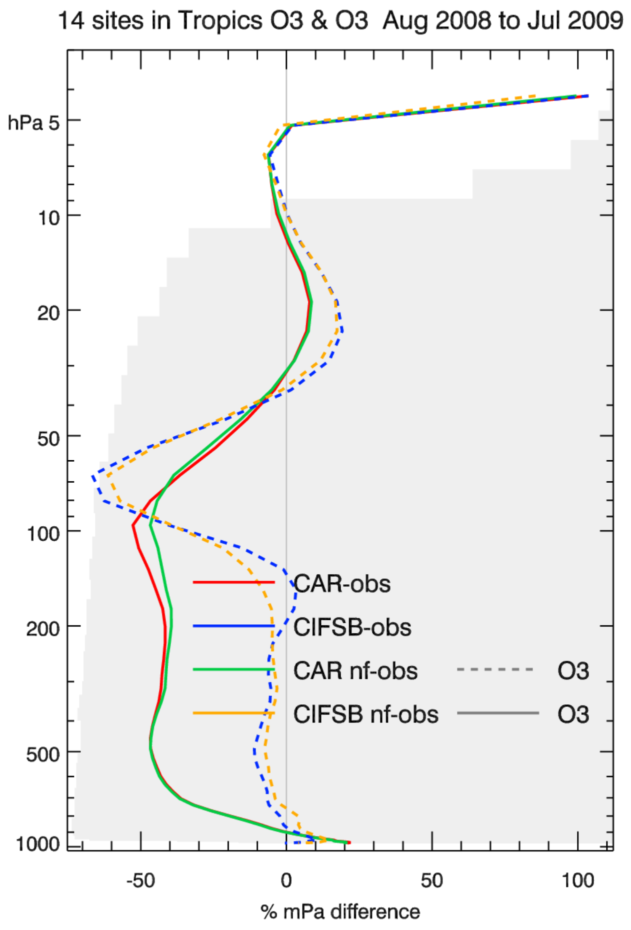
MACC-6h

C-IFS-C

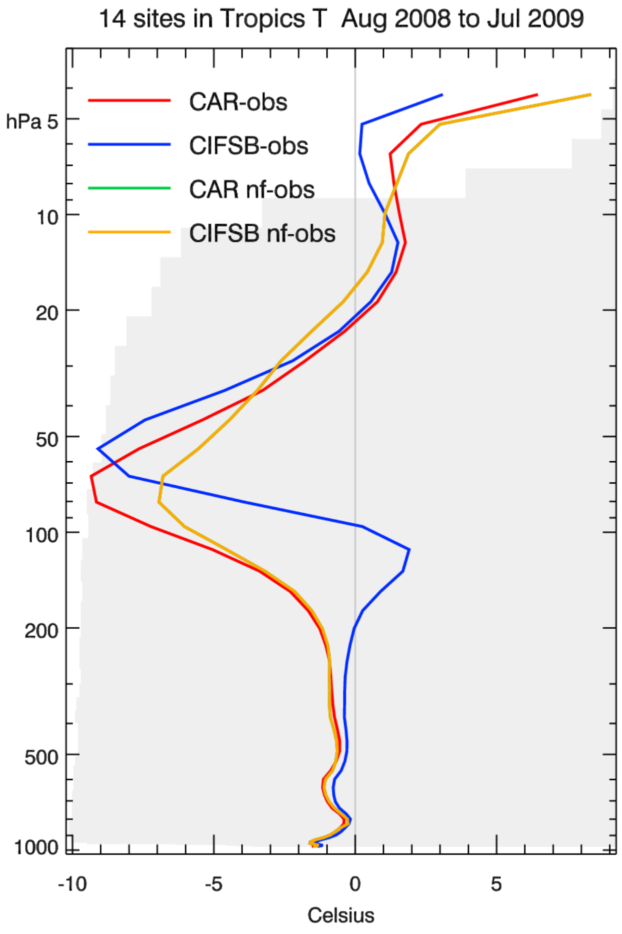
C-IFS-B

Impact of T changes on O_3 (sondes) (Tropics)

O3 bias %

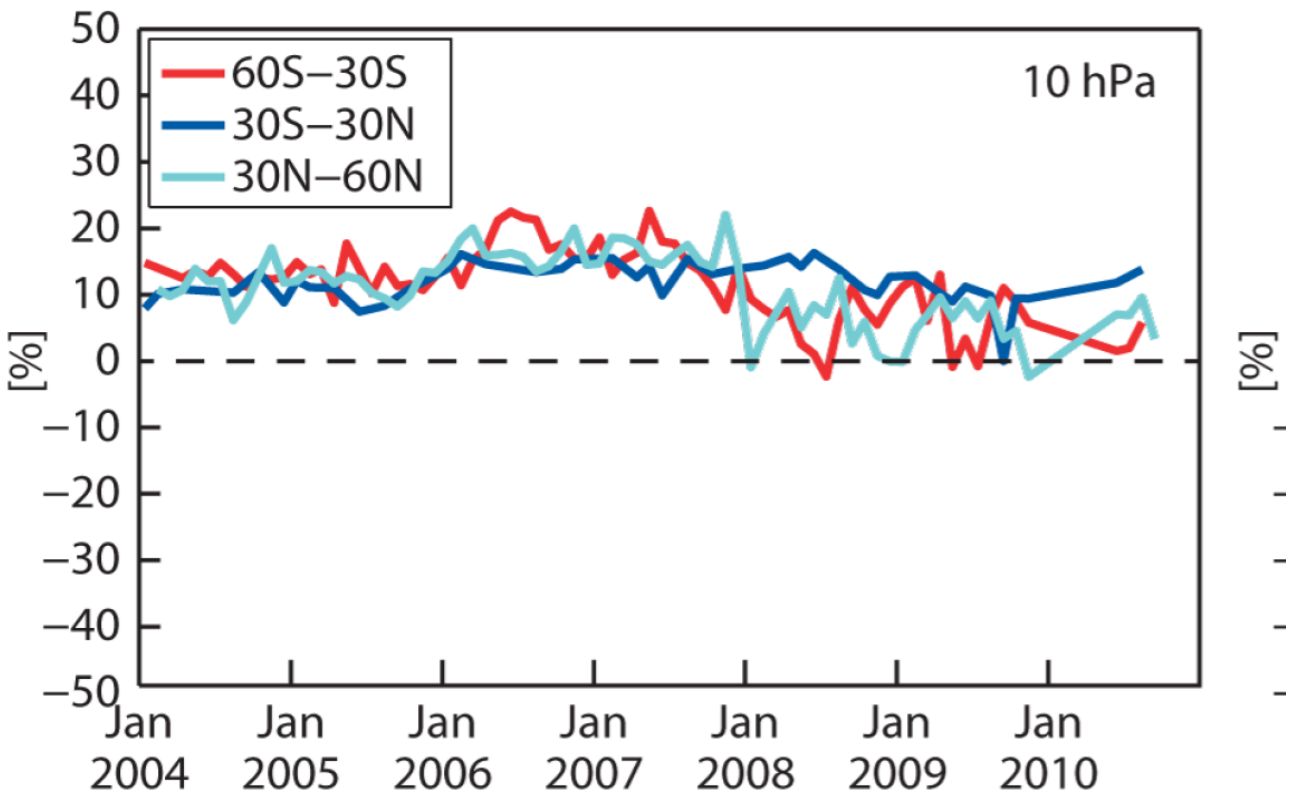


T bias K



nf
no prognostic ozone in Rad
NF CAR and nf CIFSB are the same.

Bias of MACC RA w.r.t ACE-FTS

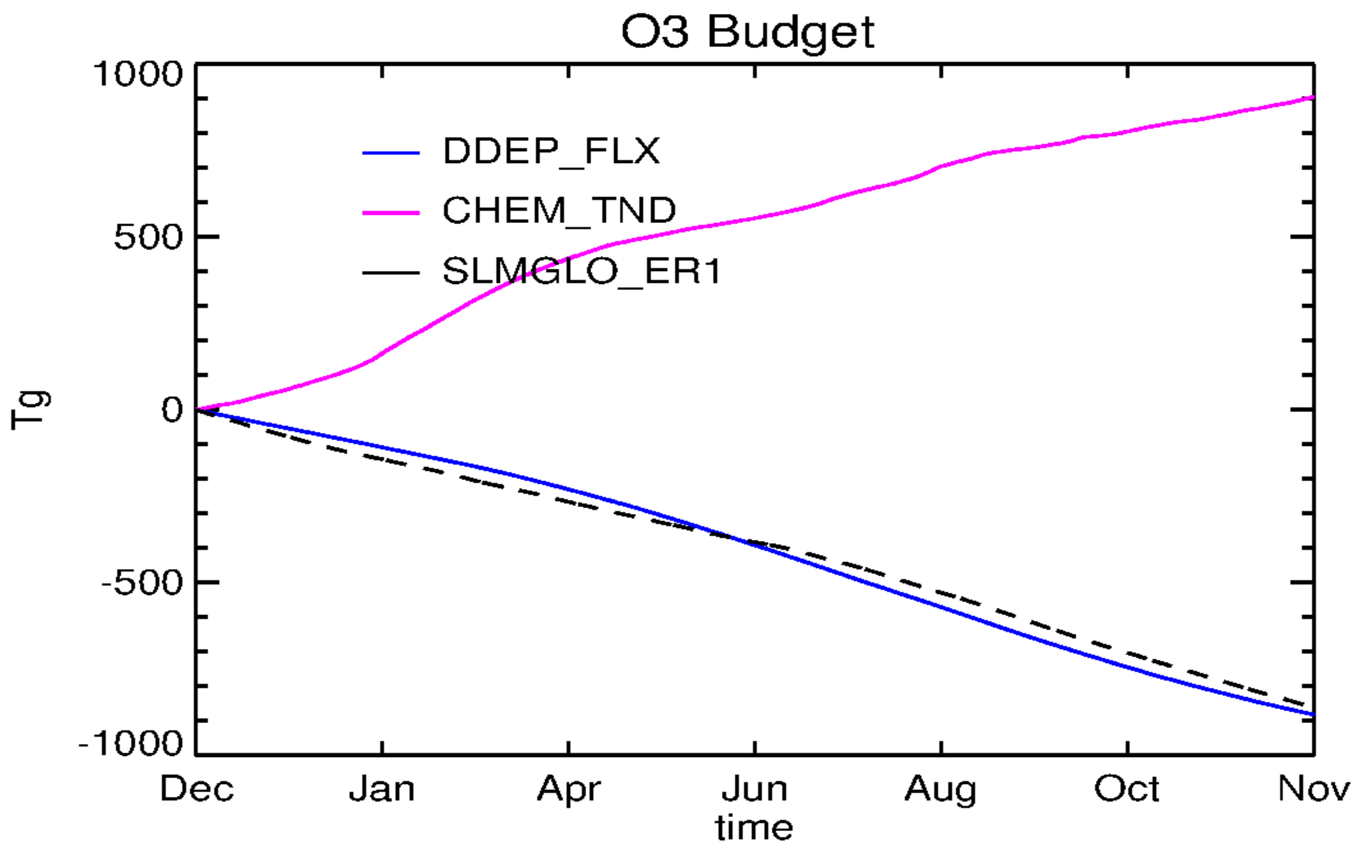


Inness et al. 2013

ECMWF

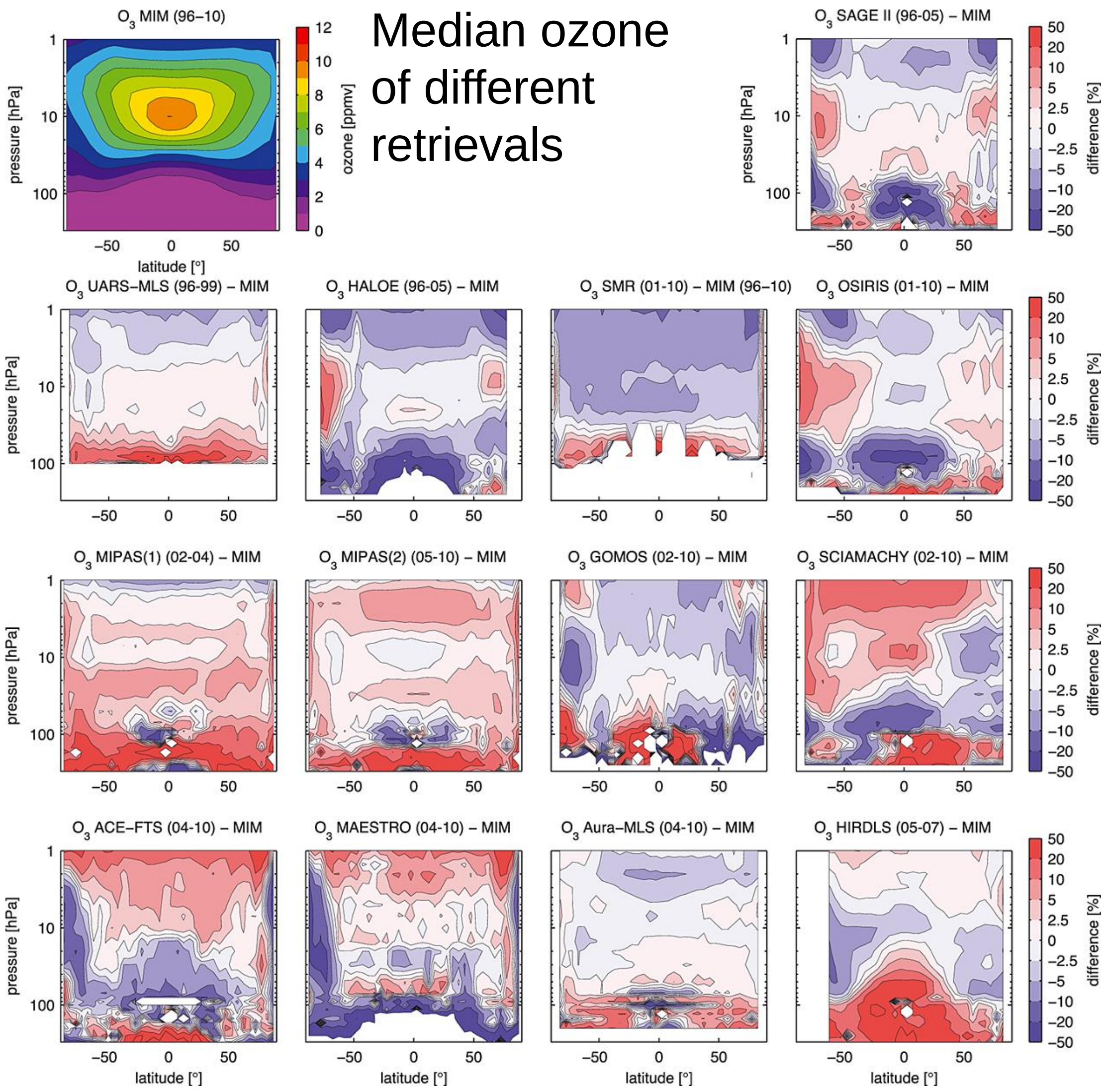
Mass Conservations

- Global Mass Fixers (Flemming and Huinen et al. 2011, Diamantakis and Flemming, 2014)
- Specific optimisation CH4 and CO2 (Agusti-Pandareda et al. 2016)



Multi instrument Ozone Retrievals

Median ozone of different retrievals

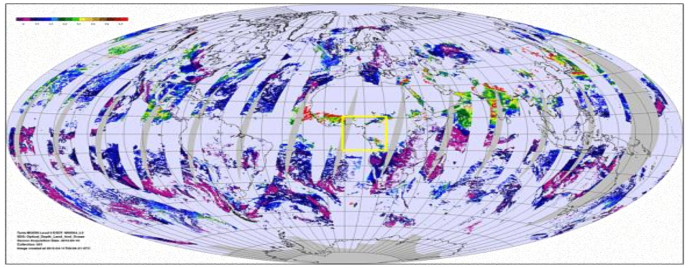


Differences of Instruments retrievals against multi-instrument median

SPARC data initiative
Tegtmeier et al. 2013, JGR

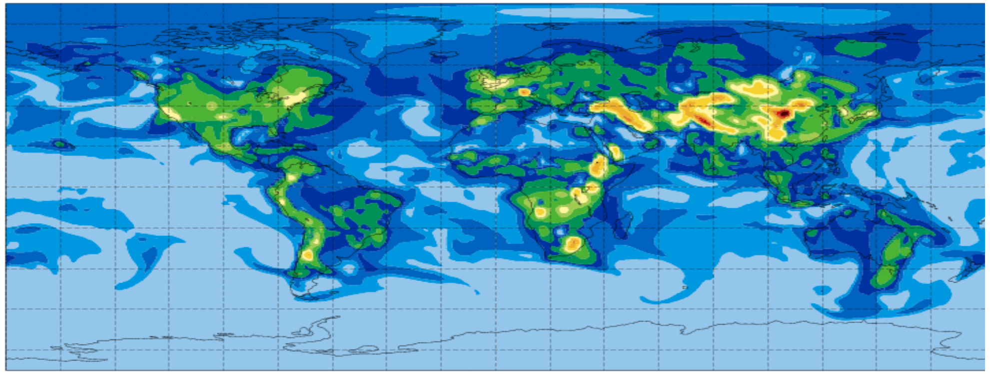
ECMWF

CAMS System: From Earth Observation to air-quality forecast



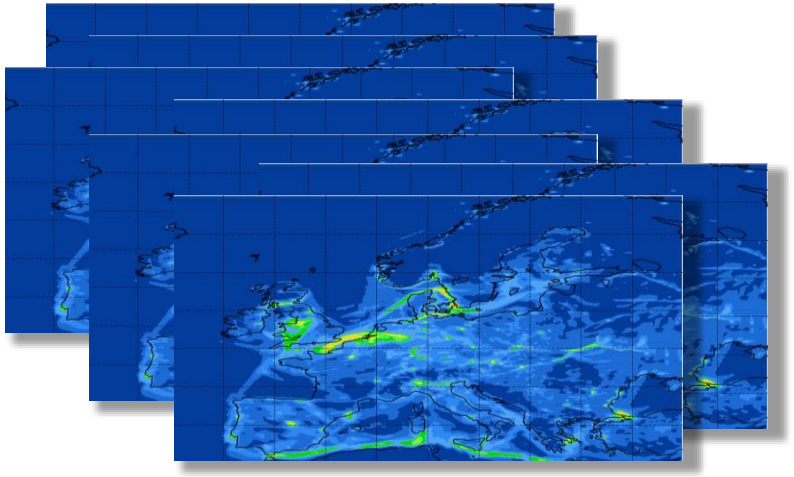
DA

Over 70 EO instruments are assimilated in the global system



Boundary conditions feed an ensemble of high-resolution European AQ systems (in order to assess uncertainties)

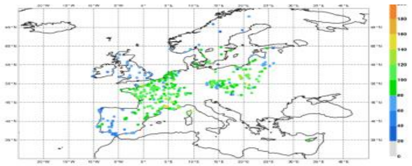
BC

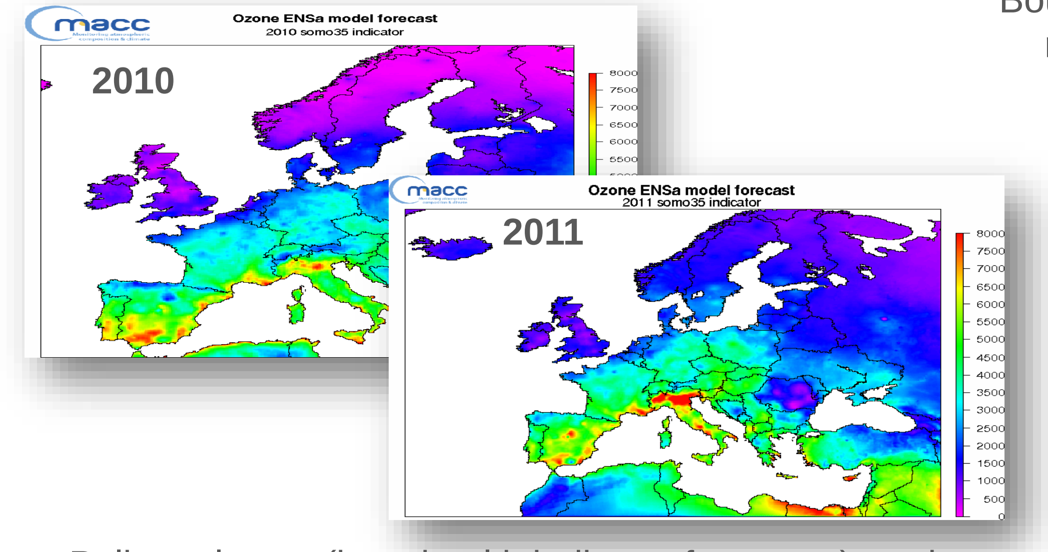


Ensemble

DA

More data are assimilated (in particular in situ) and used for extensive validation

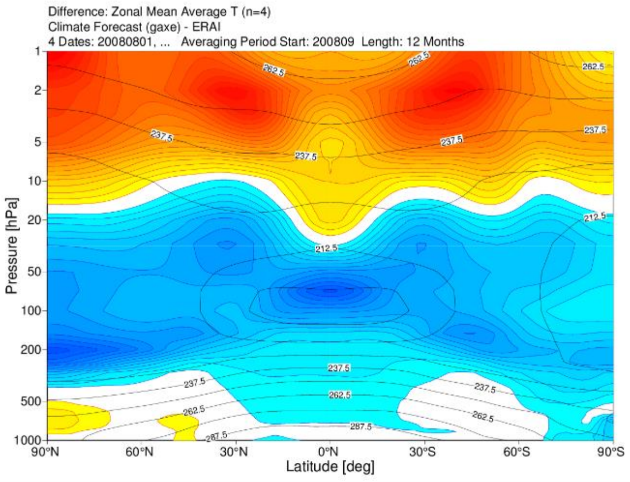




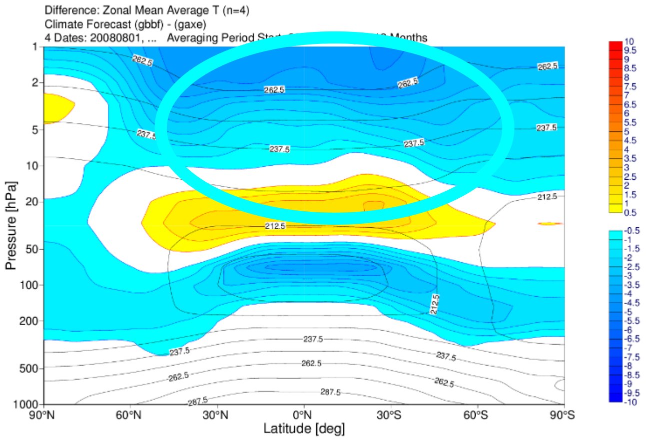
Policy-relevant (here health indicator for ozone) products are delivered. They are “maps with no gaps”, which observations alone don’t provide and are essential to assess impacts.

T vs T (BASE) (1000-1 hPa)

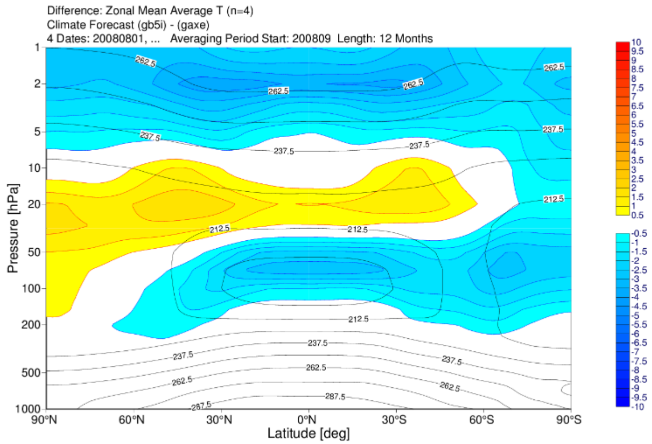
Base - era

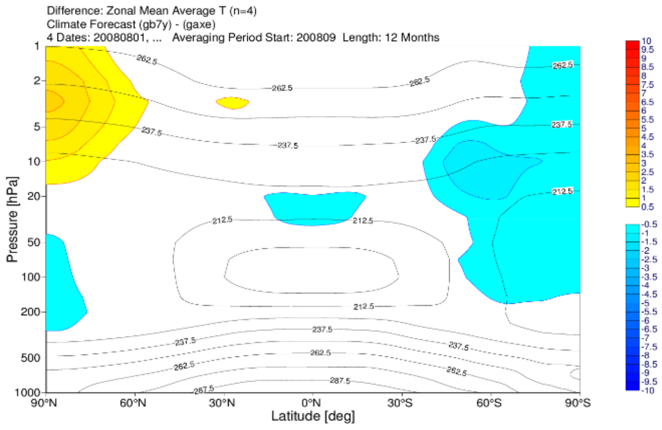


BMS

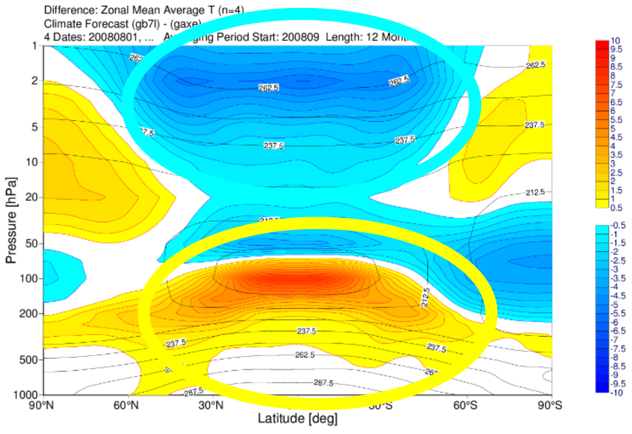


CAR

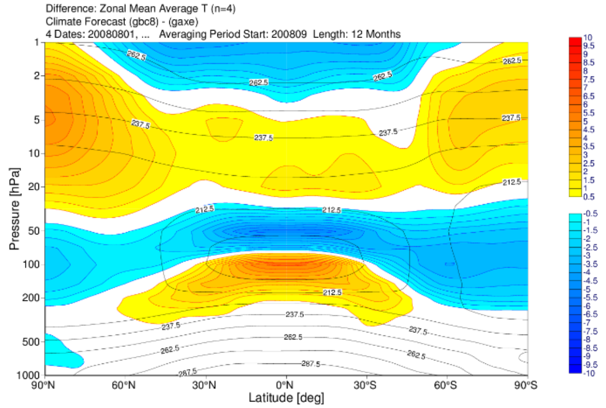




MACC-6h



C-IFS-C



C-IFS-B