ASSET
Assimilation of Envisat Data

Chemical Data Assimilation: Choices and Challenges

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NATURAL
ENVIRONMENT
RESEARCH COUNCIL

You want to do chemical DA... You ask:

What model should I use?
What DA scheme should I use?
What data should I assimilate?
How complex must chemistry be?

} CHOICES

Answer: confront observations with models

-> The ASSIC project: Comparison of ozone analyses
Geer, Lahoz et al. (2006), ACPD (accepted)
http://darc.nerc.ac.uk/asset/assic/index.html

Exercise will help reveal CHALLENGES of chemical DA

Chemical DA:

Two approaches: NWP models (GCMs) & chemical models (CTMs):

1) NWP + tracer (stratospheric methane)
NWP + parametrization of chemistry (Cariolle + cold tracer)
NWP + chemical module (coupled system)

2) CTM + tracer (no chemistry)
CTM + parametrization (Cariolle + cold tracer)
CTM + complex chemistry

Note: approaches converging (e.g. coupled NWP/CTM)

Algorithm options:

(1) Var:

3D-Var: DARC/Met Office
4D-Var: ECMWF; BIRA-IASB
3D-FGAT: MF/CERFACS

(2) KF methods:

KF + parametrization: KNMI

(3) other:

Direct inversion: Juckes

Observation options:

(1) Retrievals (L2):

Constituents:
NWP (DARC/Met Office)
CTMs (Several groups)

(2) Radiances (L1):

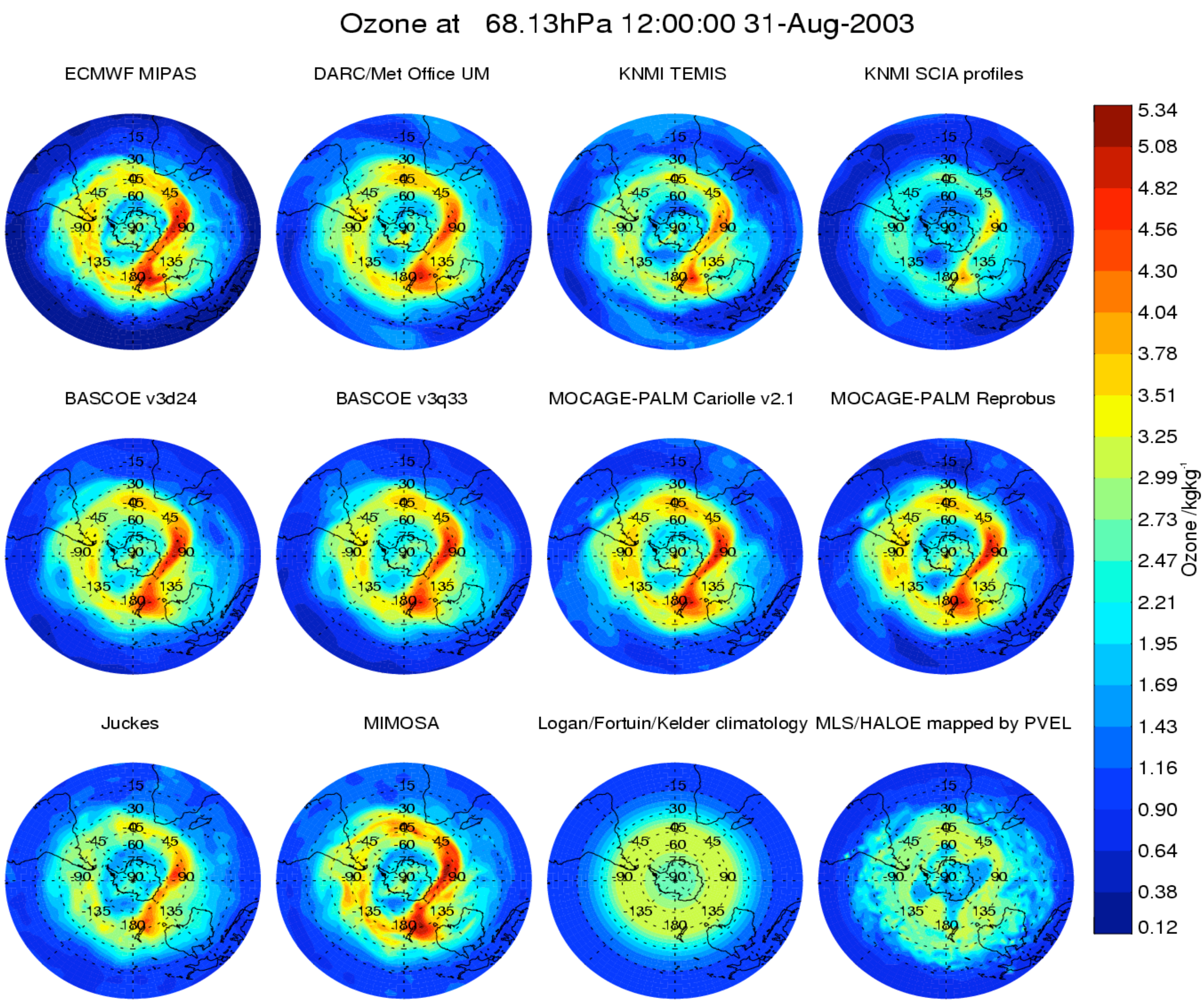
Nadir: NWP systems
Limb: ECMWF

Not investigated here

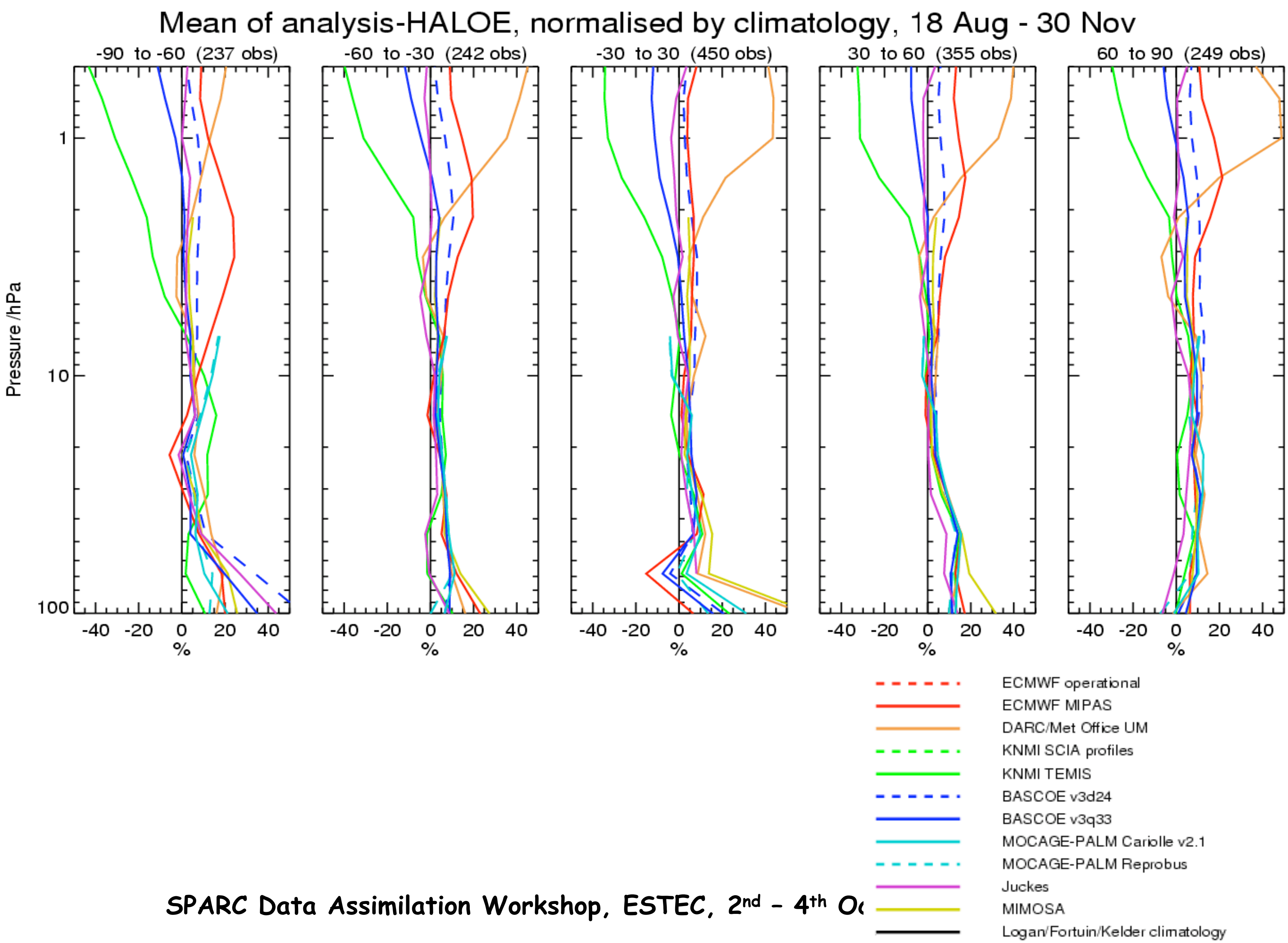
Analyses

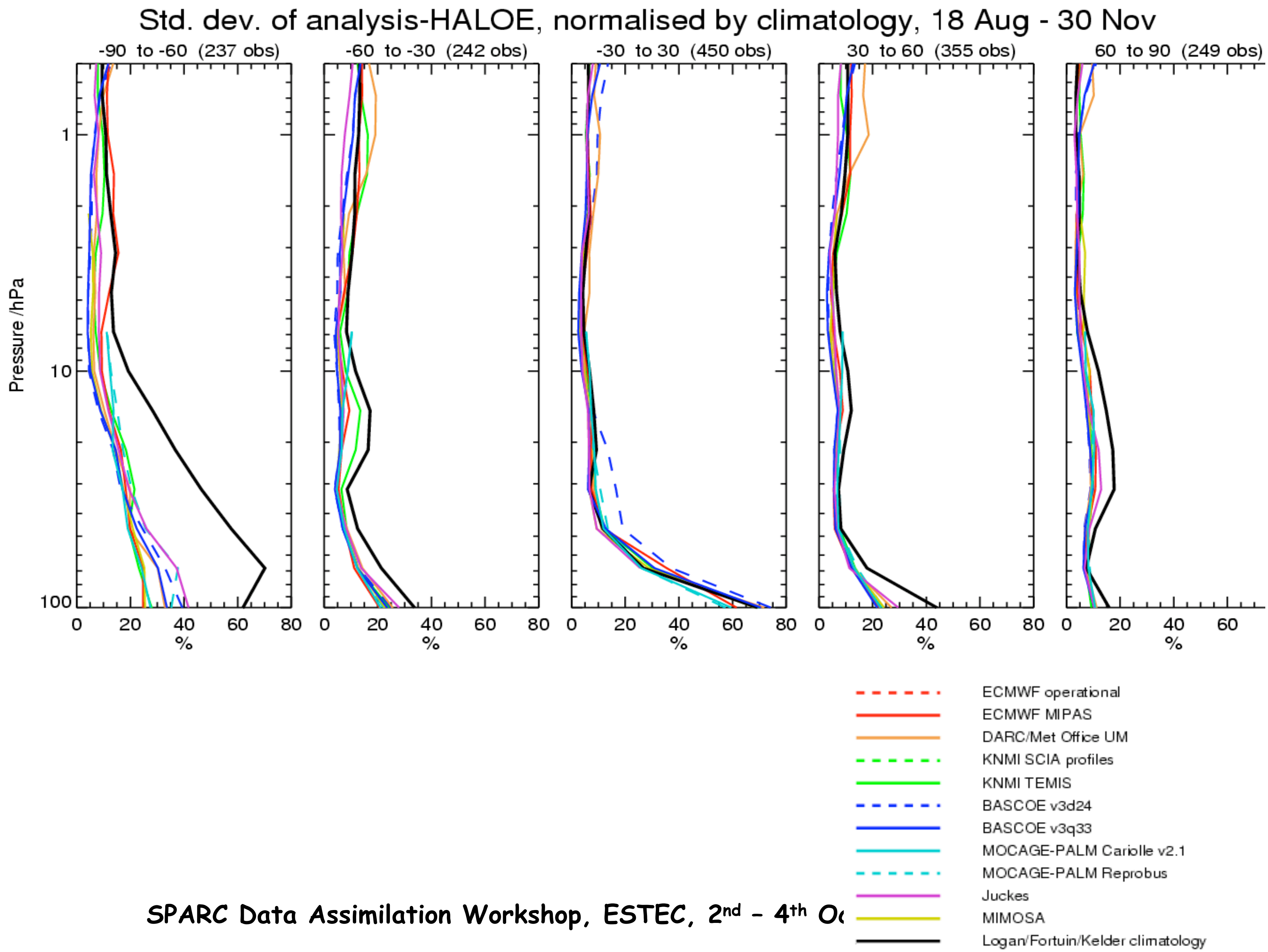
N.B. Canadian GEM analyses will be compa

- Model:
  - NWP GCM: DARC/ Met Office, ECMWF
  - CTM: KNMI, BASCOE, Meteo-France/CERFACS
  - Isentropic CTM: MIMOSA, Juckes (2006)
- Data:
  - MIPAS: all except KNMI
  - SCIAMACHY: KNMI; columns / profiles
- Ozone chemistry:
  - None: MIMOSA, Juckes
  - Cariolle scheme: (linearized ozone chemistry)
  - Full chemistry: Reprobus (reasonable troposphere), BASCOE (diurnal cycle in mesosphere)
- Assimilation techniques:
  - 3D-Var, 4D-Var, 3D-FGAT, sub-optimal KF, Direct Inversion

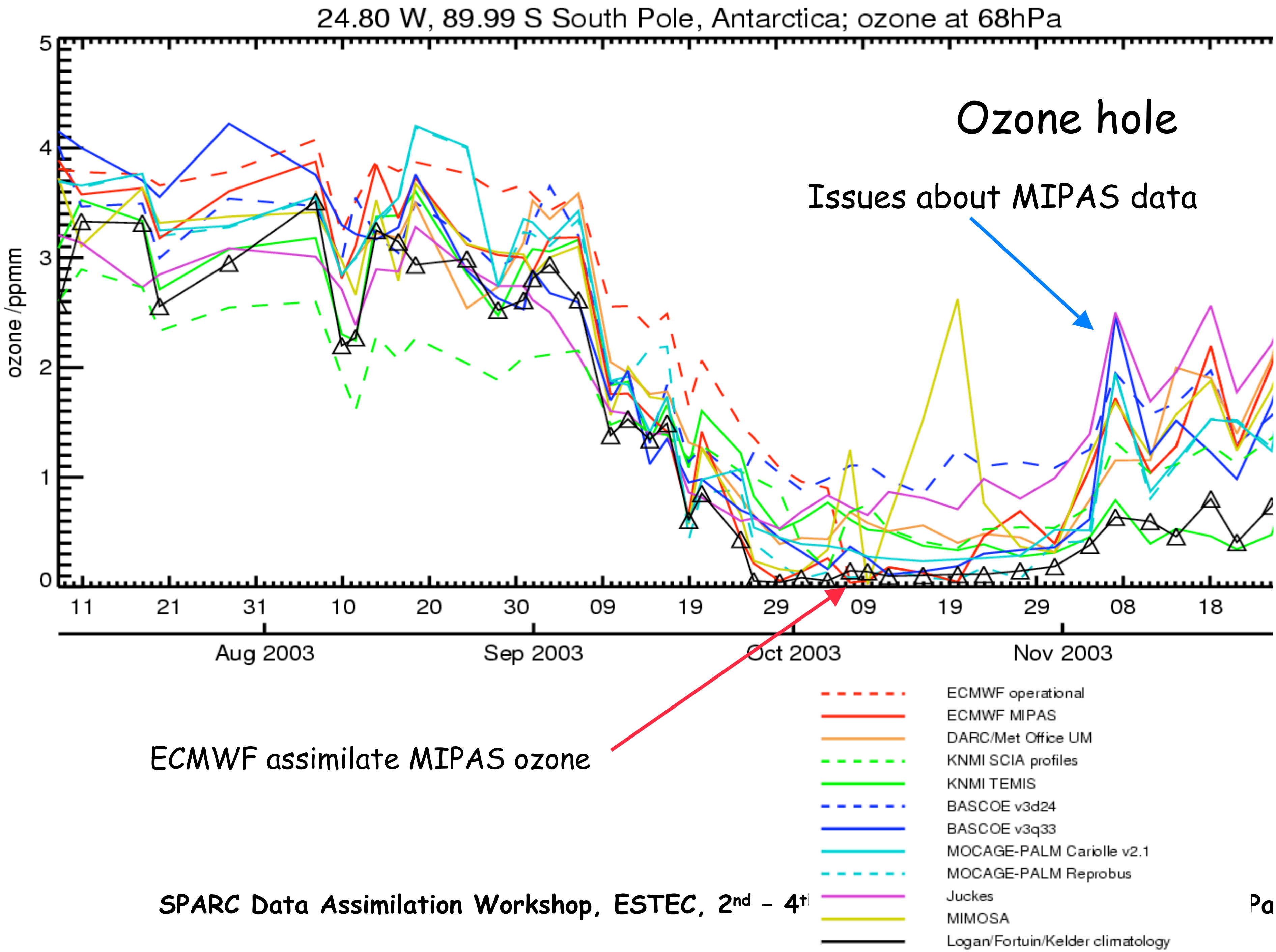

Ozone at 68.13hPa 12:00:00 31-Aug-2003
ECMWF MIPAS
DARC/Met Office UM
KNMI TEMIS
KNMI SCIA profiles
BASCOE v3d24
BASCOE v3q33
MOCAGE-PALM Cariolle v2.1
MOCAGE-PALM Reprobus
Juckes
MIMOSA
Logan/Fortuin/Kelder climatology
MLS/HALOE mapped by PVEL
5.34
5.08
4.82
4.56
4.30
4.04
3.78
3.51
3.25
2.99
2.73
2.47
2.21
1.95
1.69
1.43
1.16
0.90
0.64
0.38
0.12
Ozone /kgkg^{-1}

a


Mean of analysis-HALOE, normalised by climatology, 18 Aug - 30 Nov
-90 to -60 (237 obs)
-60 to -30 (242 obs)
-30 to 30 (450 obs)
30 to 60 (355 obs)
60 to 90 (249 obs)
Pressure /hPa
1
10
100
-40 -20 0 20 40
%
ECMWF operational
ECMWF MIPAS
DARC/Met Office UM
KNMI SCIA profiles
KNMI TEMIS
BASCOE v3d24
BASCOE v3q33
MOCAGE-PALM Cariolle v2.1
MOCAGE-PALM Reprobus
Juckes
MIMOSA
Logan/Fortuin/Kelder climatology



SPARC Data Assimilation Workshop, ESTEC, 2nd – 4th Oc


24.80 W, 89.99 S South Pole, Antarctica; ozone at 68hPa
Ozone hole
Issues about MIPAS data
ECMWF assimilate MIPAS ozone
ozone /ppmm
0
1
2
3
4
5
11
21
31
10
20
30
09
19
29
09
19
29
08
18
Aug 2003
Sep 2003
Oct 2003
Nov 2003
ECMWF operational
ECMWF MIPAS
DARC/Met Office UM
KNMI SCIA profiles
KNMI TEMIS
BASCOE v3d24
BASCOE v3q33
MOCAGE-PALM Cariolle v2.1
MOCAGE-PALM Reprobus
Juckes
MIMOSA
Logan/Fortuin/Kelder climatology

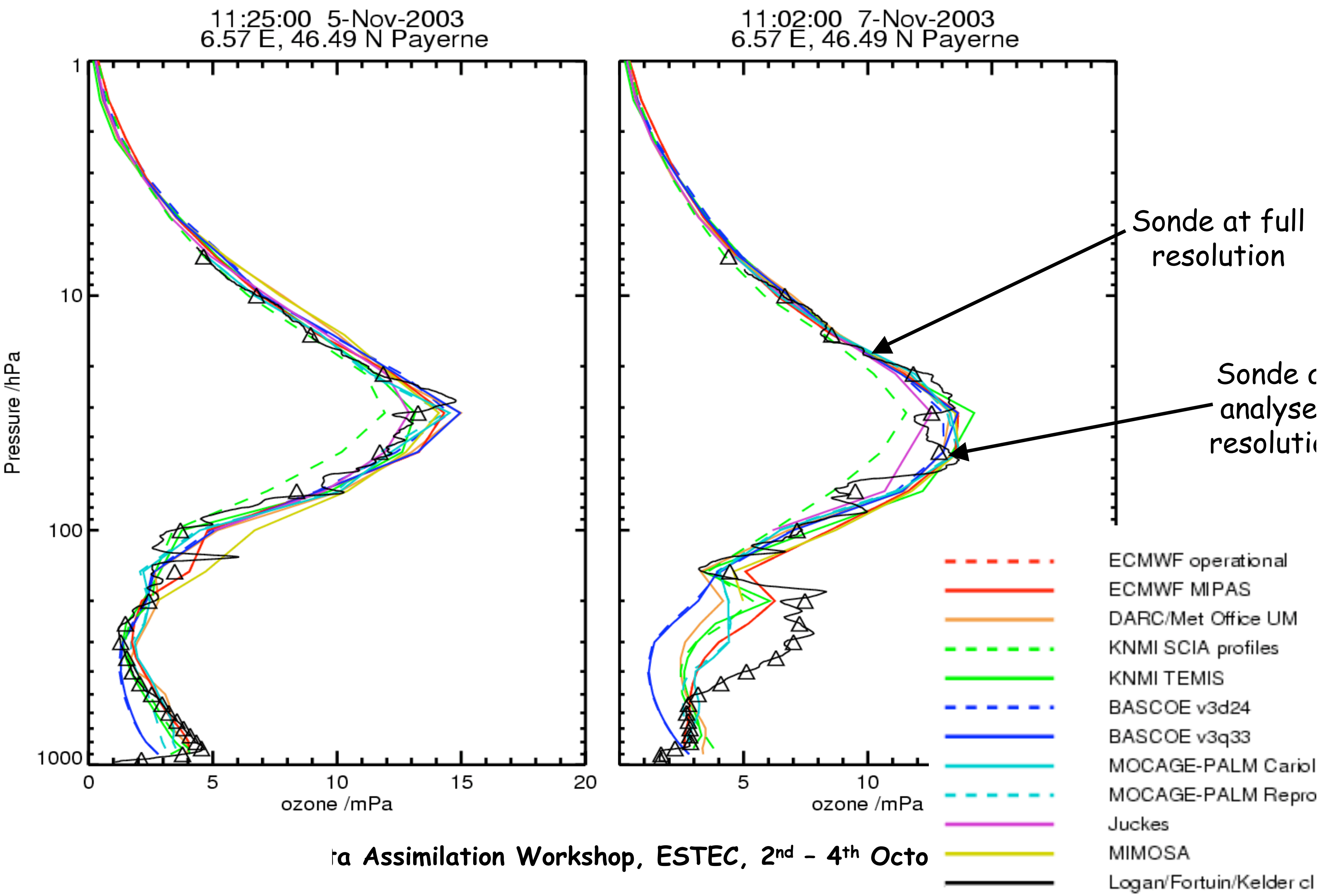
Ozone hole: heterogeneous chemistry schemes

- Correctly depleting ozone to near-zero:
  - T < 195K term (Cariolle v1.2, v2.1)
  - MOCAGE-PALM Reprobus – detailed scheme
  - BASCOE v3q33 – PSC parametrization

- 0.5 ppmm ozone remains (incorrect):
  - KNMI, DARC – cold tracer
    - Cariolle v1.0 adds too much ozone in vortex
    - KNMI?

- 1-2 ppmm ozone remains (incorrect):
  - BASCOE v3d24 – detailed PSCBox scheme
    - Affected by inappropriate aerosol formulation (Daerden et al. ACPD 2006)
  - MIMOSA, Juckes
    - No chemistry; MIPAS data limitations

Midlatitude UTLS: Payerne ozonesonde profiles



First results

- Through most of stratosphere (50 hPa-1 hPa) biases within +/- 10% and standard deviations less than 10% vs sonde & HALOE

  GOOD AGREEMENT

- Areas with worse agreement:
  - Upper stratosphere and mesosphere
  - Ozone hole
  - UTLS
  - Tropical tropopause
  - Troposphere
  - BUT at least one analysis is within 10% of independent data

These areas have issues about fidelity of transport, chemistry and observations: time-scales vs observation revisit time

Problem areas

Green -> amber -> red

- Ozone hole
  - A variety of heterogeneous chemistry schemes work well
- Upper stratosphere / mesosphere
  - Care needed to avoid biases in linear chemistry
  - Newer linear chemistry schemes work well
  - Diurnal variability?
  - Are there remaining uncertainties in chemistry and instrument calibration?
- Troposphere
  - Relaxation to climatology?
- Tropical tropopause
  - Improvements needed in modelled transport and in observations
- Extratropical UTLS
  - Needs further investigation and case studies

Conclusions from ASSIC

MIPAS profiles:

If good data quality & coverage:

Similarly good results obtained no matter DA method or system

(Current DA systems)

MIPAS ~5% higher than HALOE in mid/upper stratosphere & mesosphere (above 30 hPa), & ~10% higher than ozonesonde & HALOE in lower stratosphere (100 hPa - 30 hPa)

SCIAMACHY total columns:

Almost as good as MIPAS analyses; analyses based on SCIAMACHY limb profiles are worse in some areas -> problems in SCIAMACHY retrievals

LESSON LEARNT: FUTURE COMPARISONS

Choice of DA system:

- Current DA systems based on different approaches show broadly similar agreement vs independent data

Potential improvements:

- Improved ozone analyses can be achieved via better modelled chemistry & transport & better observations

- Likely that improvements will come through better modelling of background errors (**B**)

Chemistry complexity:

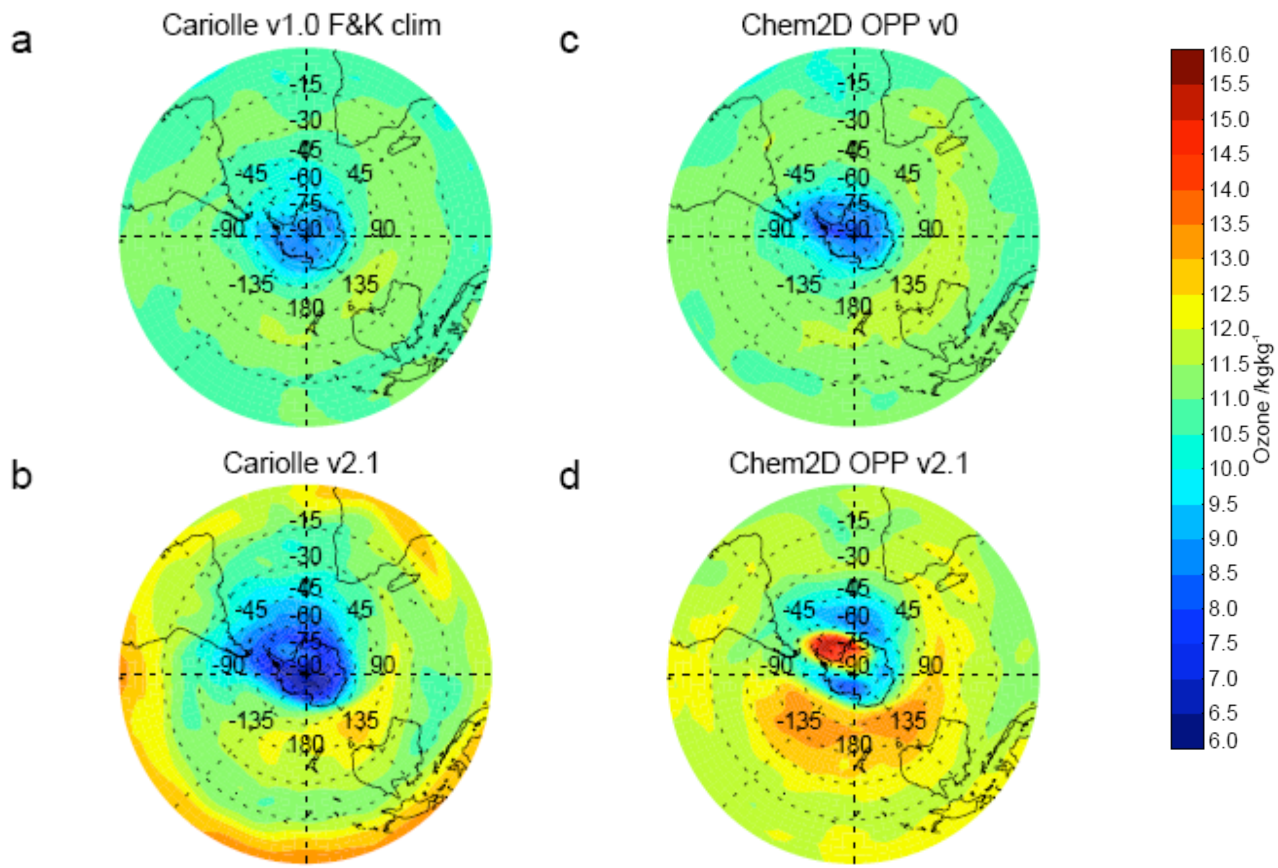
- Schemes with no chemistry do well vs. independent observations; extremely fast; depend on quality & availability of MIPAS data
- These schemes are not as good for ozone hole -> limitations with MIPAS observations; CTMs & GCMs with chemistry do better
- Linear chemistry parametrizations (Geer, Lahoz et al 2006 ACPD, accepted) -> impact in upper stratosphere

  Fast chemical time-scales – see next 2 slides

Costs:

- GCM-based analyses -> substantially more computer power than CTMs; ozone DA relatively small additional cost when included in NWP system

Cariolle schemes



Heterogeneous Chemistry fixe

Fig. 9. Ozone fields at 3.2hPa on 1/10/2003 from (a) Cariolle v1.0, (b) Cariolle v2.1, (c) Chem2D-OPP v0 and (d) Chem2D-OPP v2.1 analyses.

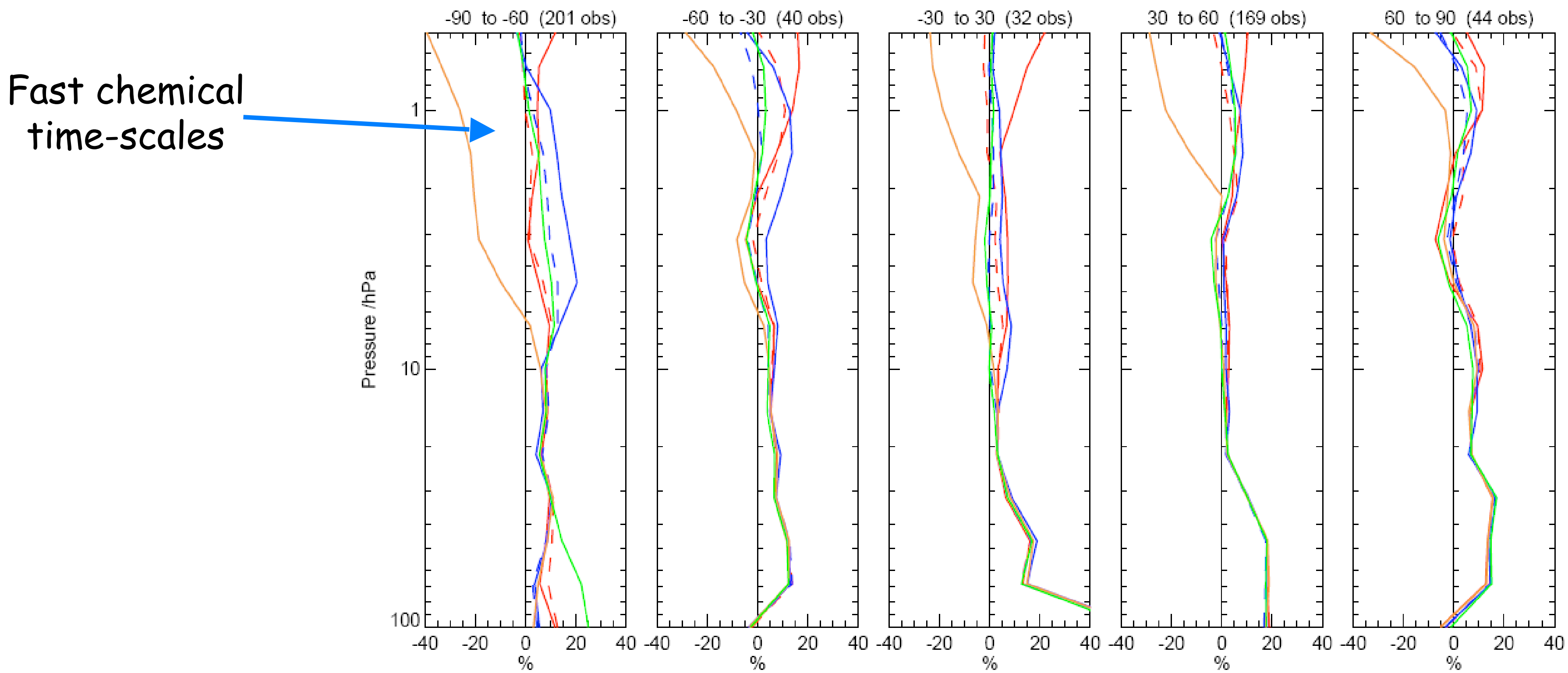
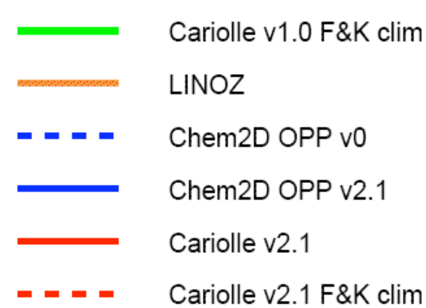
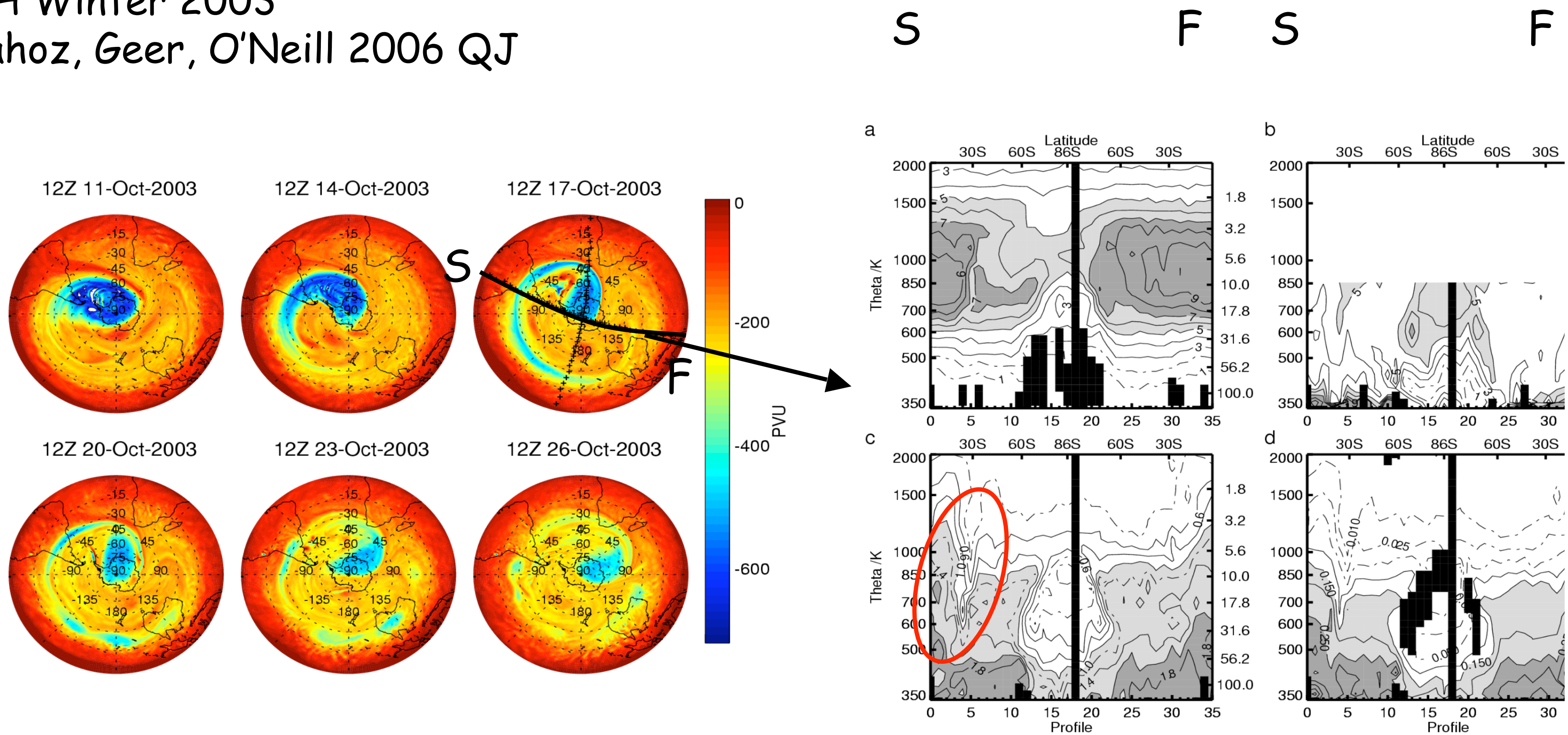


Fig. 5. Mean of (analysis - HALOE) ozone, normalised by climatology, in latitude bands for the period 27/9/2003 to 5/11/2003. See colour key in Fig. 4.



BUT Let's step back: you can also use data analyses…

SH Winter 2003
Lahoz, Geer, O'Neill 2006 QJ

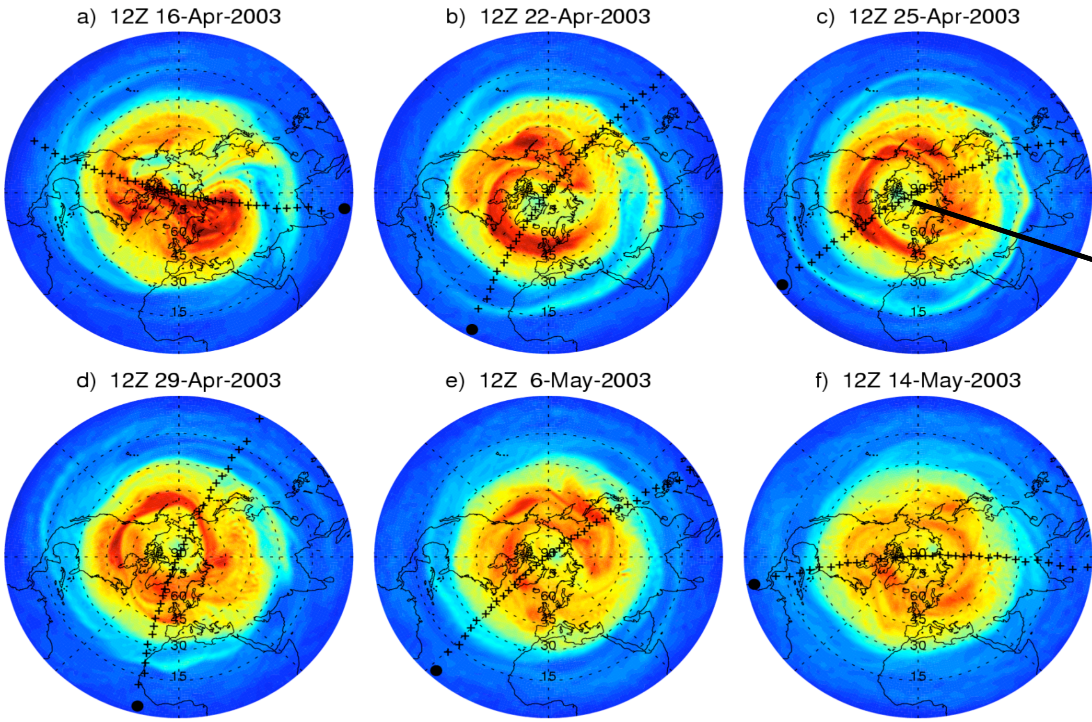


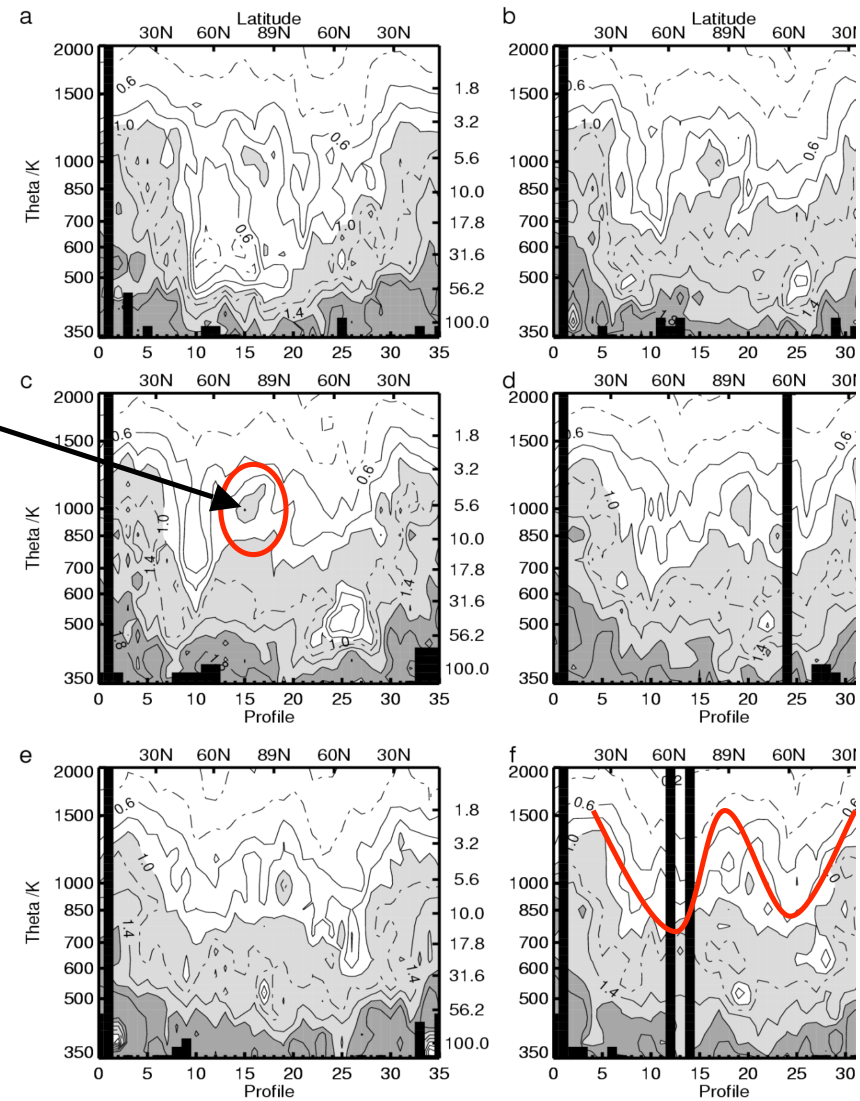
PV at 850 K

17 October x-sections:
a): O_3, b) H_2O, c) CH_4, d) N_2O

Data analysis S F

NH Summer 2003;
Lahoz, Geer, Orsolini 2006 QJ





PV at 850 K

-> CONFIDENCE IN DATA...

What comes from these studies: challenges

- Quality of data

Good quality data -> similar results from different DA/model approaches
Use approaches other than DA to look at data: consistency

- Bias in models and observations

Observations & models confronted to identify & attribute biases
Implementation of bias correction schemes active field of research

- Estimation of **B**

Needs to take account of physical & chemical principles

Model deficiencies in transport & chemistry limit value of DA

Dynamical v chemical time-scales

Chemistry applications

- Weather forecasts -> add ozone (usually with simplified chemistry) to enhance pre-existing NWP system (GCM-based): DARC/MO, ECMWF
- Chemistry-> strong arguments to build ozone DA into CTM with sophisticated chemistry, taking met. input as given: BIRA-IASB
- Ozone -> middle way: use transport model, driven by pre-existing dynamical fields, in combination with simplified chemistry scheme (e.g. Cariolle): KNMI, GMAO
- Coupled system -> chemical module embedded in GCM – still early days: BIRA-IASB and MSC Canada

CHOICE DEPENDS ON APPLICATION

Finally…

•DA invaluable for use of stratospheric constituent measurements:

- •Fills gaps between observations
- •Allows use of heterogeneous measurements

•Numerical model -> information to be propagated forward in time: combination of measurements available at different times & locations

•Properly applied, DA can add value to observations & models, compared to information that each can supply on their own

•DA underpins evaluation of impact of current observation types using OSEs, and future global observing system using OSSEs

DA ADDS VALUE

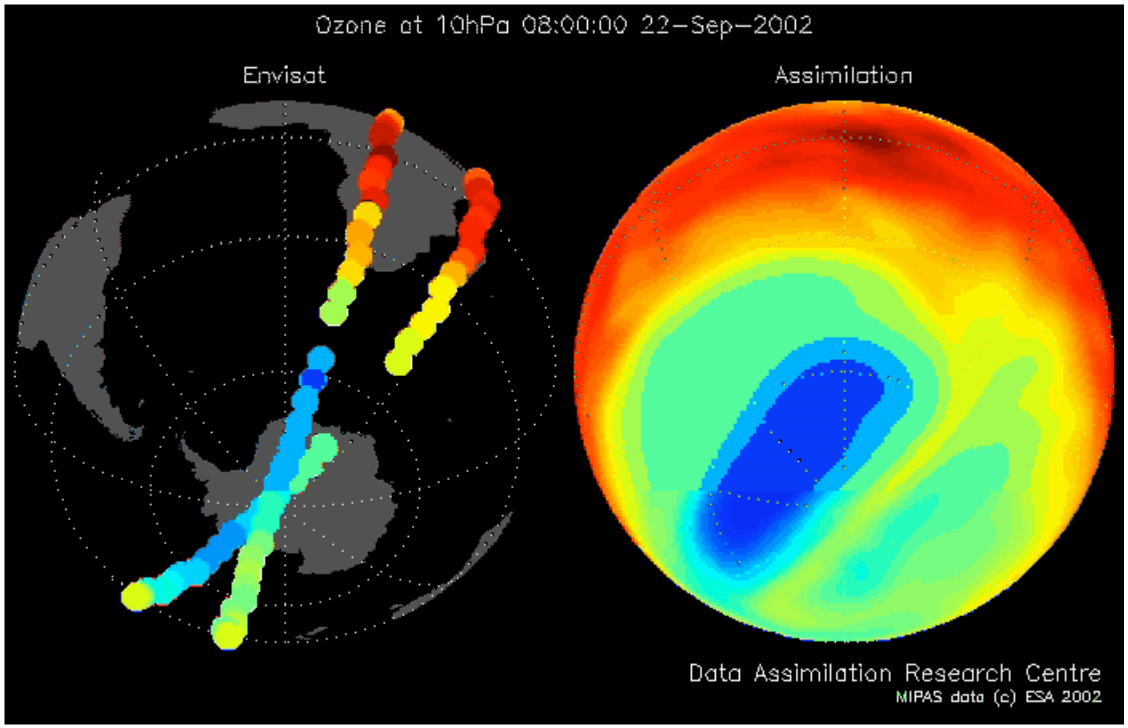
BUT, for proper use, limitations must be borne in mind

BE VERY CAREFUL HOW YOU USE DA…

HOW DA CAN ADD VALUE

The SH polar vortex split of Sep 2002: ozone at one level

MIPAS ozone



DARC analyses

Courtesy Alan Geer

Blue: low ozone; Red: high ozone; 10 hPa