NILU Norsk institutt for luftforskning
Norwegian Institute for Air Research

STAE TOULOUSE

Chemical data assimilation: Adding value to observations and models

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29-31 March 2010

Contents:

- Data assimilation: adding value to models and observations

  What is added value?

- Roles of data assimilation

  Not just analyses/initial conditions for forecasts

- Ways forward and challenges for chemical data assimilation

  Where do we go in context of:

  Understanding: science

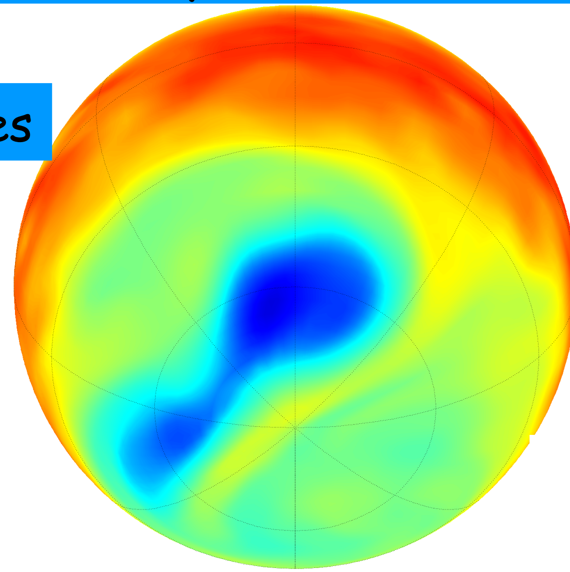
  Services: users

Data assimilation: adding value:

Ozone 10hPa, 12Z 23 Sep 2002

Red: high ozone
Blue: low ozone

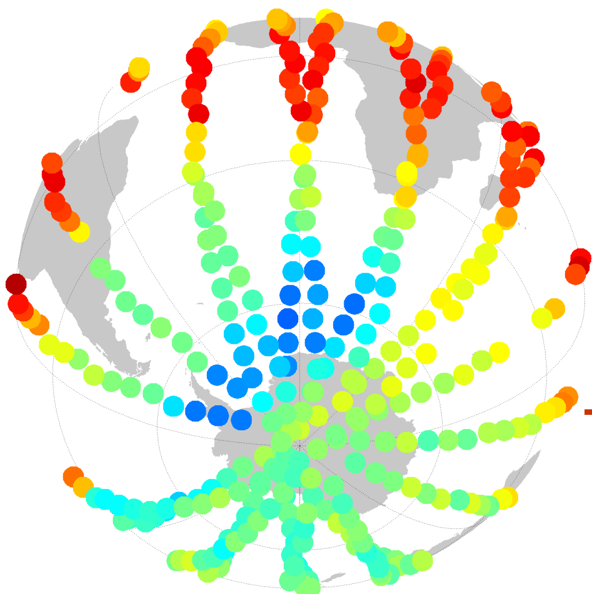
Analyses



DA adds value to both observations and model

N.B. Filling in obs gaps
Constraint of model

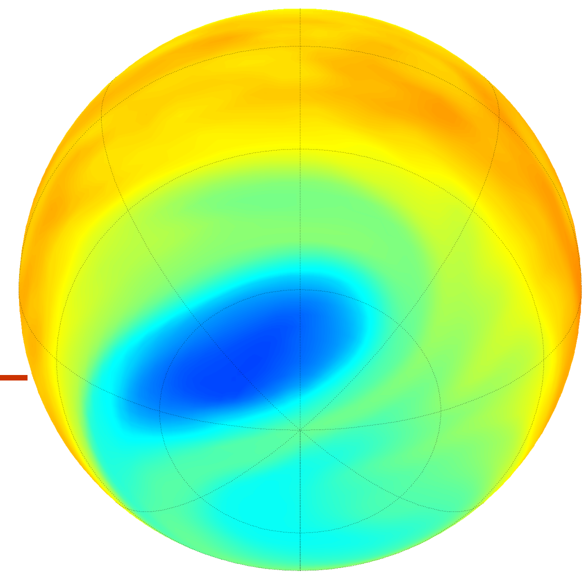
Geer et al., QJRMS (2006)
Lahoz et al., DA Book (2010)



MIPAS observations

DA

Errors



6 day forecast

Roles of data assimilation:

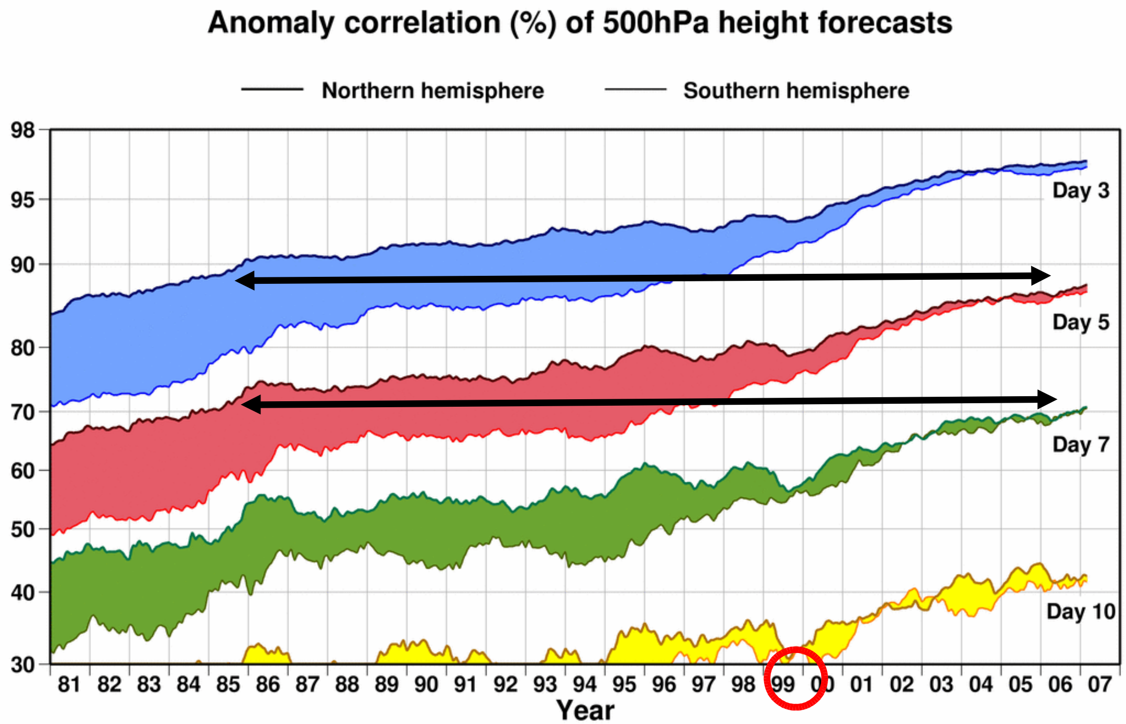
- Providing best state estimates (analyses; NWP, chemistry)
- Providing initial conditions (forecasts; NWP, Air Quality)

} NWP

- Evaluating observations and models (cal-val, OSEs, targeting)
- Monitoring Earth System (directives, protocols)
- Inverse modelling (pollutant emissions; Air Quality)
- Quantifying spatial/temporal change (O_3 loss,…)
- Evaluating future missions (OSSEs; POGEQA/MAGEAQ)

Initial conditions

(NWP: success for data assimilation)



AC coeffs, 3-, 5-, 7- & 10-day ECMWF 500 hPa ht forecasts for extra-tropical NH & SH, plotted as annual running means of archived monthly-mean scores for Jan 1980 - Nov 2006. Values plotted for a particular month are averages over that month & 11 preceding months. Colour shadings show differences in scores between two hemispheres at the forecast ranges indicated (After *Simmons & Hollingsworth, QJRMS, 2002*)

Impact of satellite observations, impact of data assimilation

Towards end of 1999: a more advanced 4D-Var developed & significant changes in the

GOS mainly due to launch of 1st ATOVS instrument onboard NOAA satellites

Data assimilation and NWP:

Key idea: Confronting models with observations
Apply to other areas, e.g., chemistry

Progress in NWP has been a combination of:

- Better models: higher resolution, better processes
- Better observations: satellites
- Better use of observations: bias correction, quality-control, radiances
- Better computing power
- Data assimilation: better use of observations and models; use of 4d-var

This has allowed observations and models to be evaluated and improved

This has allowed improvement in NWP forecasts (e.g. ECMWF)

Best state estimates

GEMS: chemical species, reanalysis of CO columns

Coupled IFS-MOZART system, assimilate MOPITT CO column data (validate vs MOZAIC)

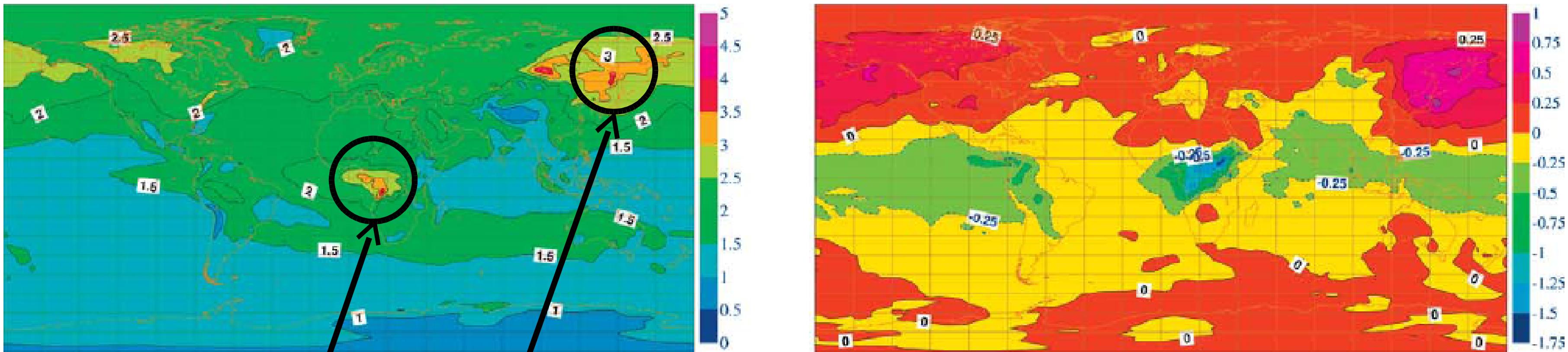


FIG. 7. Mean total columns of CO (10^{18} molecules cm^{-2}) for the period of 15–30 Jul 2003. (left) Reanalysis using MOPITT data and (right) difference between the reanalysis and the unconstrained model simulation.

Biomass burning

Tropical Africa, E. Siberia

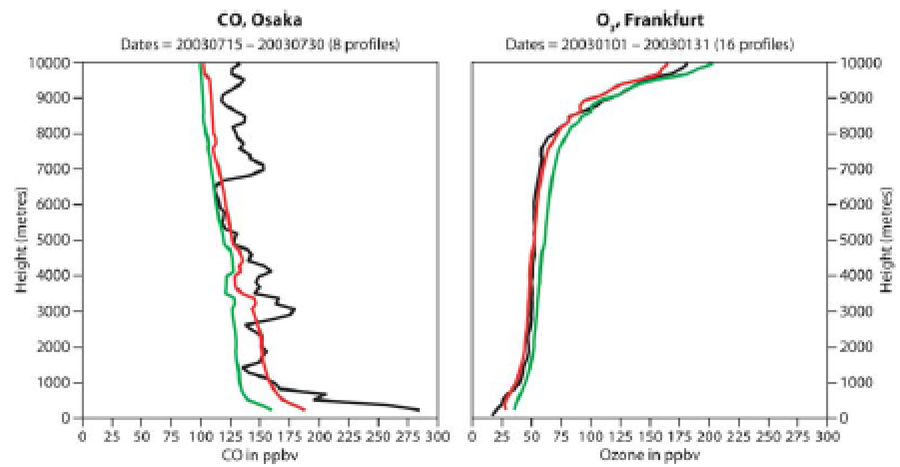
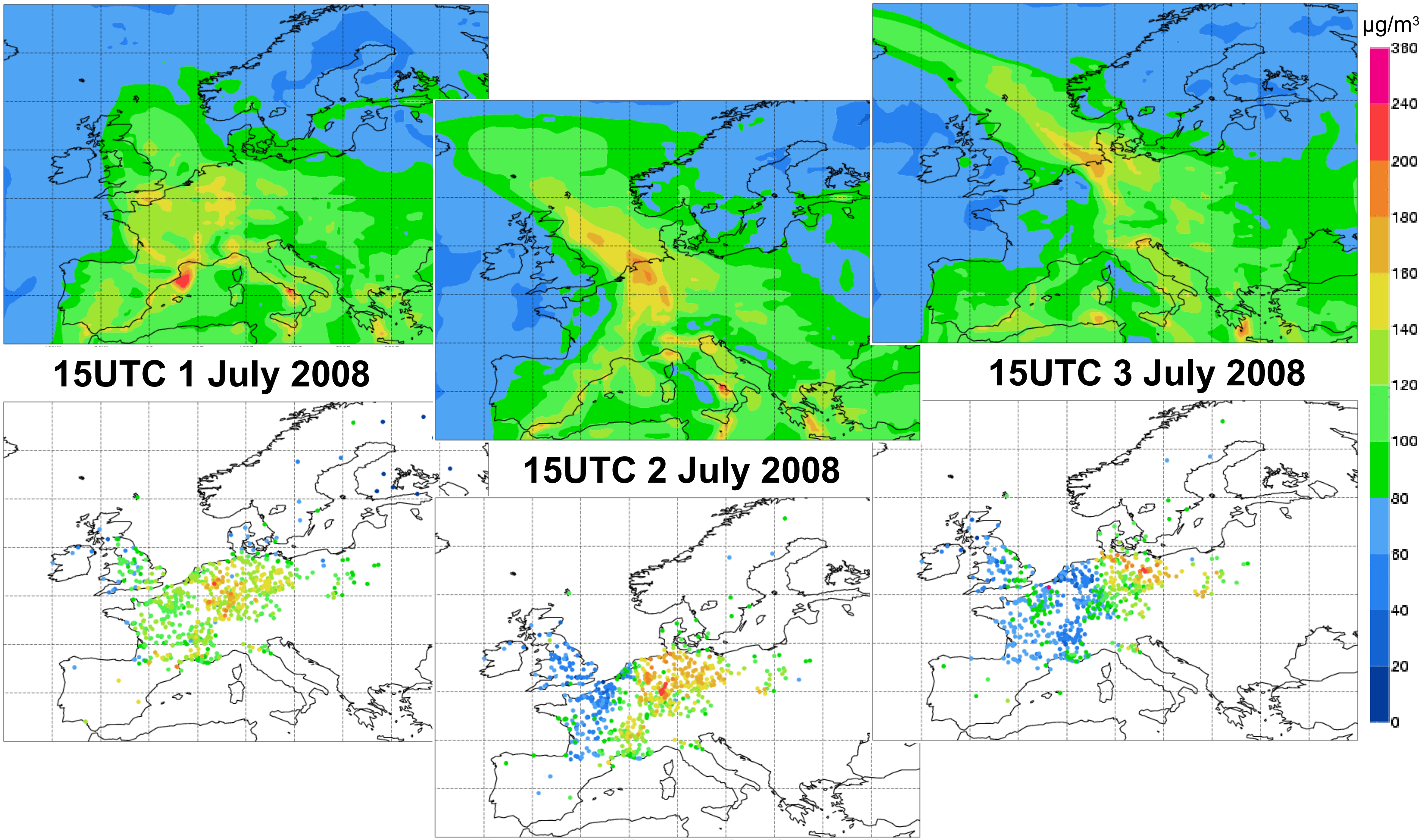


FIG. 8. Average vertical profiles of (left) CO over Osaka, Japan, and of (right) O_3 over Frankfurt, Germany, from MOZAIC observations (black), the control run (green), and the assimilation run (red).

Hollingsworth et al. , BAMS (2008)

From Simmons et al., MACC

Regional air quality: successive 63h surface ozone forecasts from CHIMERE and verifying observations



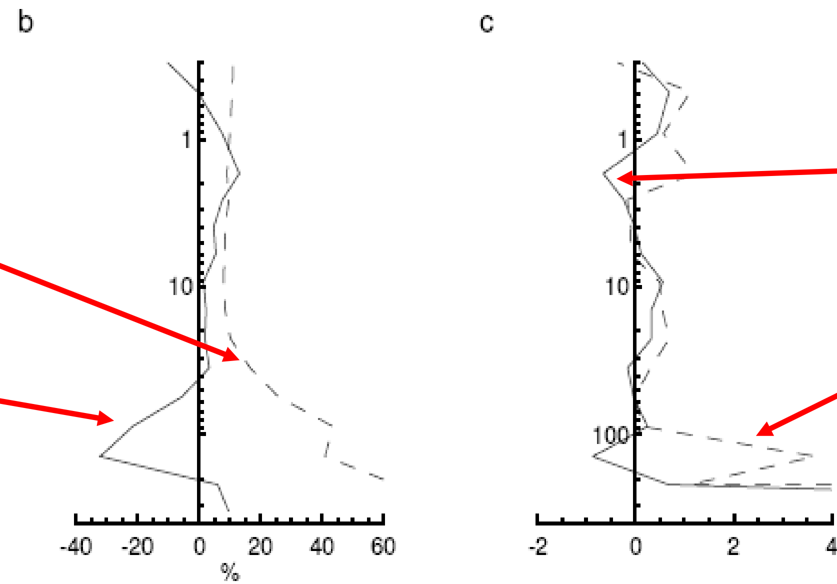
Obs quality:

Statistics: 14-28 Sep 2002

Data assimilation:

Self-consistency of MIPAS ozone data

Obs (MIPAS) minus short-range Forecast (model), OmF



Standard Deviation

Bias

Skewness

Kurtosis - 3

OmF ~ 0 in stratosphere

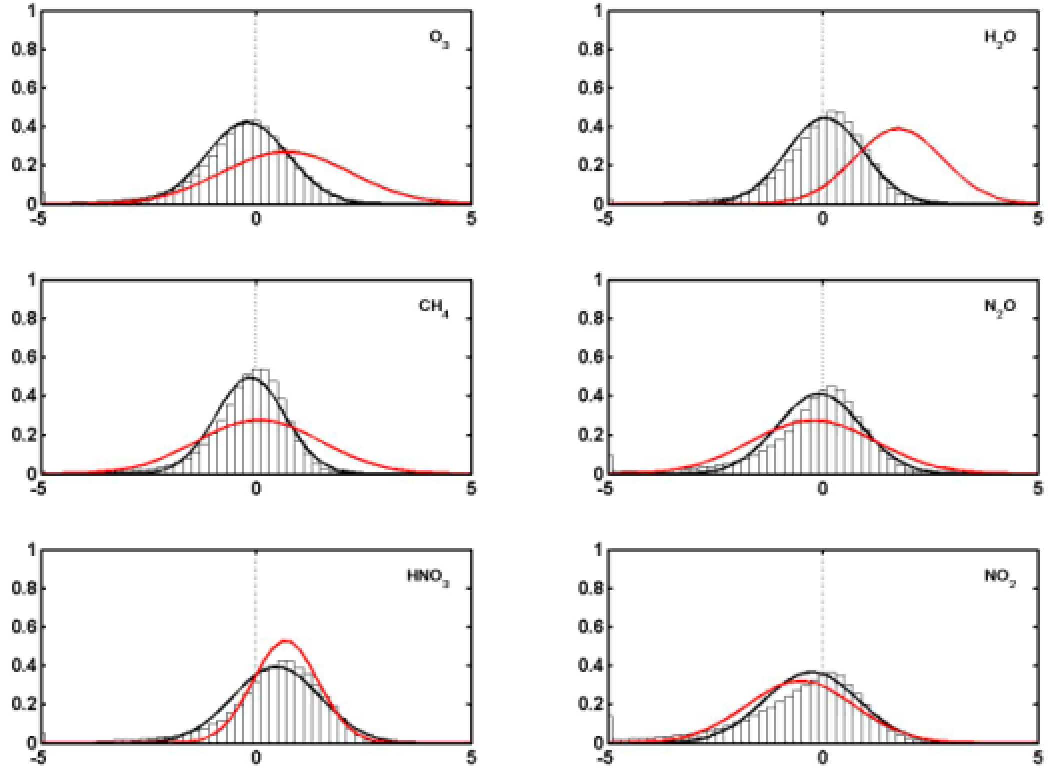
Consistent with Gaussian errors in stratosphere

Struthers et al. JGR (2002); Geer et al. QJRMS (2006)

Self-consistency & added value

OmF:

Observation minus forecast



Evaluation of analyses using histograms of OmF differences (normalized by observation error) averaged for stratosphere, globe & August 2003 for six stratospheric constituents: O_3 (top left), H_2O (top right), CH_4 (middle left), N_2O (middle right), HNO_3 (bottom left) and NO_2 (bottom right). Constituent observations rom ESA MIPAS off-line retrievals. Frequency of histograms normalized to lie between 0 and 1. Black line is Gaussian fit to histograms; red line is Gaussian fit from model run without assimilation.

Results support assumption of Gaussian errors in observations & forecast, & show analyses are closer to observations than simulations from model run without assimilation. Experiments performed at BIRA-IASB. With permission from *Lahoz et al., ACP (2007)*

See also *Lahoz and Errera, DA Book (2010)*

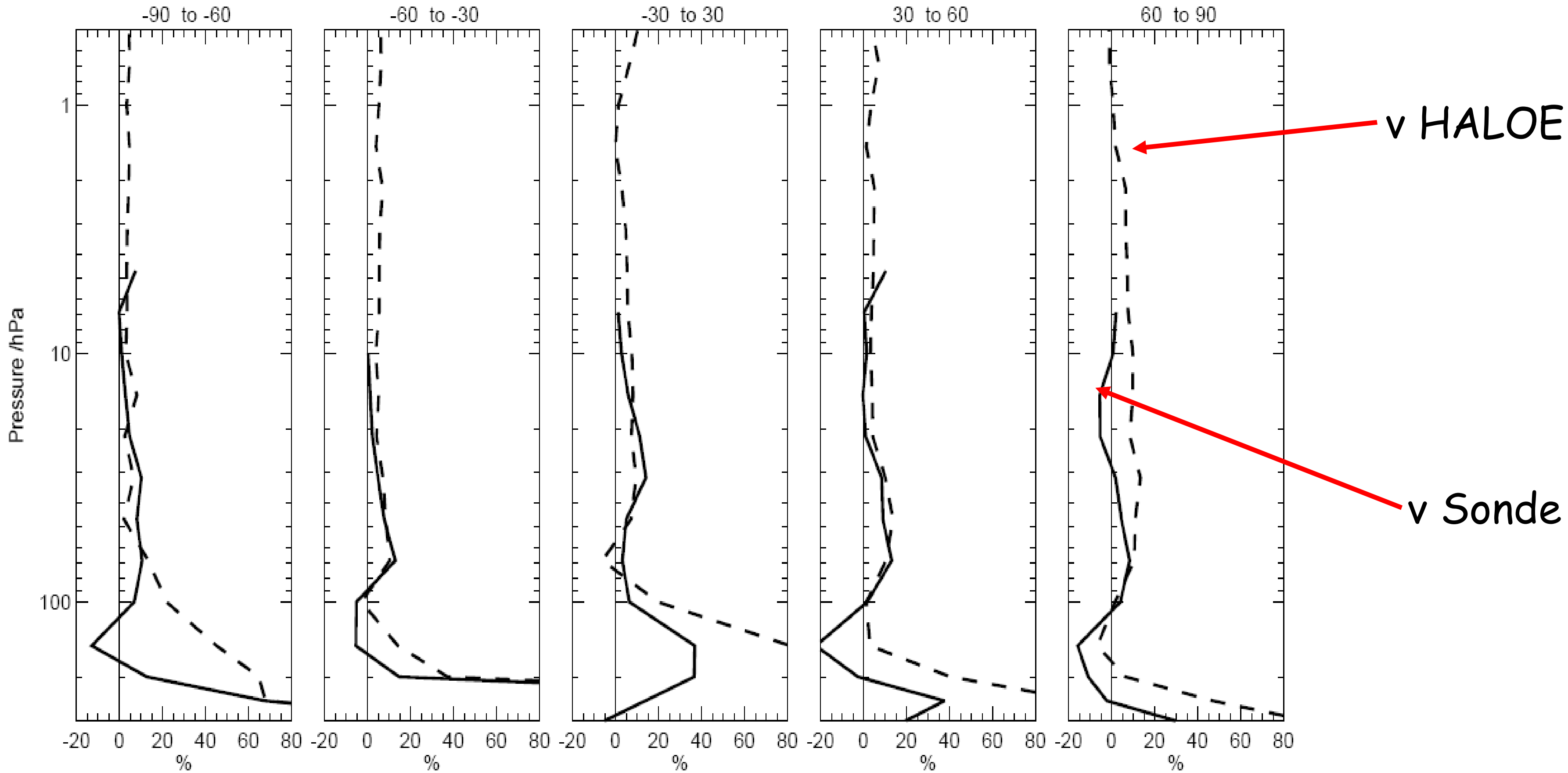
Obs bias:

DA: Evaluation of MIPAS ozone using independent data

BASCOE used as "interpolating" analysis

Statistics: 18 Aug – 30 Nov, (Obs1-Analysis) – (Obs2-Analysis):

Geer et al. ACP (2006); Lahoz et al. ACP (2007)



Bias in MIPAS ozone generally positive: ~5% - ~10% -> feedback to MIPAS team

OSEs:

OSEs: combined assimilation of UARS MLS ozone and GOME total column ozone

Struthers et al., JGR (2002)

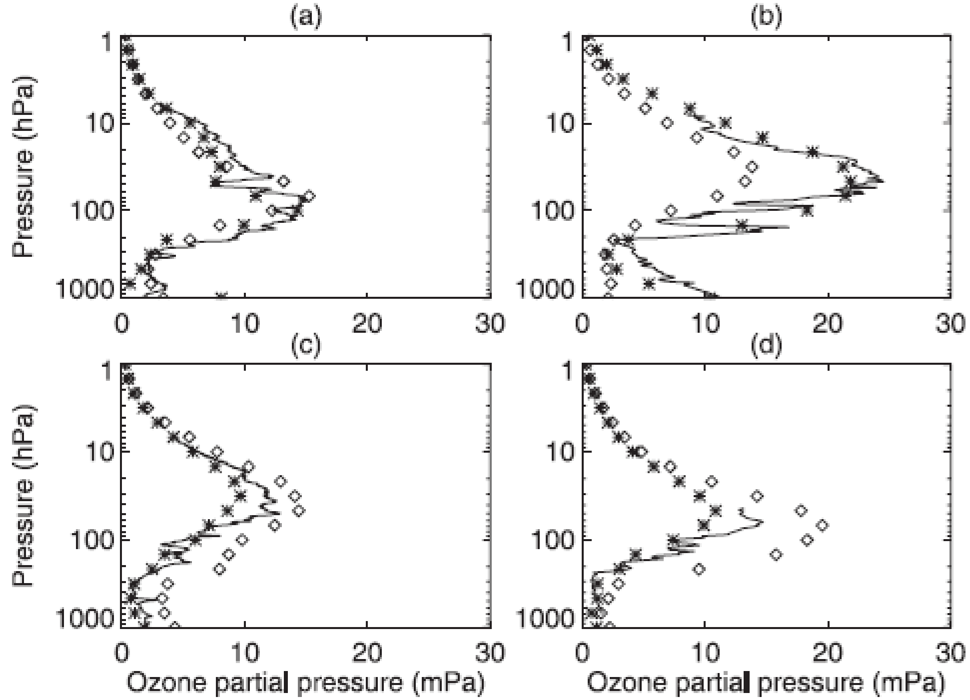


Figure 6. Four examples of co-located ozonesonde profiles, analysis profiles for assimilation run 3 and profiles of the Fortuin climatology (milliPascals, mPa). The stars represent analysis values plotted on standard UARS pressure levels. The diamonds represent Fortuin climatology values plotted on standard UARS pressure levels. (a) Ny Alesund 27 April 1997 (12 GMT). (b) Payerne 25 April 1997 (12 GMT). (c) Lauder 16 April 1997 (12 GMT). (d) South Pole 18 April 1997 (12 GMT). See text for details.

Better agreement with independent data (sondes) than if assimilate on their own:

(i) UARS MLS (poor troposphere), or (ii) GOME data (poor vertical structrure)

Evaluate models:

Accuracy of combined ozone information (obs/model)

ASSET project

Geer et al., ACP (2006, 2007)
Lahoz et al., ACP (2007a, b)

Good performance in stratosphere:
Within 5-10% of HALOE instrument

Complexity of chemistry:
Parametrization v comprehensive (e.g. ECMWF v BASCOE)

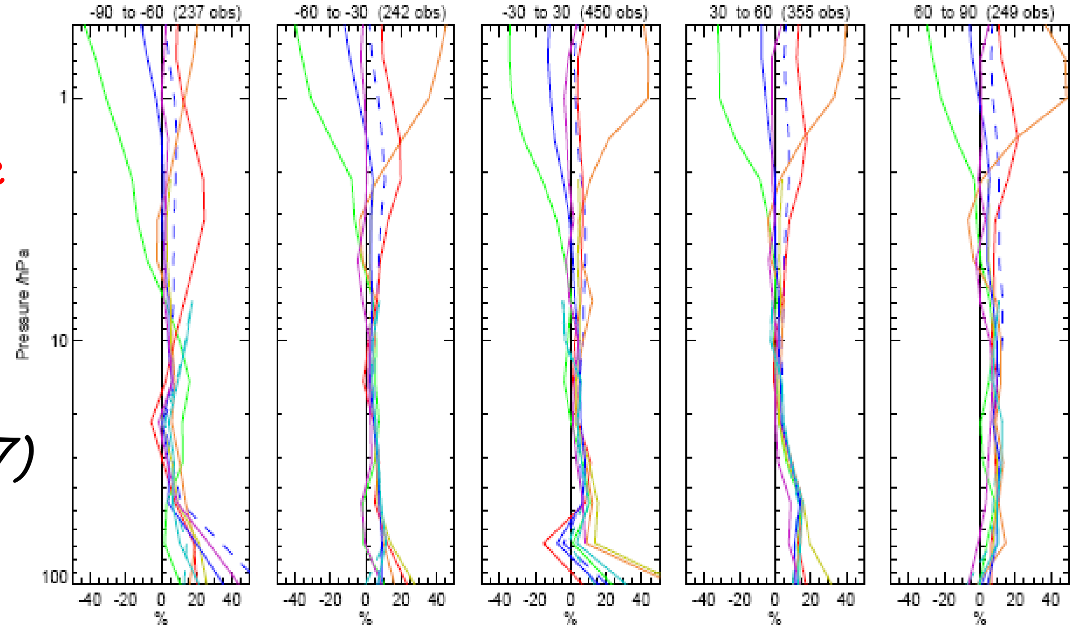


Fig. 10. Mean of analysis minus HALOE differences, normalized by climatology, for the period 18 August–30 November 2003. See Fig. 9 for colour key. The numbers in brackets indicate the HALOE/analysis coincidences within each latitude bin. Units: percent. These data are used to evaluate the performance of the ozone analyses. Based on Geer et al. (2006).

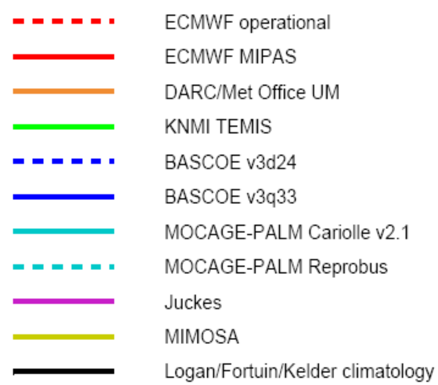
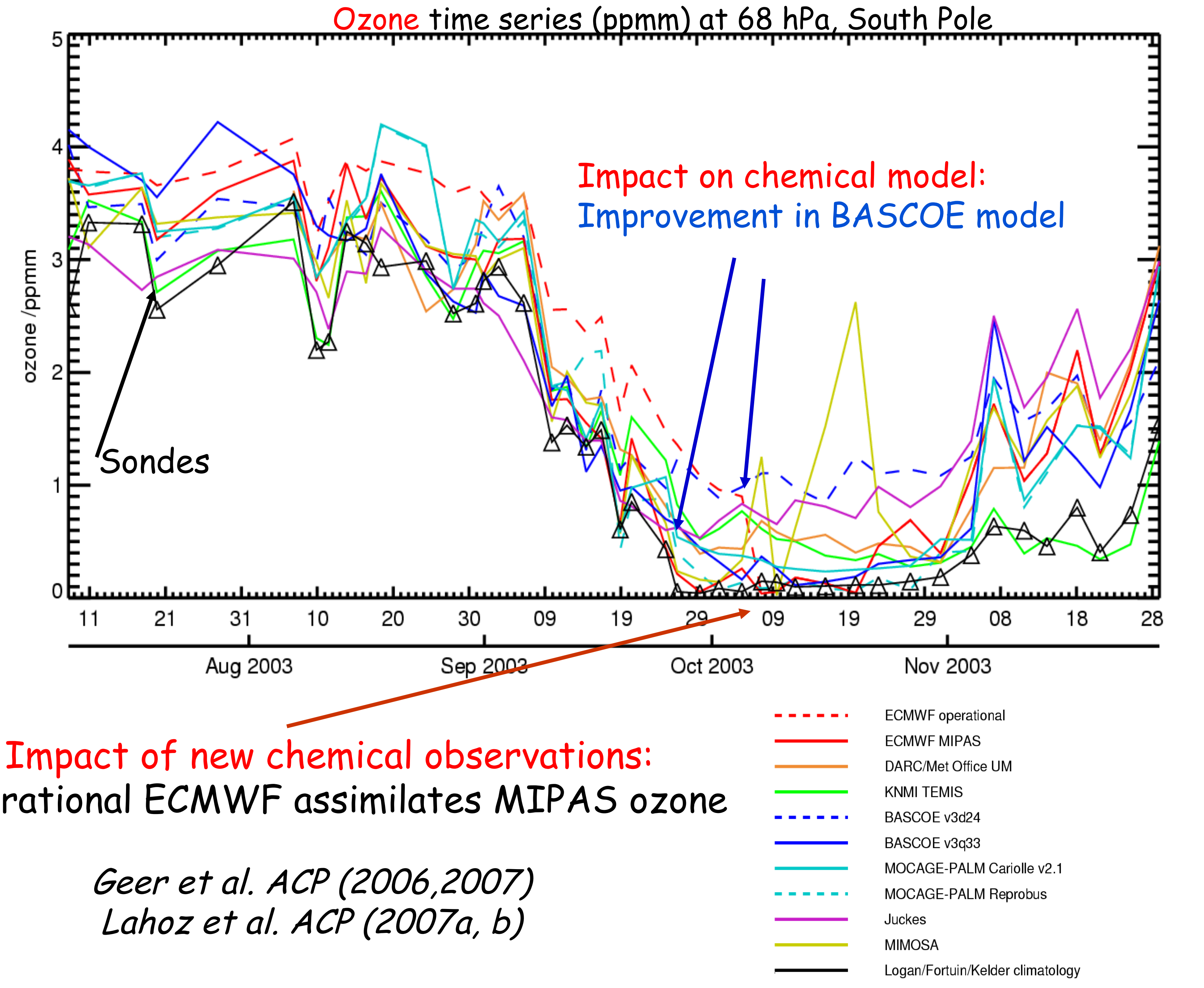


Fig. 9. Colour key used in Figs. 10–11.



Impact of new chemical observations:
Operational ECMWF assimilates MIPAS ozone

Geer et al. ACP (2006,2007)
Lahoz et al. ACP (2007a, b)

Accuracy of combined water vapour information (obs/model)

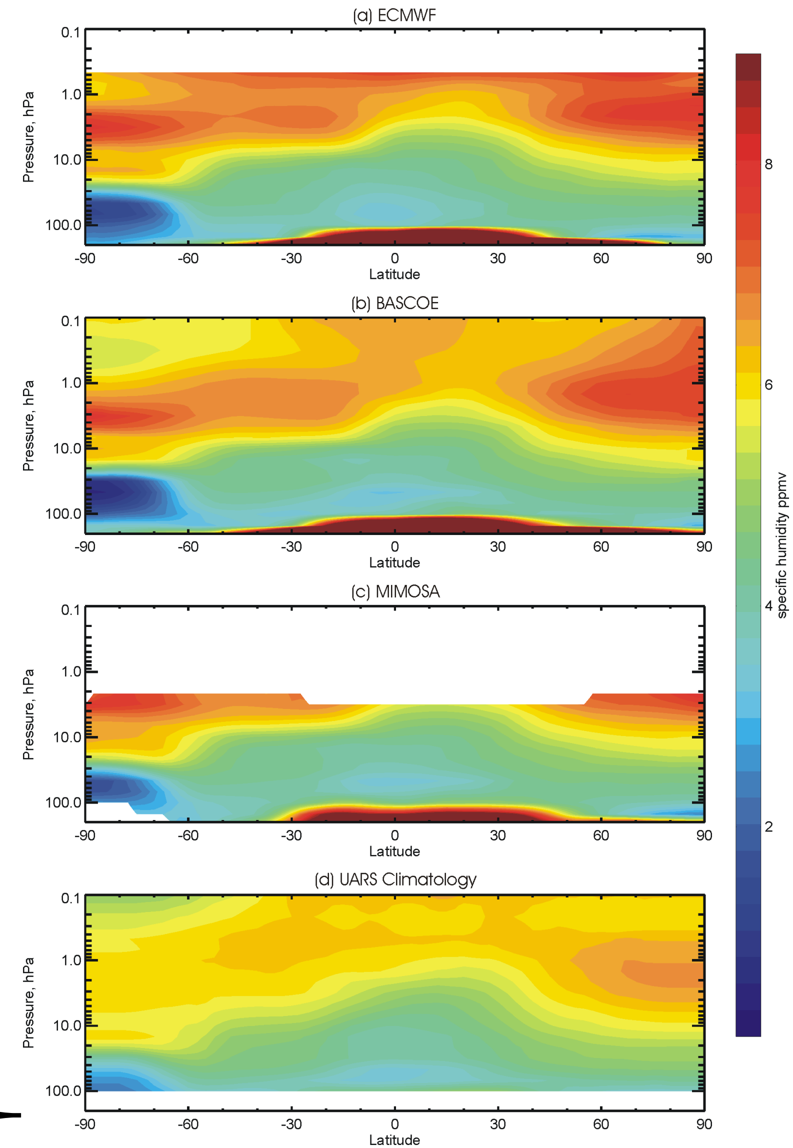
ASSET project

Lahoz et al., ACP (2007a, b)
Thornton et al., ACP (2009)

Main features of stratospheric WV captured:

- Tropical WV minimum,
- SH polar vortex WV minimum
- Brewer-Dobson circulation
- Mesosphere: analyses wetter than UARS clim & reflect wet bias of MIPAS obs

Monthly zonal mean specific humidity analyses, Sep 2003: (a) ECMWF, (b) BASCOE, (c) MIMOSA; (d) UARS clim
MIPAS WV profiles assimilated in ECMWF, BASCOE & MIMOSA analyses.
Blue: relatively low specific humidity values
Red: relatively high specific humidity values. Units: ppmv.



Forecast error evaluation

GEMS: chemical species, NO_2 forecasts

Emissions, boundary conditions, forcing same for all models. Spread: forecast error

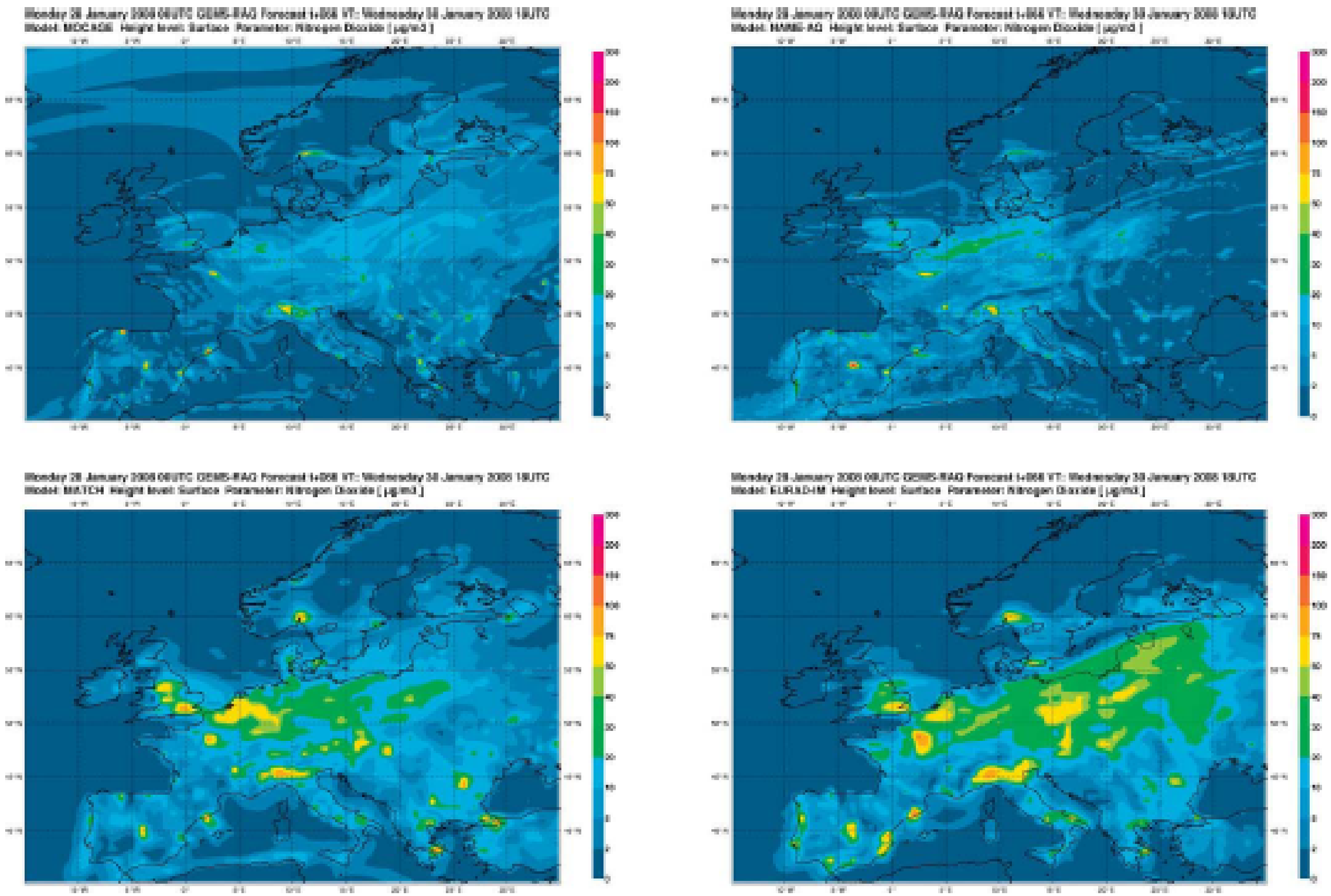


FIG. 12. Ensemble regional air quality forecasts: 66-h forecast of nitrogen dioxide (μg m^{-3}) valid at 1800 UTC 30 Jan 2008 from four European air quality model systems: (top left) MOCAGE, (top right) Numerical Atmospheric dispersion Modeling Environment (NAME), (bottom left) Multiscale Atmospheric Transport and Chemistry Model (MATCH), and (bottom right) European Radar (EuRAD).

Hollingsworth et al. , BAMS (2008)

Monitoring

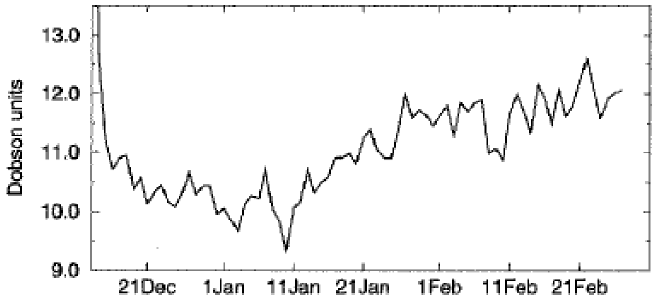


Figure 5. The evolution of daily global root-mean-square of TOMS observed-minus-forecast residuals in the GEOS ozone Data Assimilation System during the validation period in winter 1992.

Ozone monitoring:

Štajner et al. QJRMS (2001), JGR (2004)

TOMS: OmF rms residuals

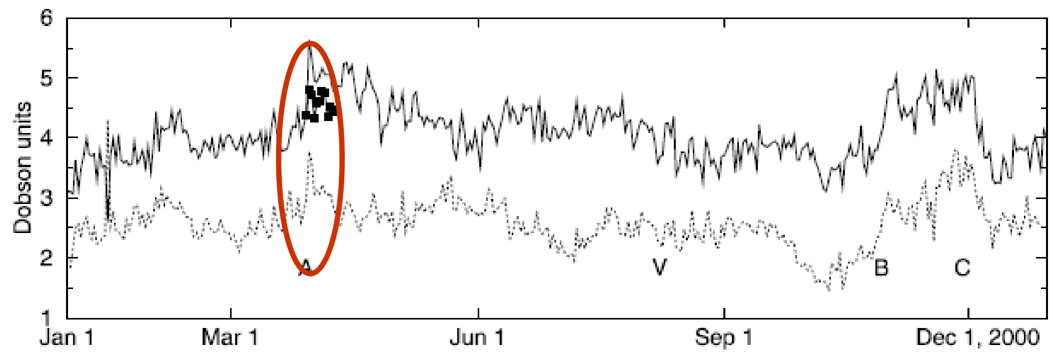


Figure 2. Time series of daily global mean of NOAA 14 SBUV/2 O-F residuals in Umkehr layer 5 for operational SBUV/2 data (solid line) is shown for the system driven by GEOS-3 winds. The same quantity from the ozone assimilation driven by winds from a prototype GEOS-4 system, and including parameterized ozone chemistry is shown by the dotted line. Note the sharp jump near the mark "A" exceeding the typical day-to-day variability followed by a downward trend in the mean of O-F residuals. This feature is coincident with the instrument calibration change on March 31. Near the mark "A" the same quantity is shown for assimilation driven by GEOS-3 winds and using reprocessed SBUV/2 data (line with squares). An increase between marks "B" and "C" coincides with a change in the grating position of the instrument.

SBUV/2: OmF mean residuals

Quantify variability:

Use data assimilation to estimate vortex-averaged quantities

Ozone loss in polar vortex

Fill in observational gaps

Jackson & Orsolini, QJRMS (2008)

DA Run: Cariolle scheme
(no heterogeneous chem)
EOS MLS, SBUV/2 Assim

Ref run: DA run but no O_3 assim
Cariolle scheme off

Difference: chemistry

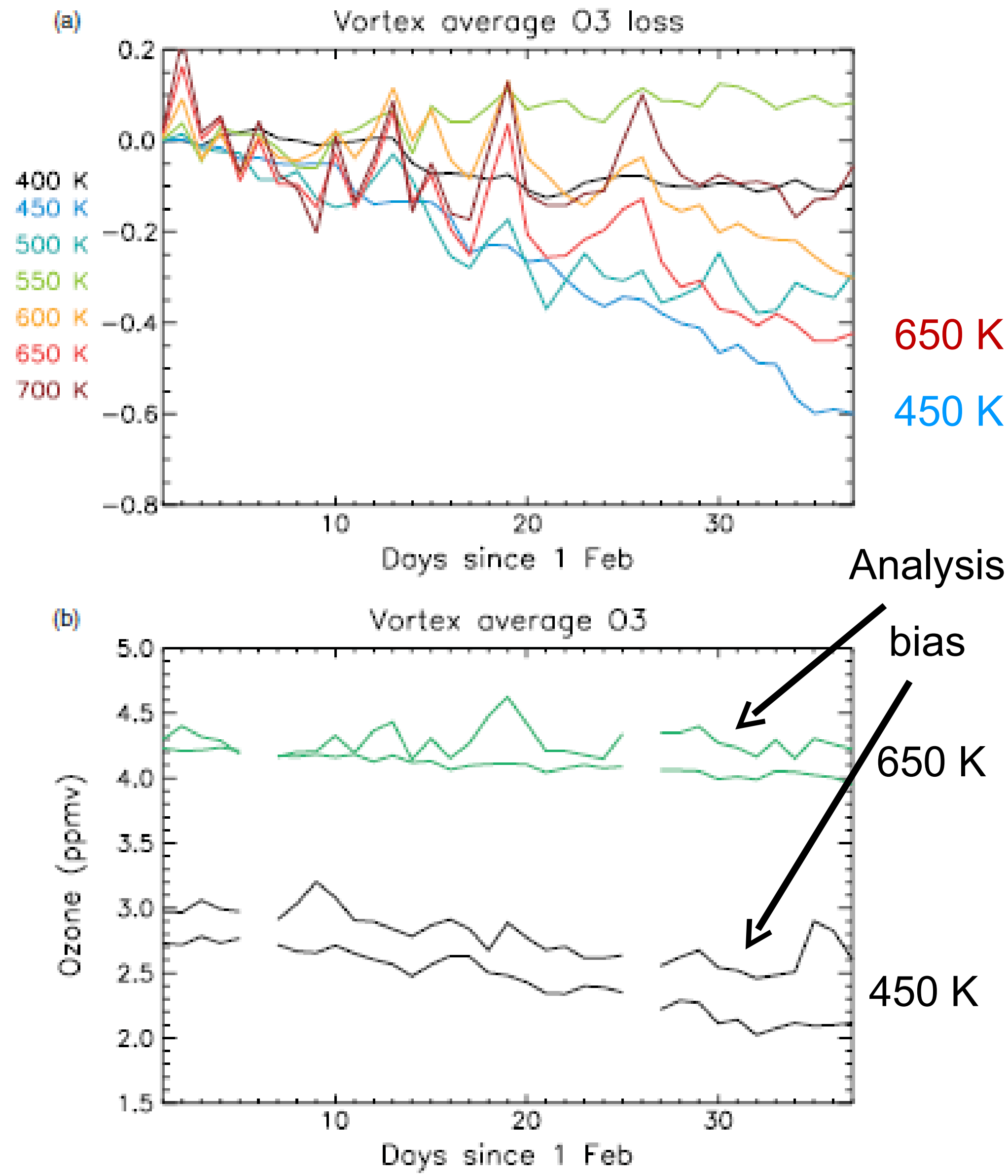


Figure 1. (a) Vortex average ozone loss for selected isentropic levels from 400 to 700 K (the levels are indicated by the colour key). The y-axis shows ozone loss in ppmv, the x-axis shows days from 1 February 2005. Negative values indicate ozone loss. (b) Vortex average ozone for the assimilation run (thin lines) and from EOS MLS observations (thick lines) for the 450 K (black) and 650 K (green) isentropic levels. Units are ppmv.

Use data assimilation to estimate vortex-averaged quantities

Ozone loss in polar vortex

Fill in observational gaps

El Amraoui et al., GRL (2008)

O_3 data assimilation

Diabatic descent estimated from N_2O

Vortex-averaged O_3 loss in NH winter

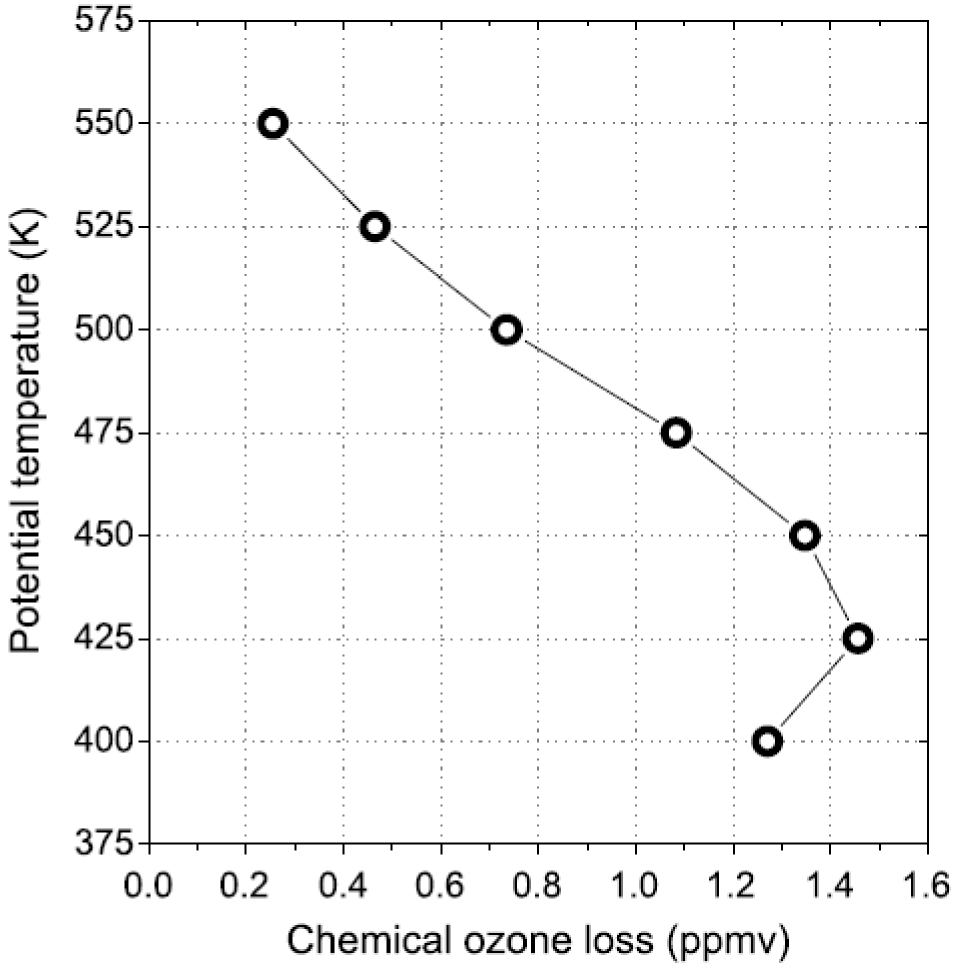


Figure 4. Estimated ozone loss mixing ratio between 10 January and 10 March 2005 versus potential temperature after removing the effects of diabatic descent. The maximum ozone loss of ~1.5 ppmv is observed at 425 K.

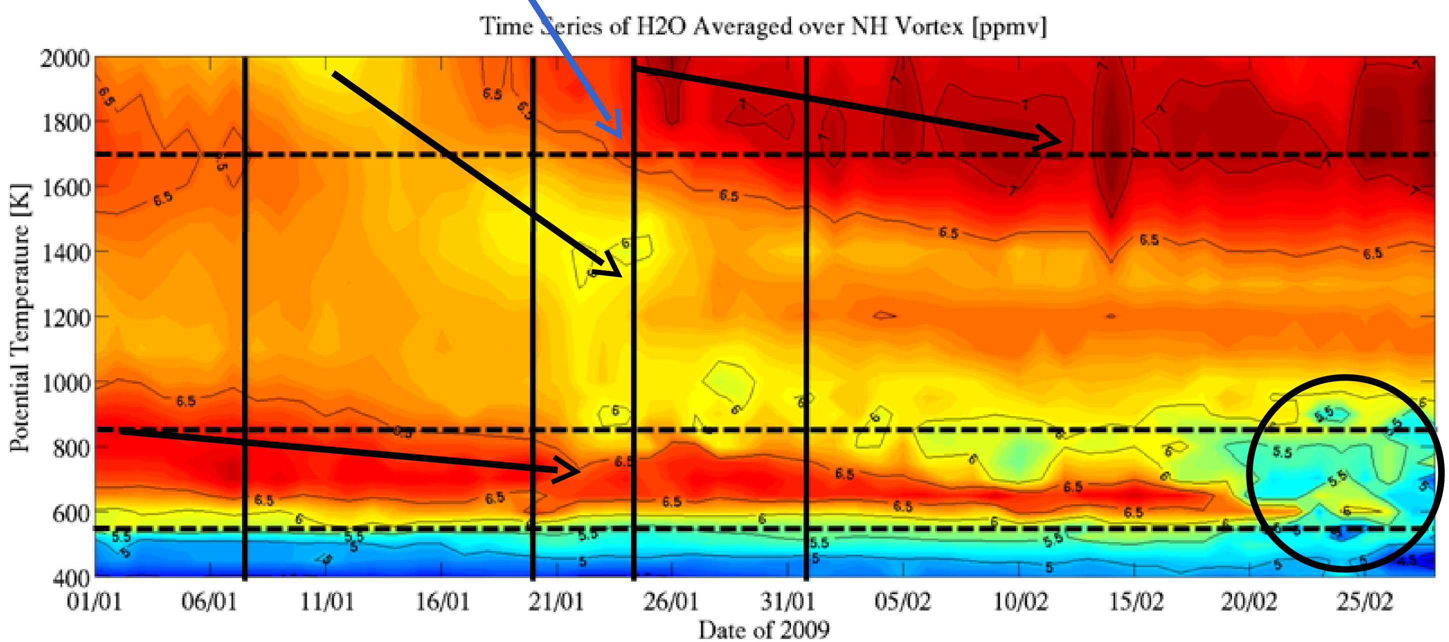
BASCOE system

Use data assimilation to estimate vortex-averaged quantities

H_2O changes During a major warming

Confirm obs features

Major warming, *Manney et al., GRL (2009)*



Time series of vortex-averaged BASCOE water vapour analyses (400 K – 2000 K) for the period 1 January – 28 February 2009. The vortex average is computed for PV values identified to be within the polar vortex, the edge of the vortex estimated to be at the location of the strongest gradients in PV at a given isentropic level, following the criterion of Nash et al. (1996). The vertical black solid lines identify the dates 8 January, 20 January, 24 January and 1 February. The horizontal black dashed lines identify the theta levels 550 K, 850 K and 1700 K.

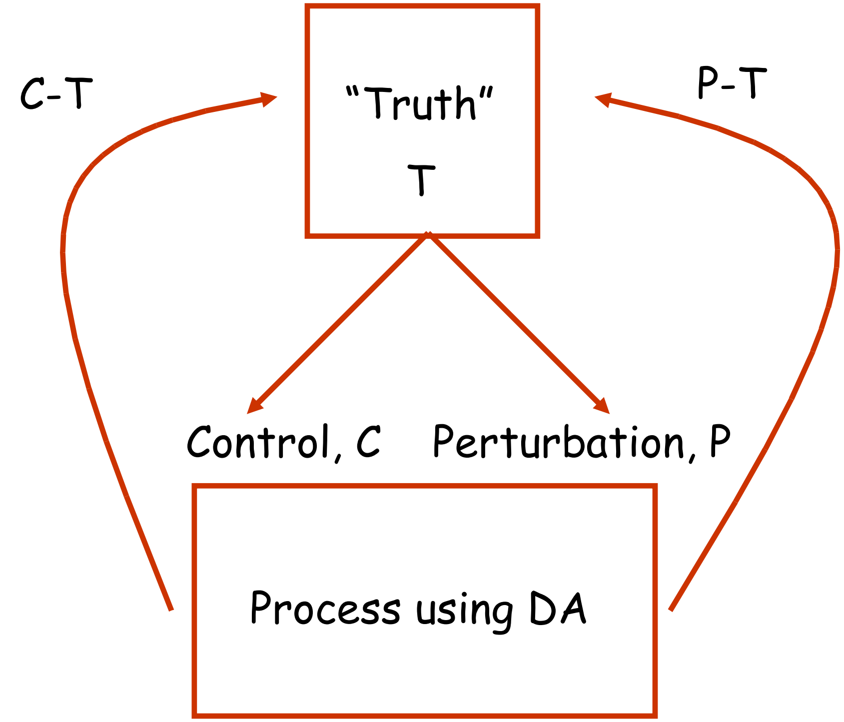
Fill in observational gaps

Lahoz, Viscardy, Errera

Evaluation of future observations: OSSEs

Structure of an OSSE

- Simulated atmosphere ("truth"; T): using a model, analyses
- Simulated observations of instruments appropriate to the study, including errors: using T
- Assimilation system: using a model
- Control experiment C: all observations except those under study
- Perturbation experiment P: all observations



OSSE goal: evaluate if the difference P-T (measured objectively) is significantly smaller than the difference C-T

Note shortcomings of an OSSE - *Masutani et al., DA Book (2010)*

- Expensive (cost ~ assimilation system) -> alleviate problem: simplify OSSE

- Difficult interpretation (model dependence) -> alleviate problem: conservative errors, several methods to investigate impact

- Incest -> alleviate problem: different models to construct "truth" & perform assimilation (BUT there could be bias between models)

Despite shortcomings, high cost of EO missions means that OSSEs often make sense to space agencies

- Use for POGEQA/MAGEAQ: proposed GEO AQ platform

OSSE: evaluate proposed SWIFT instrument

Lahoz et al., QJRMS (2005)

SWIFT:

- Based on UARS WINDII principle (Doppler effect)
- 2 wind components using 2 measurements at ~90°
- Thermal emission (mid-IR) of ozone (1133 cm^{-1})
- Technology difficult to implement
- Global measurements of wind and ozone profiles (~20-40 km)

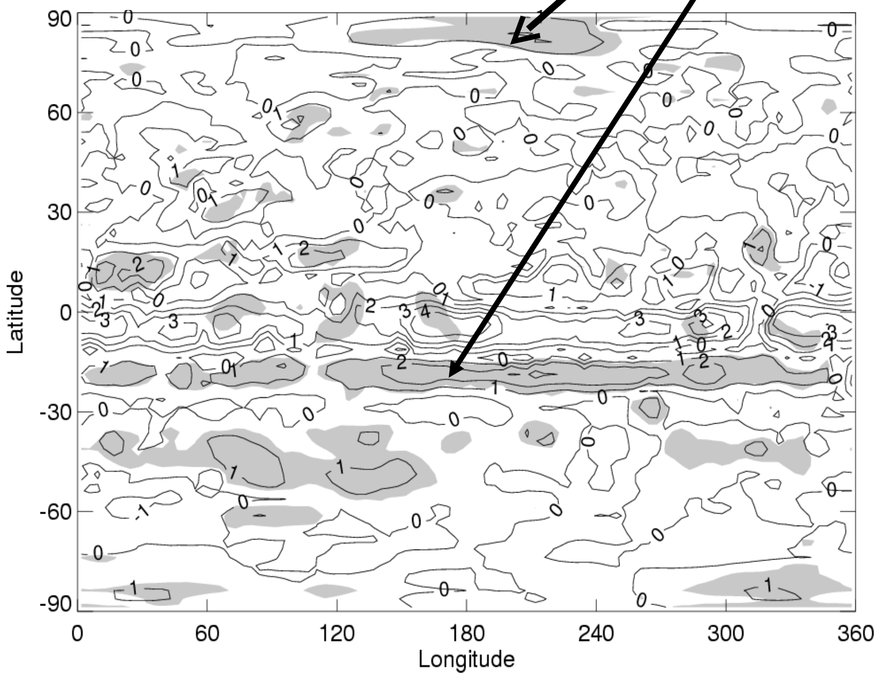
Addresses concerns about GOS winds

Provides information for scientific studies: e.g. tropical winds, transport, wintertime variability

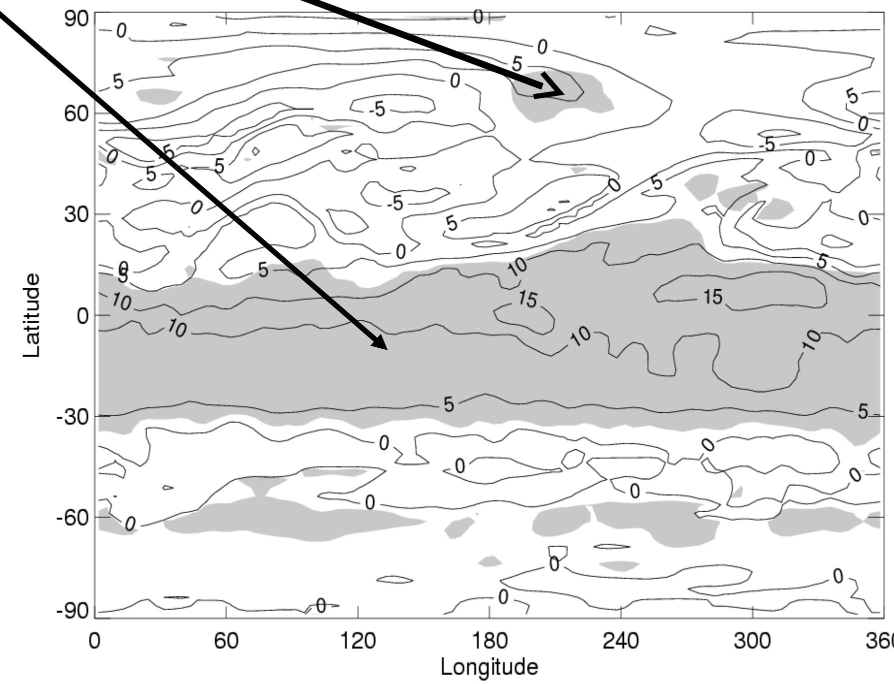
Significance tests

Areas > 5%

Positive impact for zonal wind



10 hPa



1 hPa

Y=Abs(C-T) -Abs(P-T); Zonal-wind (m/s); January 2000;
Shaded:95% C.L. & Y>0. Similar results for April 2000.

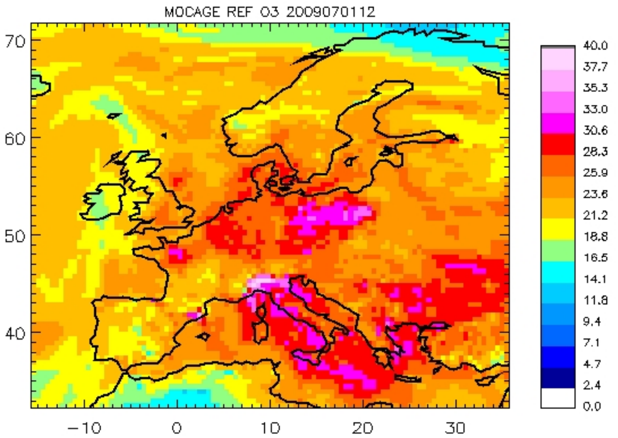
N.B. Some areas of -ve impact (information on data assimilation system)

New observations can degrade data assimilation system - not significant

An OSSE with MTG/IRS (ozone)

Peuch et al. & MAGEAQ Team

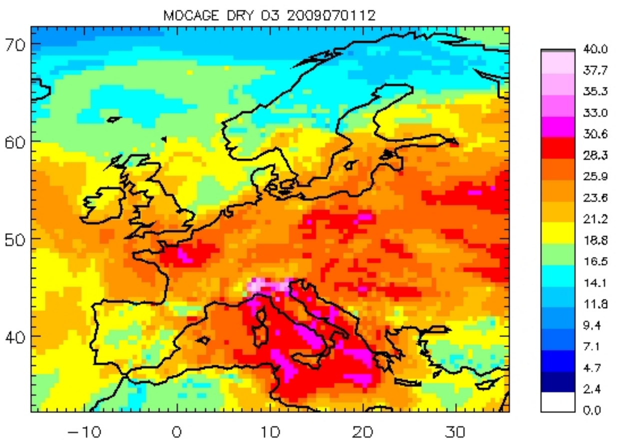
EUMETSAT and ESA have initiated joint preparatory activities for the MTG definition to be available in the 2016-2018 timeframe. In particular, MTG-IRS specifications result from a compromise between meteorology and chemistry needs, with a priority on Numerical Weather Prediction.

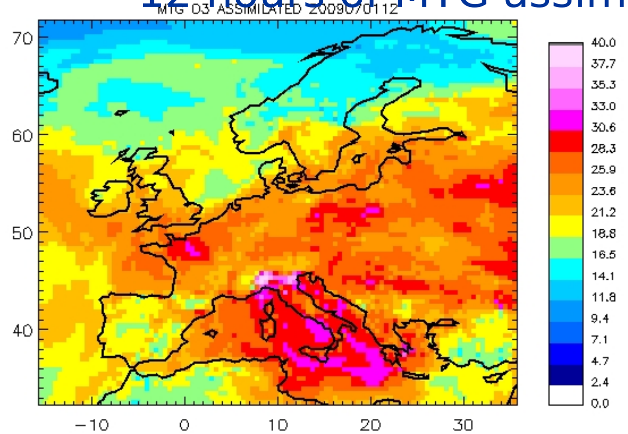


Target species	OPD (cm)	NeDL $(W/cm^2.sr.cm^{-1})$	Spectral resolution
O_3	0.8	2.45 10^{-8}	0.625
CO	0.8	6.12 10^{-9}	0.625

Impact on initial conditions after

12 hours of MTG assimilation





There is a very limited impact of the assimilation of the ozone partial column 0-6km. We confirm that **there is a need for a dedicated geostationary Air Quality sensor for O_3 and CO.**

Ways forward and challenges:

Data assimilation (DA) adds value to observations/models

Success in NWP, carried over to chemical species (AQ forecasts)

What is chemical data assimilation for? Other than for AQ forecasts?

What did it ever do for us? (© Life of Brian)

Why not just use a model or observations? Several examples in this talk:

DA is useful for: Cal-val, monitoring, quantification, OSEs, OSSEs,…

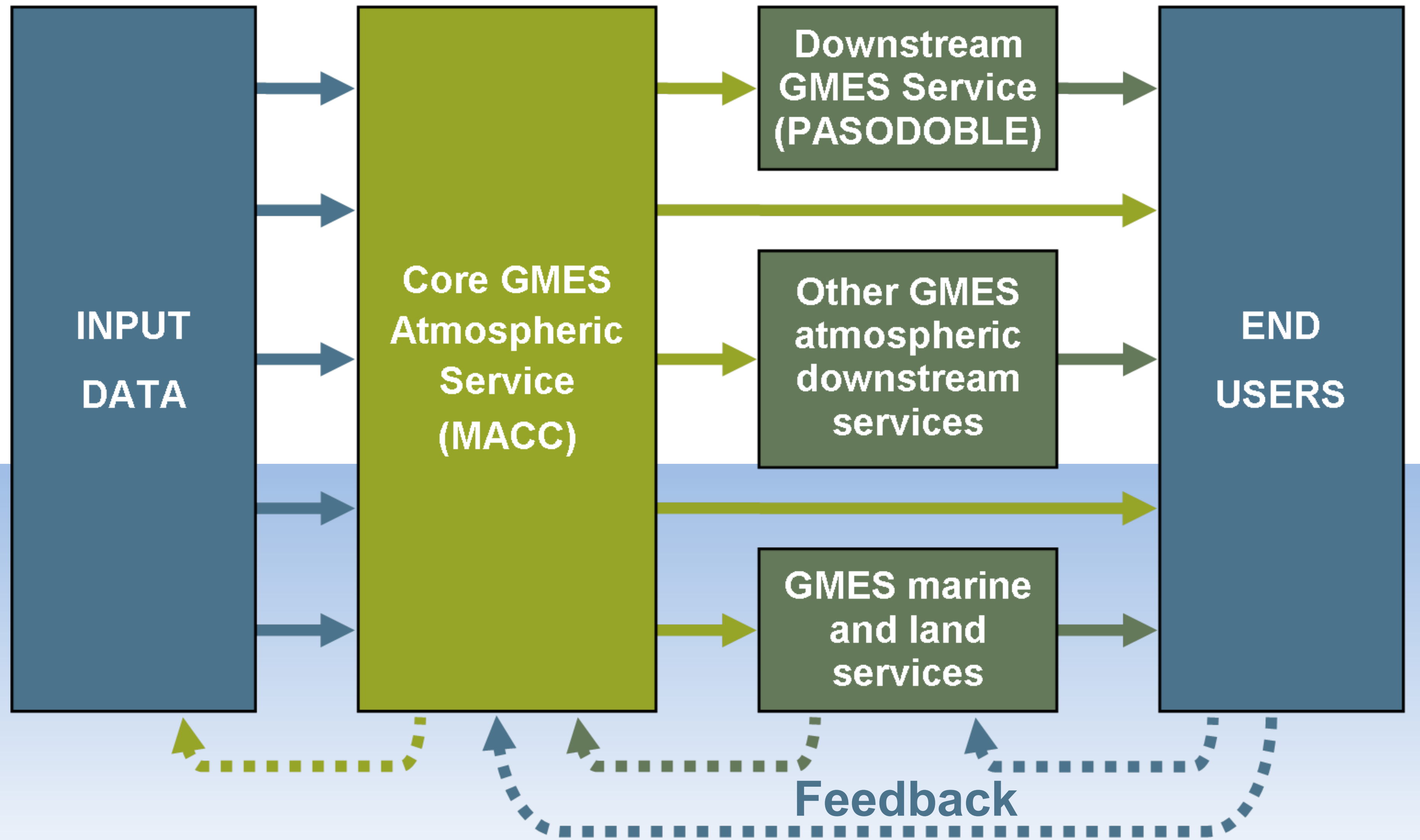
Key point: DA allows confrontation of observations and models (in a consistent, objective way)

Way forward: integrate observations & models using data assimilation

Data Assimilation must be a key element in EO science (e.g Concordiasi)

Data Assimilation key role for: services – users (from Simmons et al., MACC)

Overall service structure (from MACC viewpoint)



Challenge for data assimilation:

What is added value? Discussion with Q. Errera & S. Viscardy

What does data assimilation do better than model/observations?

"Improved" information – e.g. analysis closer to independent data

What does data assimilation do differently than model/observations?

"Extra" information – e.g. something not provided by model/obs: Confrontation of models & observations

Does this give a better estimate - higher accuracy?

Quantification (errors, monitoring, ozone loss, vortex averages,…)?