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Data assimilation: A tool for evaluating chemistry models

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Contents:

- Data assimilation: adding value to models and observations
- NWP: success for data assimilation
- Applying NWP ideas to evaluating models:

  Chemistry models; climate models; chemistry-climate models
- Ways forward

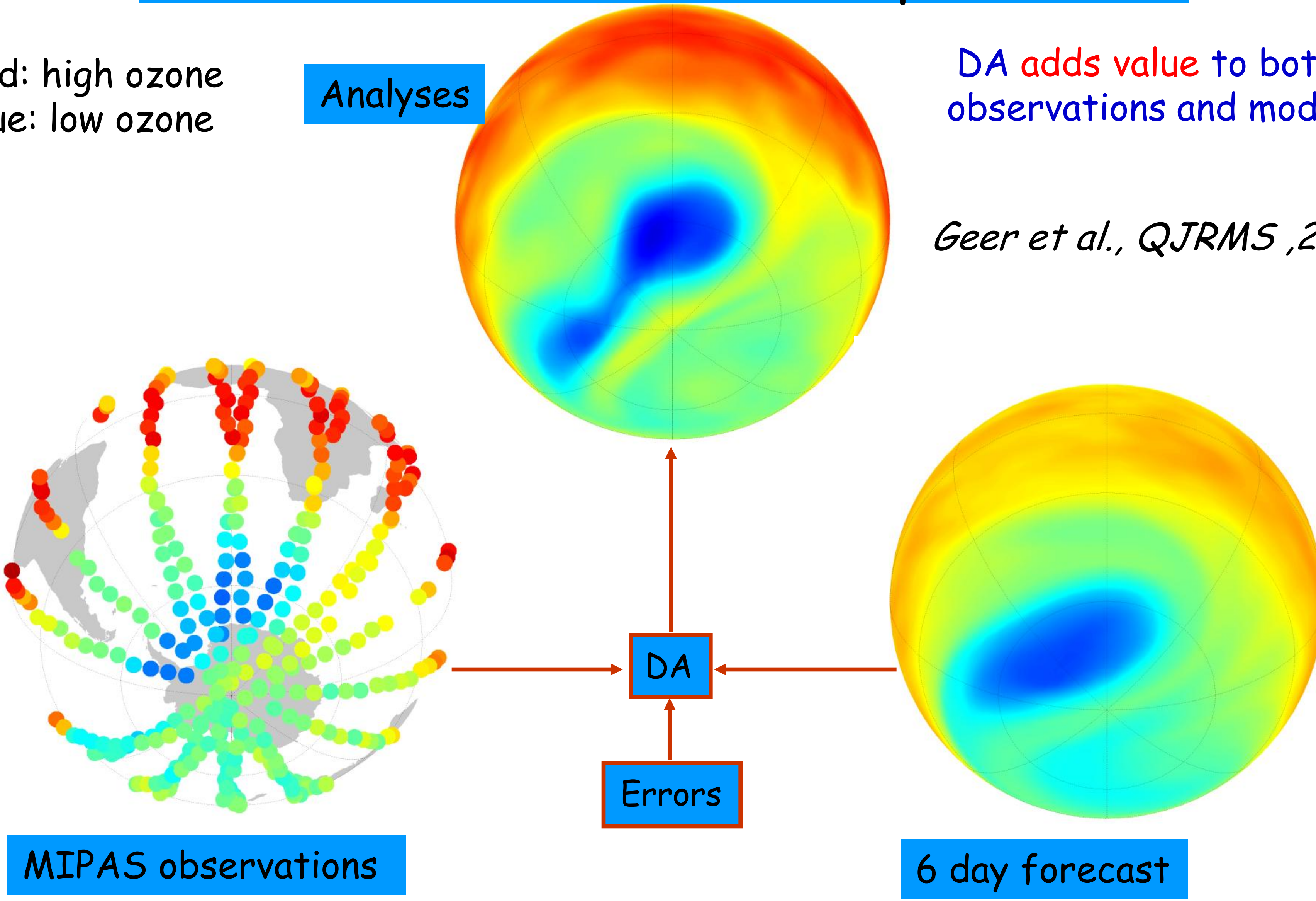
Data assimilation: adding value:

Ozone 10hPa, 12Z 23 Sep 2002

Red: high ozone
Blue: low ozone

DA adds value to both observations and model

Geer et al., QJRMS ,2006



Data assimilation and NWP:

Key idea: Confronting models with observations

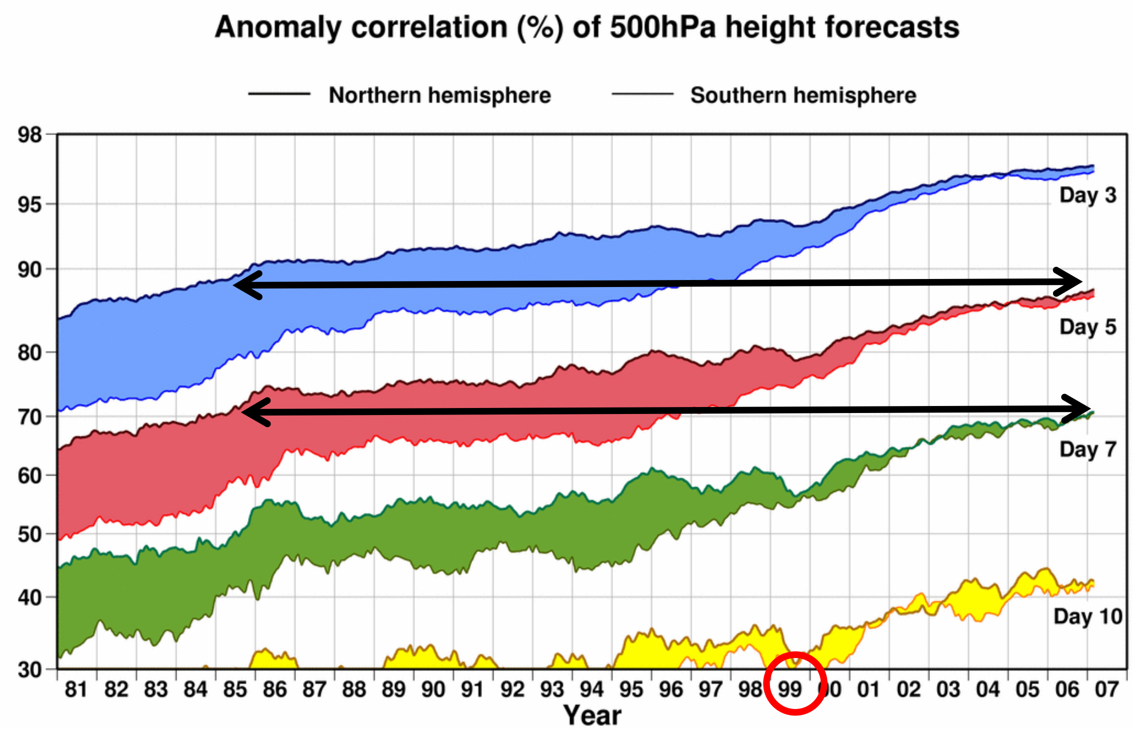
Progress in NWP has been a combination of:

- 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)

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

Applying NWP ideas to other areas:

- Chemistry models

  Chemistry-transport models (CTMs)

- Climate models

  General circulation models (GCMs)

- Climate-chemistry models (CCMs)

Can extend ideas to other models: Earth System models (ESMs)

Chemical models:

Accuracy of combined ozone information (obs/model)

ASSET project

Geer et al., ACP, 2007
Lahoz et al., ACP, 2007a, b

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

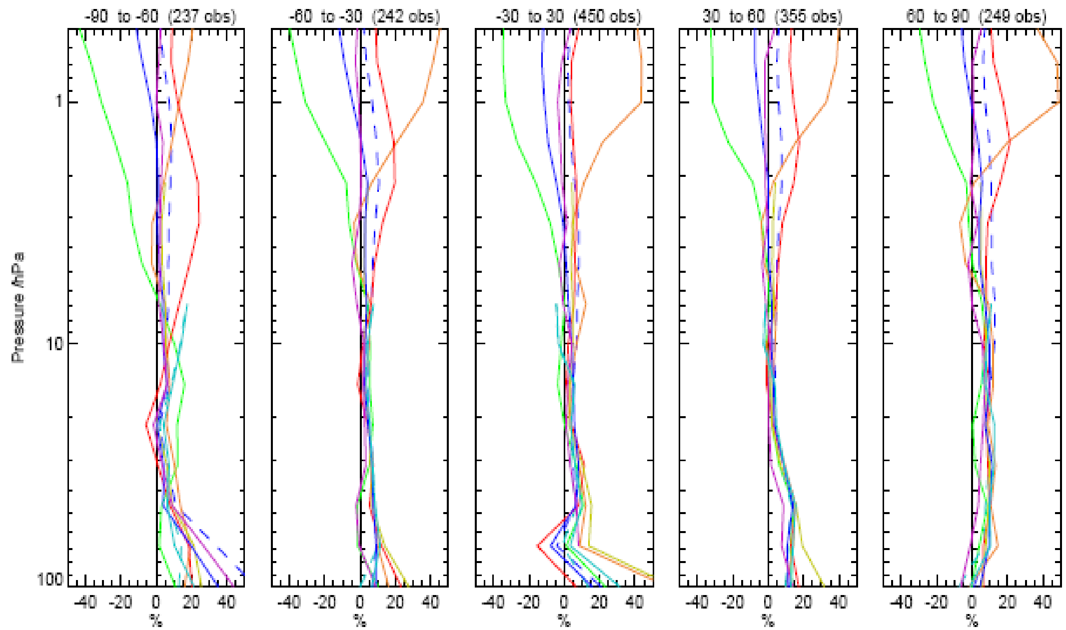


Fig. 10. Mean of analysis minus HALOE differences, normalized by climatology, for the period 18 August–30 November 2003. See Fig. 9 for colour key. The numbers in brackets indicate the HALOE/analysis coincidences within each latitude bin. Units: percent. These data are used to evaluate the performance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

Information on complexity of chemistry:
Parametrization v comprehensive
(e.g. ECMWF v BASCOE)

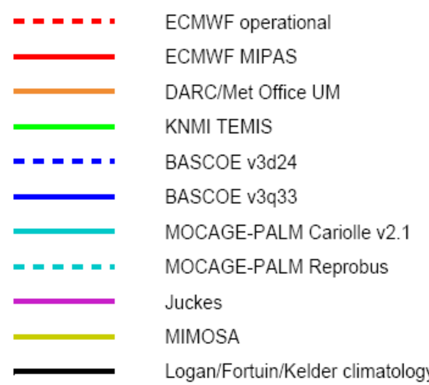
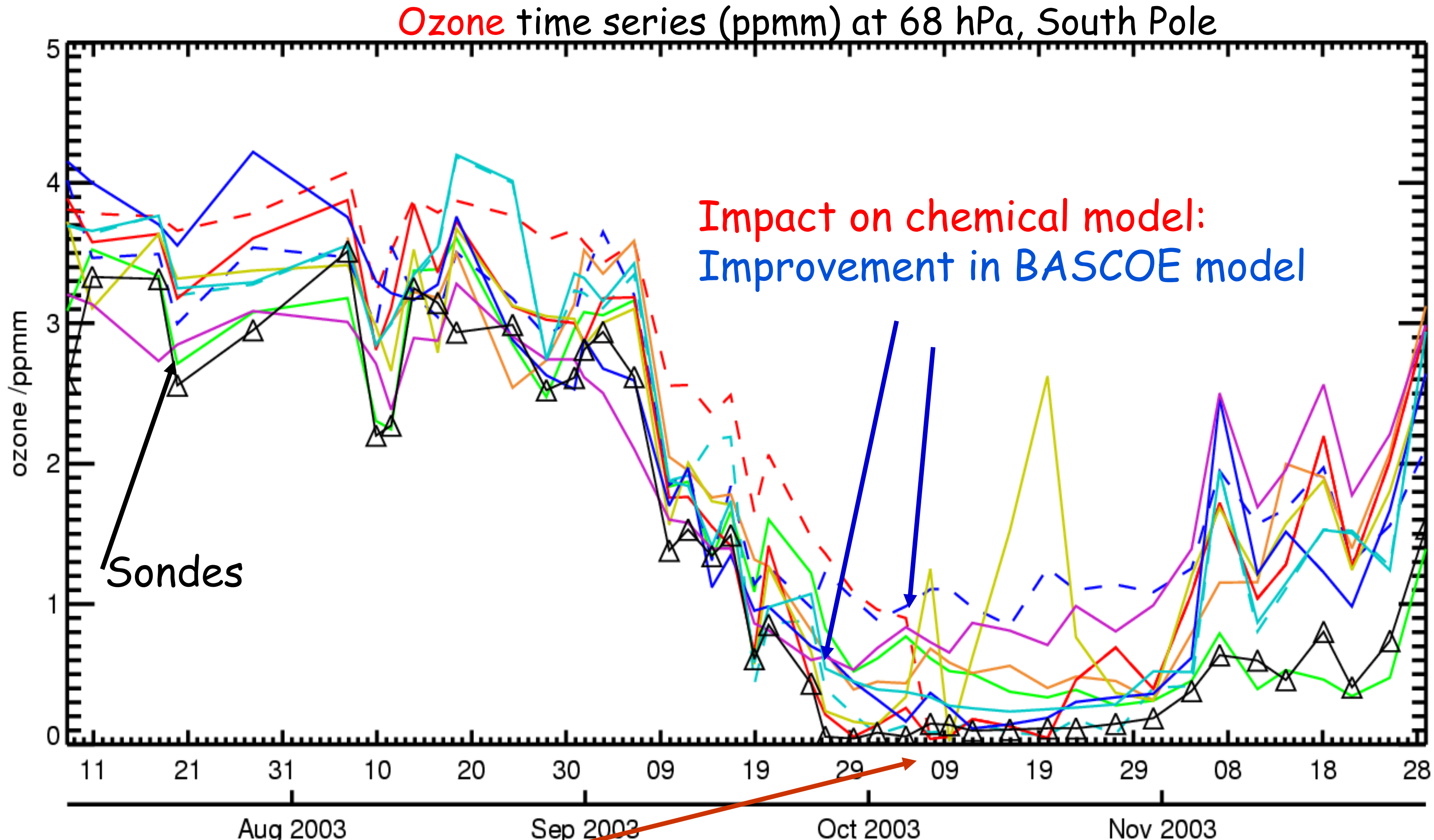
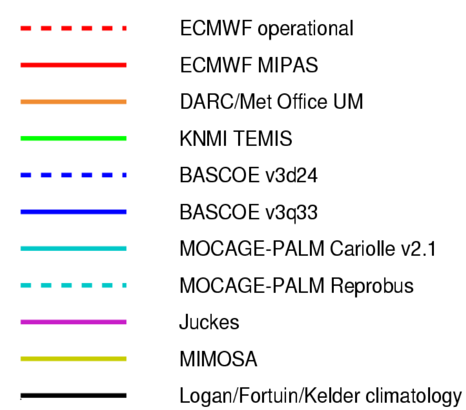


Fig. 9. Colour key used in Figs. 10–11.





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

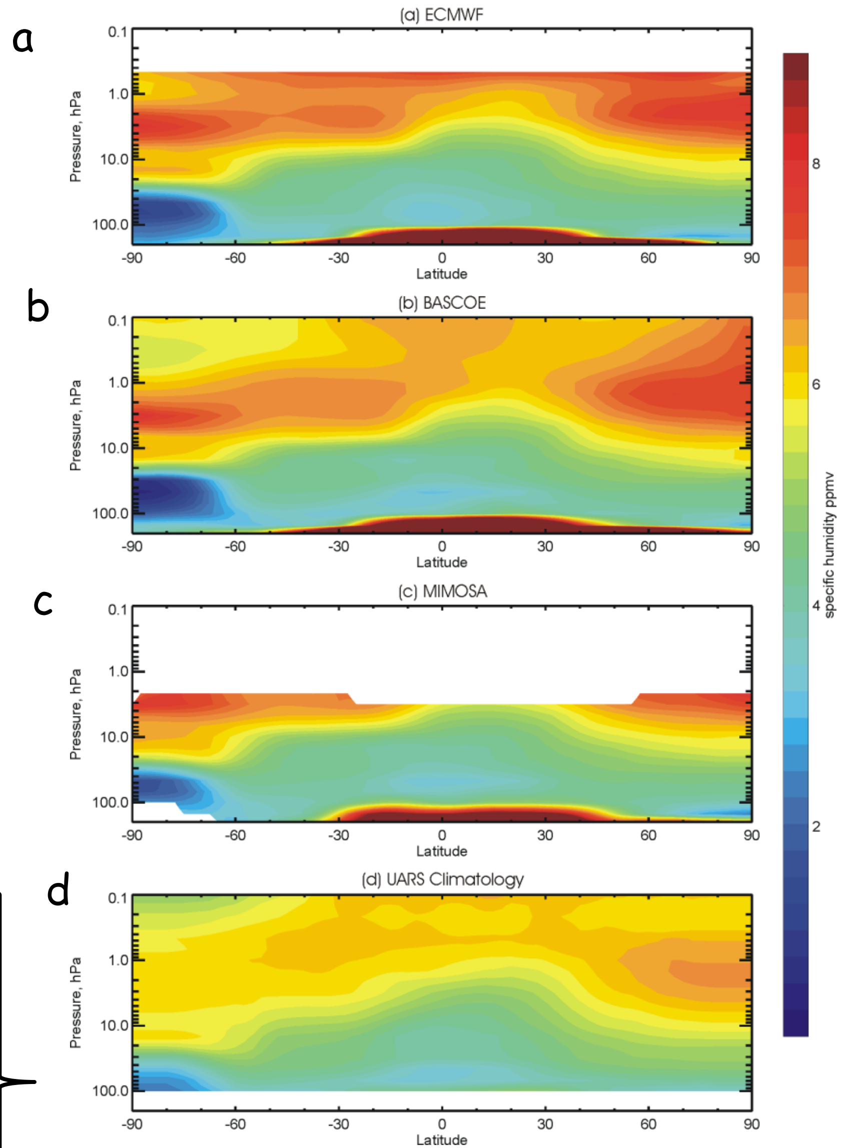
Lahoz et al., ACP, 2007a, b
Thornton et al., ACP, 2009

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

Information on DA system

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.



Climate models:

Recent NWP-based ideas to evaluate climate models:

- CAPT initiative – improve parametrizations in GCMs (*Phillips et al. 2004*) – requires accurate NWP analyses; systematic error can be largely attributed to parametrization deficiencies

- Seamless prediction – fundamental physical/dynamical processes common to both weather & seasonal forecasts, & climate-change timescales (*Palmer et al. , BAMS, 2008*)

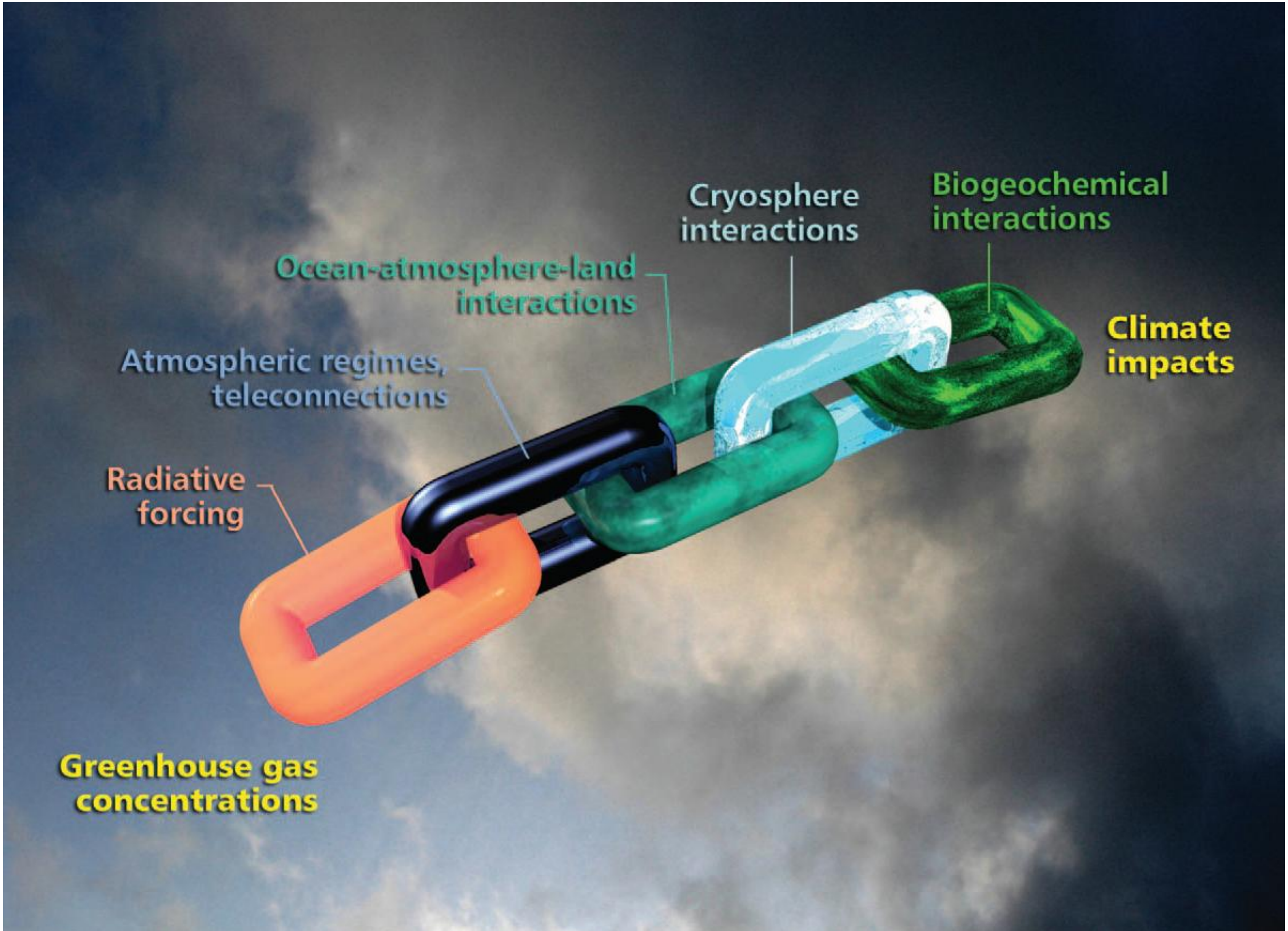
    - Proposal: probabilistic validation of models at timescales where validation data exist (e.g. daily, seasonal,...) can be used to calibrate climate-change probabilities at longer timescales.
    - Need for calibration reflects a need for model improvement

- Parameter estimation – e.g. climate model parameters (GWs…)

SPARC DA Meeting at IAMAS

See also efforts to quantify uncertainty in CCMs (*Waugh & Eyring 2008*)

Palmer et al., BAMS, 2008



Estimating climate model parameters using DA:

M. Pulido - see SPARC DA meeting at IAMAS

DA offers a reliable way to determine objectively parameters of a climate model

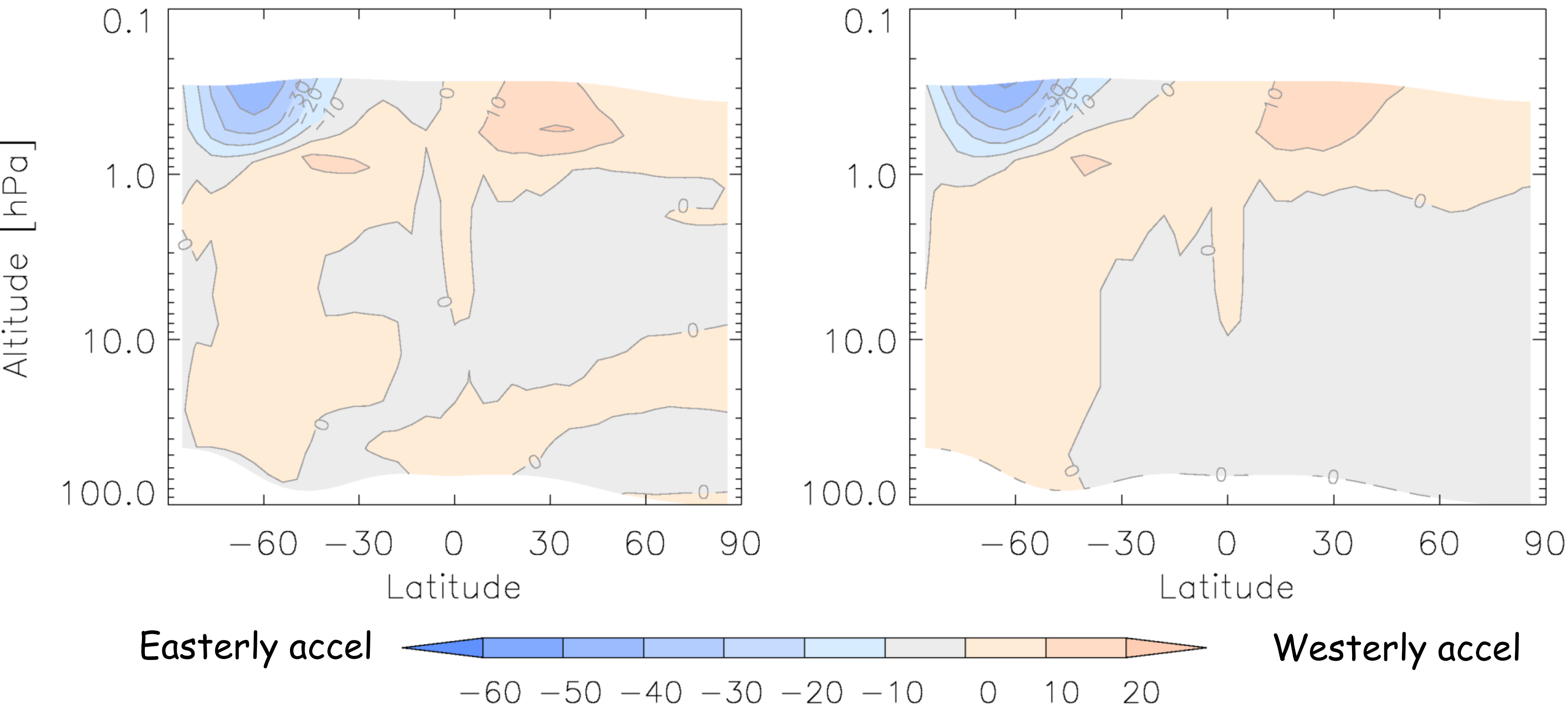
Details of approach:

- Parameters form the control space
- Observed variables that show sensitivity to parameters needed
- Optimum parameters are those that minimize a cost function

Differences from standard DA:

- Low-dimensional control space (10-100 parameters)
- Parametrizations usually contain highly non-linear regimes as function of parameters (affects choice of algorithm)

An example: missing force (ms^{-1}day^{-1}) due to small-scale waves



Left: Missing zonal force, Jul 2002, estimated with Assimilation System for Drag Estimation, ASDE (*Pulido & Thuburn, JC ,2008*), 4D-Var used to estimate drag/missing forces due to under/unresolved waves

Right: Forcing from a gravity wave drag scheme (*Scinocca, JAS, 2003*) using optimum parameters. Parameters estimated using a genetic algorithm (*Pulido et al. 2009 , in preparation).* Cost function contains multiple local max/min, but a well-defined global min (difficult for 4D-Var, but genetic algo can deal with this)

- Evaluate CCMs – quantify uncertainties in predictions

(1) SPARC-CCMVal & grading (*Waugh & Eyring, ACP, 2008*) – observationally-based diagnostics

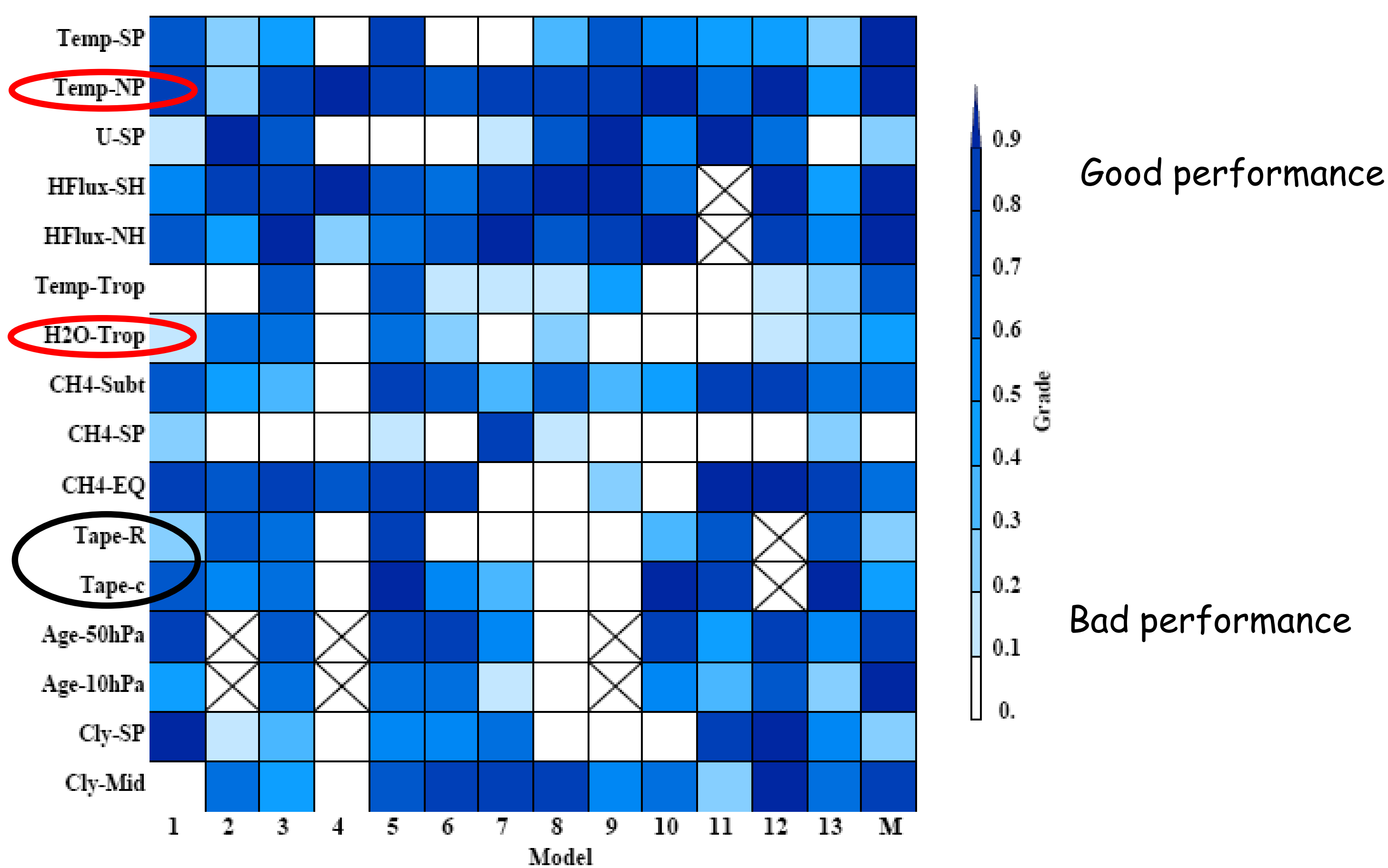


Fig. 2. Matrix displaying the grades (see color bar) for application of each diagnostic test to each CCM. Each row shows a different test, and each column a CCM. The right most column is the "mean model". A cross indicates that this test could not be applied, because the required output was not available from that model. See Table 1 for model names.

- CCMs – Models used in Waugh & Eyring

Table 1. CCMs used in this study. The models discussed in this paper are numbered alphabetically.

Name	Reference
AMTRAC	Austin et al. (2006)
CCSRNIES	Akiyoshi et al. (2004)
CMAM	Fomichev et al. (2007)
E39C	Dameris et al. (2005)
GEOSCCM	Pawson et al. (2008)
LMDZrepro	Lott et al. (2005)
MAECHAM4CHEM	Steil et al. (2003)
MRI	Shibata and Deushi (2005)
SOCOL	Egorova et al. (2005)
ULAQ	Pitari et al. (2002)
UMETRAC	Austin (2002)
UMSLIMCAT	Tian and Chipperfield (2005)
WACCM	Garcia et al. (2007)

- *CCMs* – Diagnostics used in Waugh & Eyring

Eyring et al., JGR, 2006

Table 2. Diagnostic tests used in this study.

Short Name	Diagnostic	Quantity	Observations	Fig. E06
Temp-SP	South Polar Temperatures	SON, 60° –90° S, 30–50 hPa	ERA-40	1
Temp-NP	North Polar Temperatures	DJF, 60° –90° N, 30–50 hPa	ERA-40	1
U-SP	Transition to Easterlies	U, 20 hPa, 60° S	ERA-40	2
HFlux-SH	SH Eddy Heat Flux	JA, 40° –80° S, 100 hPa	ERA-40	3
HFlux-NH	NH Eddy Heat Flux	JF, 40° –80° N, 100 hPa	ERA-40	3
Temp-Trop	Tropical Tropopause Temp.	T, 100 hPa, EQ	ERA-40	7a
H_2O-Trop	Entry Water Vapor	H_2O, 100 hPa, EQ	HALOE	7b
CH_4-Subt	Subtropical Tracer Gradients	CH_4, 50 hPa, 0–30° N/S, Mar/Oct	HALOE	5
CH_4-SP	Polar Transport	CH_4, 30/50 hPa, 80° S, Oct	HALOE	5
CH_4-EQ	Tropical Transport	CH_4, 30/50 hPa, 10° S–10° N, Mar	HALOE	5
Tape-R	H_2O Tape Recorder Amplitude	Amplitude Attenuation R	HALOE	9
Tape-c	H_2O Tape Recorder Phase Speed	Phase Speed c	HALOE	9
Age-50 hPa	Middle Stratospheric Age	10 hPa , 10° S-10° N and 35° –55° N	CO_2 and SF_6	10
Age-10 hPa	Lower Stratospheric Age	50 hPa , 10° S-10° N and 35° –55° N	ER2 CO_2	10
Cl_y-SP	Polar Cl_y	80° S, 50 hPa , Oct	UARS HCl	12
Cl_y-Mid	Mid-latitude Cl_y	30° –60° N, 50 hPa , Annual mean	multiple	–

- Evaluate CCMs – quantify uncertainties in predictions

(2) Use of data assimilation to evaluate uncertainties

One possible approach (not exhaustive):
Uncertainty analysis: input uncertainties -> output uncertainties
Perturbed chemistry ensemble: sample parameter space

(i) uncertainties in key parameters for stratospheric ozone chemistry (CCM inputs) using a DA system (e.g. CTM-based);
(ii) uncertainties in CCM outputs as a function of CCM inputs;
(iii) ensembles of DA experiments to estimate input uncertainties
(iv) ensembles of CCM experiments to estimate output uncertainties

Ideas under discussion: approach needs testing

Need:
- Observations/parameters to be simulated in a model
- Observations to constrain observations/parameters

A possible strategy for implementing DA to evaluate/improve CCMs and assess uncertainties in predictions:

1. Use theory & simple model expts
   Which chemical parameters to be evaluated?

2. Multi-model DA CTM expts to evaluate chemical parameters (e.g. onset of Cl activation, formation rate of HOCl, denitrification via PSC sedimentation, total Br_y) – model variables (chemical species & parameters) to be updated
   Parameters such as ClOOCl photolysis could be validated
   CTM must represent variables; observations must constrain variables

3. Could supplement DA expts with multi-model CTM expts (e.g. Polar Stratospheric Cloud parameters; transport)
   Extra information on input uncertainties

4. CCM multi-model expts with input uncertainties (mean, high, low) -> output uncertainties (temperature, ozone, water vapour,…)
   Output uncertainties as a function of input uncertainties

Question: for what aspects of photochemistry can DA best contribute?

Ways forward:

Data assimilation (DA) adds value to NWP models: ECMWF forecasts

By confronting models with observations & building on NWP heritage:

DA can add value to other models (chemical, climate, CCM, ESM)

- Desirable to have an NWP system developed parallel to climate model (But not necessary - e.g. input/output uncertainties approach)
- Ensemble approach useful (minimize model dependence of results), e.g. use an ensemble of DA systems & CCMs (expense?)
- Possible proposal to evaluate CCM uncertainties with DA: needs testing: roadmap, feasibility, cost… (note there may be other approaches)
- DA could be used to evaluate climate model parameters (early days…)

Note: WAVACS COST Action (www.isac.cnr.it/~wavacs) has plans for a workshop on evaluating climate models (incl. DA approach) - date TBC