



# The impact of ground based ozone monitoring on stratospheric ozone assessments: A case study using sequential and variational data assimilation

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Deutsches Zentrum  
für Luft- und Raumfahrt e.V.  
in der Helmholtz-Gemeinschaft

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# Motivation

- ↗ Satellite instruments: lack of limb/occultation sounder >2010 ?
- ↗ LIDAR: few instruments, expensive in sustained operation
- ↗ Ozone sondes: mature, relatively cheap, many stations  
(500-700\$ total costs per sounding)
- ↗ Umkehr retrieval: high potential but only low vertical resolution

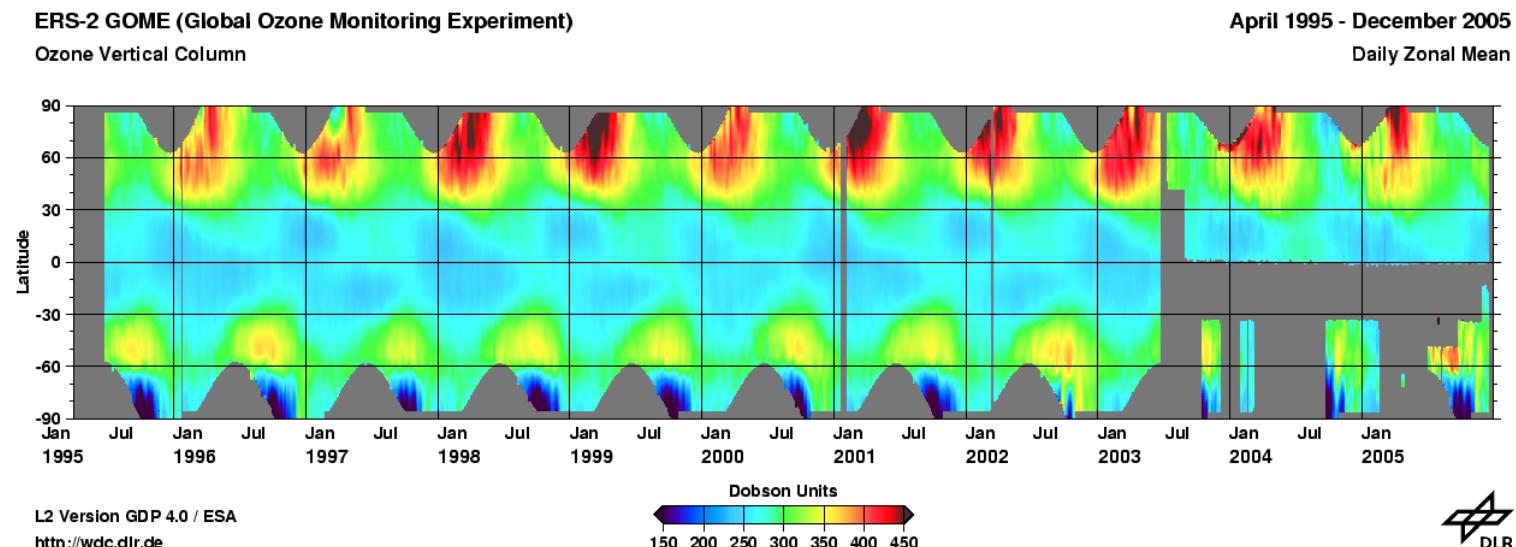
(see, e.g., WMO/IGACO ozone and UV recommendations)

Bulk of ozone below 10 hPa!

--> assess current ozone sonde networks (this study)

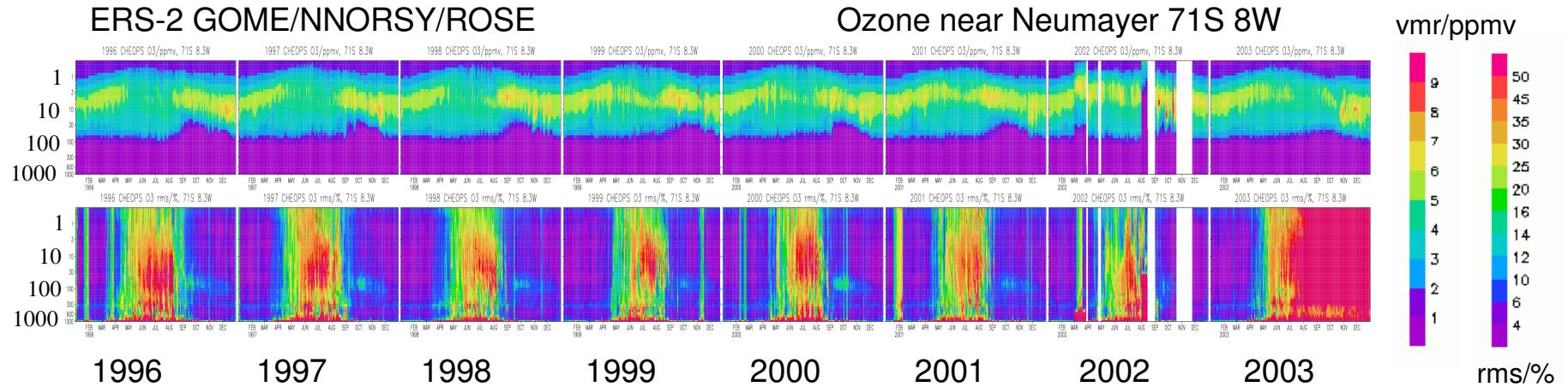
## ERS-2 GOME total ozone column heritage

- ↗ Nadir looking UV instrument giving 320 x 40km<sup>2</sup> footprints
- ↗ Global coverage / 3 days since January 1996, reduced since July 2003
- ↗ Retrieval version 4 data within 5% c.t. NDSC (e.g., Spurr et al., 2005)
- ↗ Application projects: ESA CHEOPS, GSE PROMOTE



# CHEOPS vertical ozone profile record

- ↗ Vertical O<sub>3</sub> profiles using neural network approach (NNORSY)  
(Müller et al., 2003)
- ↗ Approximately 10 years of data available since 1996
- ↗ Sequential assimilation as consistency check / fill gaps
- ↗ Analyzed profiles show very low bias with most rms <10%



# PROMOTE long-term 3D stratospheric ozone record

## a joined service by BIRA and DLR

**Best affordable description of chemical state** by combination of satellite data, meteorological data and chemistry-transport models

**Long-term synoptic 3D ozone analyses** to identify trends in reactive trace gases and inorganic reservoir species

### Target products:

- ↗ O<sub>3</sub> and related (destructive) species (ClO<sub>x</sub>, NO<sub>x</sub>, BrO<sub>x</sub>)
- ↗ Polar-stratospheric clouds (PSCs)
- ↗ Reservoir species: eg., Cl<sub>y</sub>, Br<sub>y</sub>
- ↗ Quantification of chemical ozone loss

**Temporal coverage:** 1992-2004 (phase 1), 2005 – to date

**Core user:** SPARC CCMval, WMO (negociations)

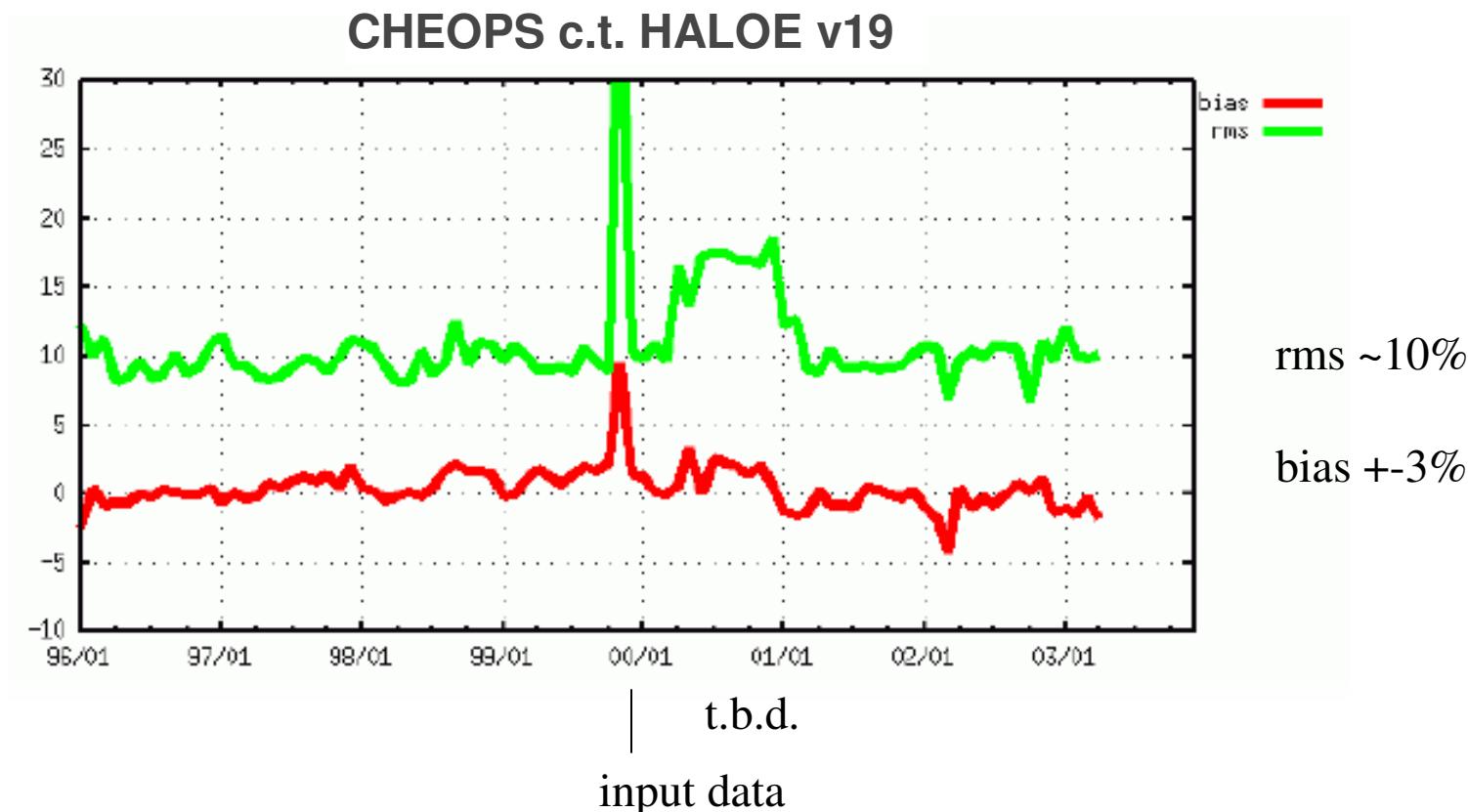
# GOME/NNORSY V3 ozone profiles

## Neural Network Ozone Retrieval System (Müller et al., 2003)

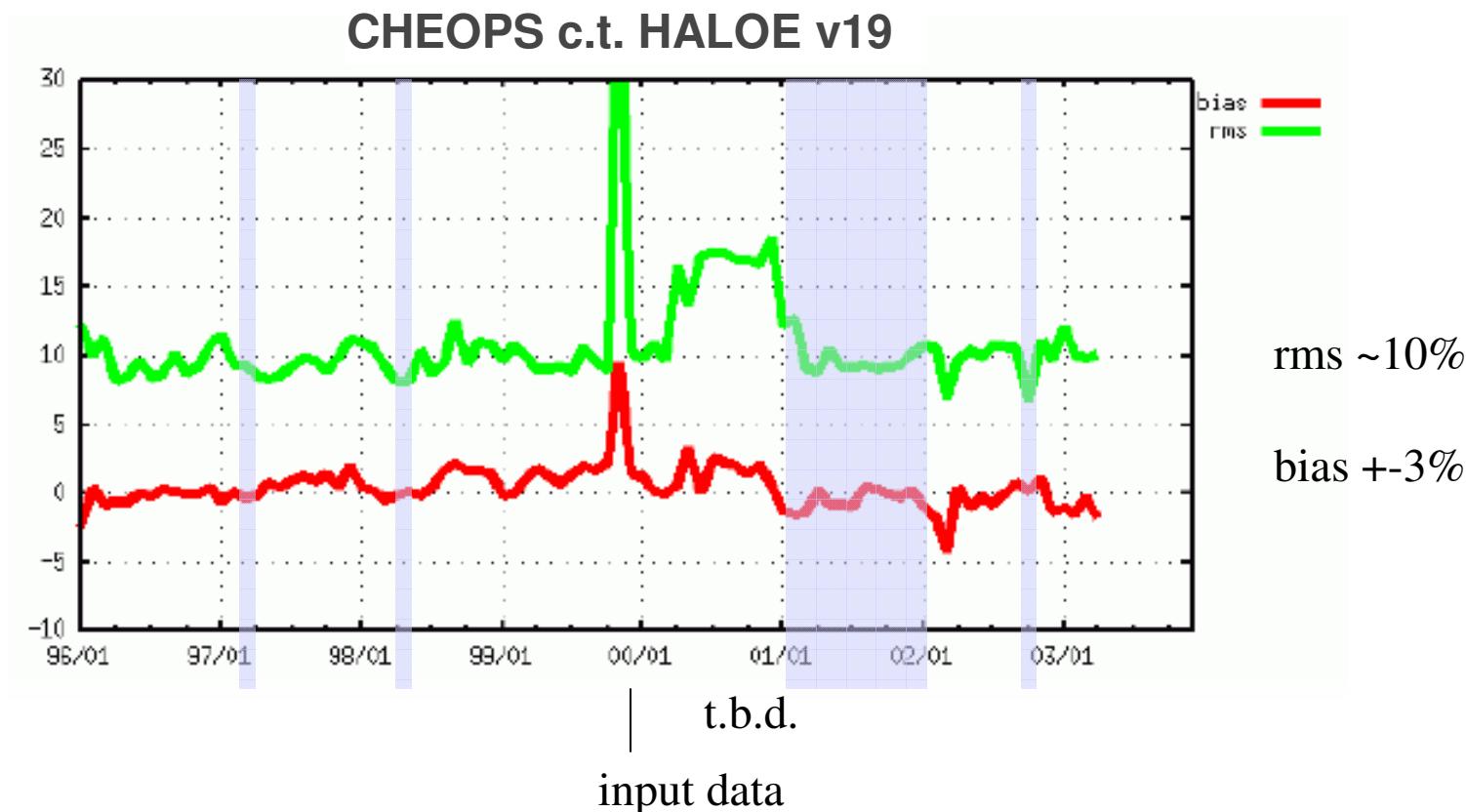
- ↗ feed forward 3-layer neural network
- ↗ spectral, temperature (GEOS4) and climate data as input
- ↗ trained by additional spectral and profile measurements

<b>Training data</b>	GAW and NDACC ozone sondes HALOE, SAGE II, POAM III and SBUV
<b>Data volume</b>	ca. 30,000 profiles per day
<b>Spatial resolution</b>	320km x 40km, 3-5km between 15-32km alt.
<b>Profile errors</b>	bias <<5%, rms <10% for stratosphere independent study (Meijer et al. 2006): 5-10%
<b>Caveats</b>	tropopause region, high zenith angles

# CHEOPS analyzed ozone record 1996-2003: GOME/NNORSY/ROSE sub-opt KF approach



# CHEOPS analyzed ozone record 1996-2003: GOME/NNORSY/ROSE sub-opt KF approach



data used for this study

# Observation Simulation System Experiments (OSSEs)

Simulated ozone soundings using CHEOPS data

## Ozone radio sondes

several networks, currently ca. 2 soundings per day

## 10hPa max altitude

ca. 30min per ascend, >100km drift possible

-> instantaneous ‘measurement’ on 2.5° model grid

## WMO and NASA registered stations (#15, 73, 125 total)

location derived from WOUDC data center:

<http://www.msc-smc.ec.gc.ca/woudc>



# Observation Simulation System Experiments (OSSEs)

Two experiment sets

## 'short-term'

- 1997 April 01-18th: low-ozone streamer from north of Europe
- 1998 Febr. 01-18th: North Atlantic low-ozone streamer
- 2002 Sept. 11-28th: Antarctic vortex-split episode

## 'long-term'

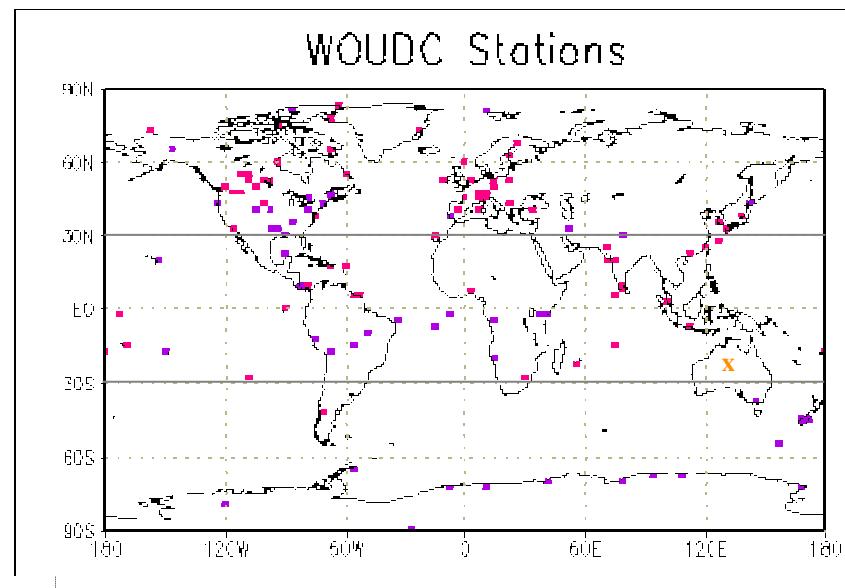
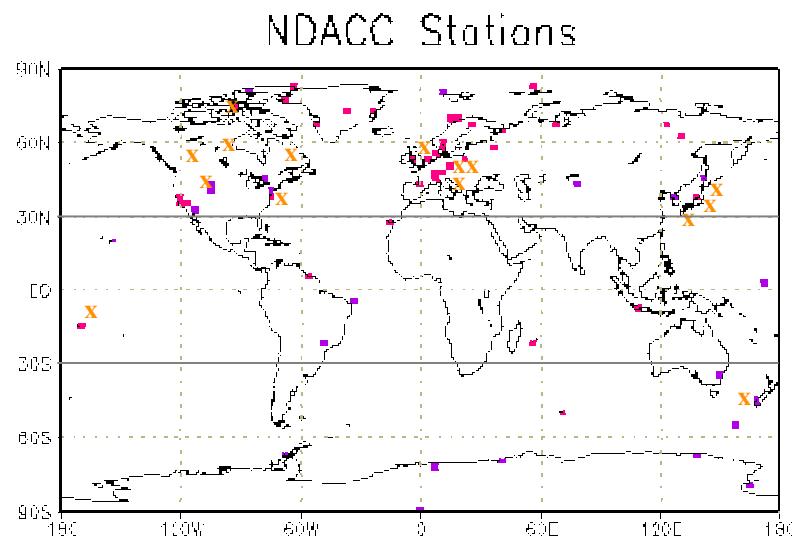
- 2001 January-September (Q1-Q3): cold persistent both hemispheres

Three *pseudo* networks (CHEOPS ozone record as input)

- GAW(A)** 15 active stations, mostly North America and Europe
- NDACC** 73 stations, global, Greenland, Scandinavia, Antarctica
- WOUDC** 125 stations, global, all registered including SHADOZ



# Ozone sonde station networks



X : active GAW stations

# Observation Simulation System Experiments (OSSEs)

Two experiment sets

## 'short-term'

1997 April 01-18th:	network	WOUDC	1/day	>30 °N
1998 Febr. 01-18th:		WOUDC	1/day	<30 °NS
2002 Sept. 11-28th:		WOUDC	1/day	>30 °S

## 'long-term'

2001 01-09:	network	GAW	1/day
		NDACC	1/week
		WOUDC	1/week
		Reference	no sounding



# CHEOPS/ROSE ozone sonde profile OSSE

Resolution =  $2.5 \times 3.7^\circ$ , 1.3km, 43 levels (1000-0.3hPa)

Meteorological analyses: UKMO 24h wind and temp. fields

Finite-volume transport scheme (Lin and Rood, 1996)

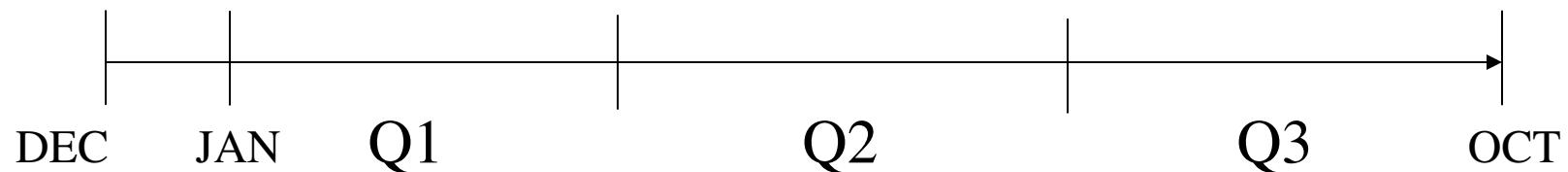
Non-QSSA chemistry (JPL14), NAT, ICE, sulphate aerosols

Sequential assimilation of vmr/rms from CHEOPS analyses  
(instantaneous ‘observations’ from surface up to 10 hPa at 7am LT)

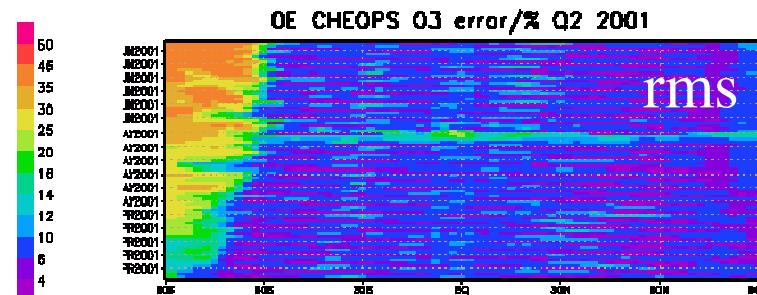
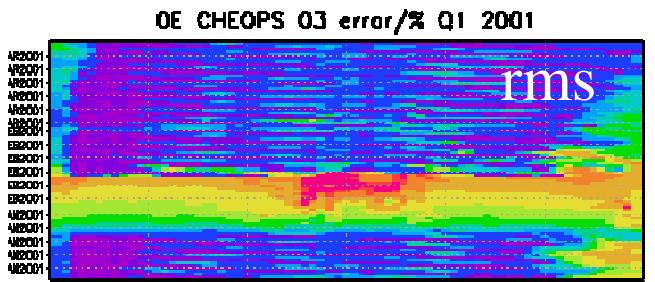
KF: propagation of analysis errors (e.g., Khattatov et al., 2002)

## **'long-term' experiments: 2001 Q1-Q3**

*initialization*

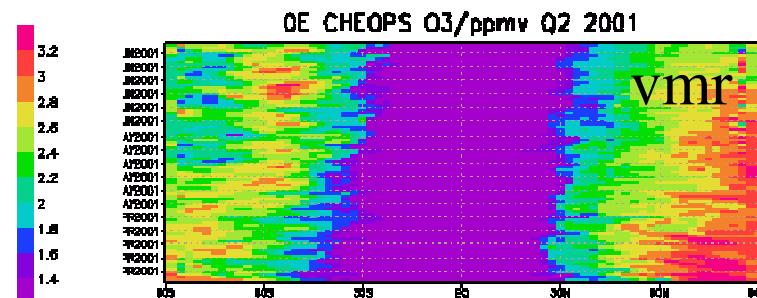
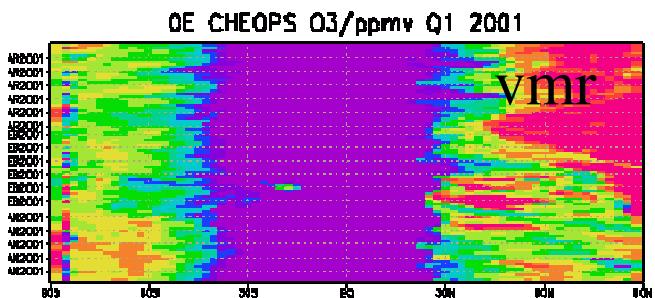


Q1



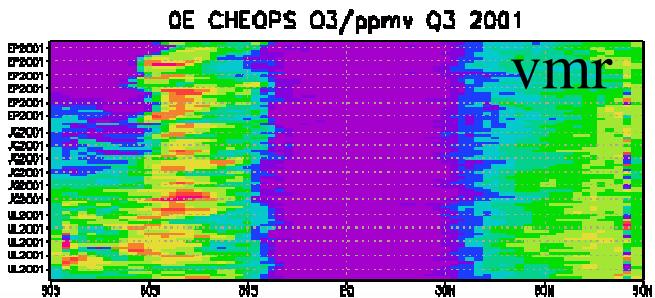
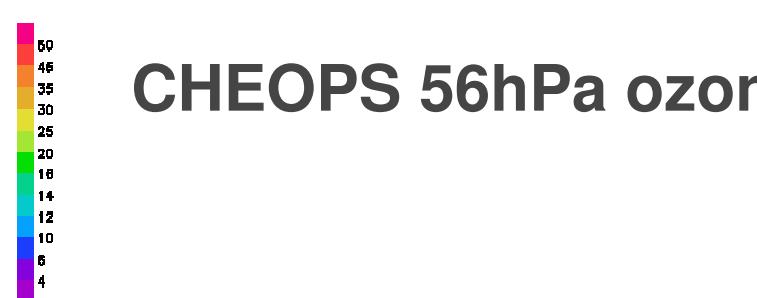
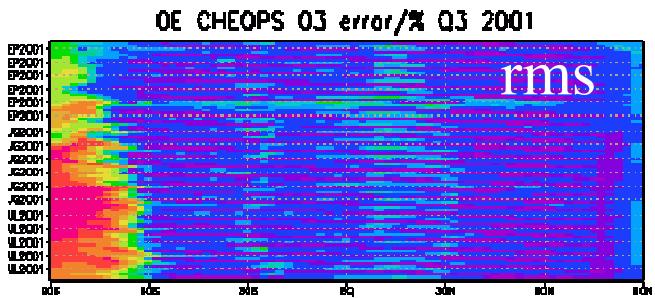
Q2

1/%



1/ppmv

Q3



## CHEOPS 56hPa ozone



## Total residuals: Reference - HALOE\* (>100hPa)

Reference Q1				Reference Q2				
	#	mean	bias	rms	#	mean	bias	rms
SH	27064	3.46	-5.43	23.83	28333	3.67	5.07	16.89
TP	16942	3.73	-8.04	26.20	24471	3.82	-3.62	21.56
NH	25279	3.71	-4.24	17.17	7527	3.54	-1.04	12.87

Reference Q3				
	#	mean	bias	rms
SH	14733	3.82	7.88	19.77
TP	8961	3.96	-0.74	20.43
NH	18186	3.25	-1.07	15.26

## Total residuals: GAW - HALOE

	GAW Q1				GAW Q2			
	#	mean	bias	rms	#	mean	bias	rms
SH	27064	3.46	-5.45	23.15	28333	3.65	4.40	16.22
TP	16942	3.73	-7.97	25.36	24471	3.81	-3.75	21.12
NH	25279	3.71	-4.18	15.36	7527	3.51	-2.10	11.21

	GAW Q3			
	#	mean	bias	rms
SH	14733	3.77	6.66	17.82
TP	8961	3.92	-1.25	19.85
NH	18186	3.23	-1.79	14.64

## Total residuals: NDACC - HALOE

	NDACC Q1				NDACC Q2			
	#	mean	bias	rms	#	mean	bias	rms
SH	31801	3.43	-3.28	19.14	28333	3.60	3.12	15.03
TP	17014	3.82	-5.34	21.03	24471	3.87	-2.05	18.14
NH	29948	3.72	-3.57	14.40	7527	3.48	-2.83	11.07

	NDACC Q3			
	#	mean	bias	rms
SH	12468	3.82	5.53	15.49
TP	1314	3.80	2.75	17.45
NH	6986	3.01	-1.48	11.04

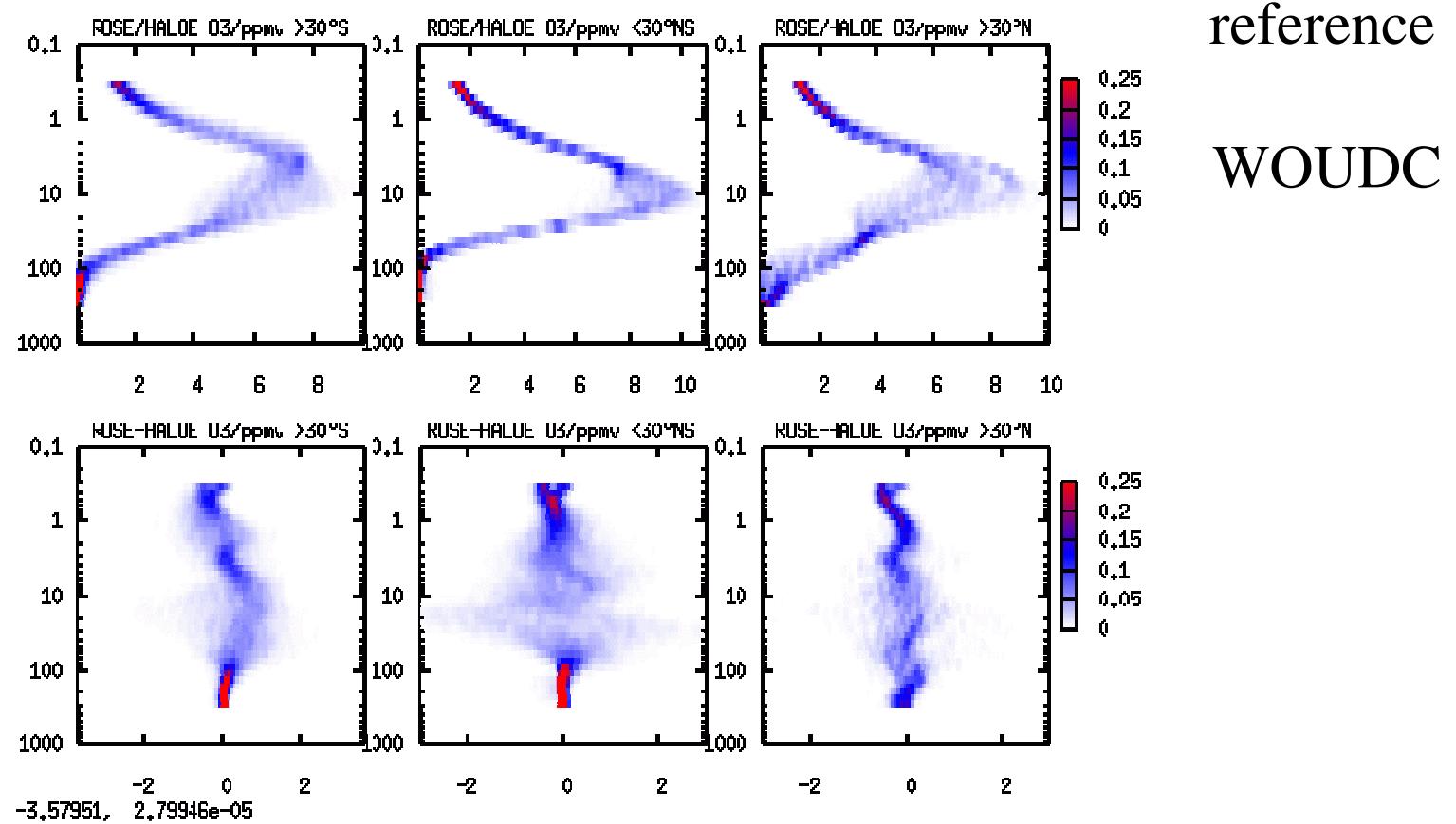
## Total residuals: WOUDC - HALOE

	WOUDC Q1				WOUDC Q2			
	#	mean	bias	rms	#	mean	bias	rms
SH	31801	3.45	-2.93	18.13	28333	3.60	3.12	14.89
TP	17014	3.84	-4.72	19.70	24471	3.89	-1.75	16.90
NH	29948	3.71	-3.69	14.33	7527	3.50	-2.30	10.92

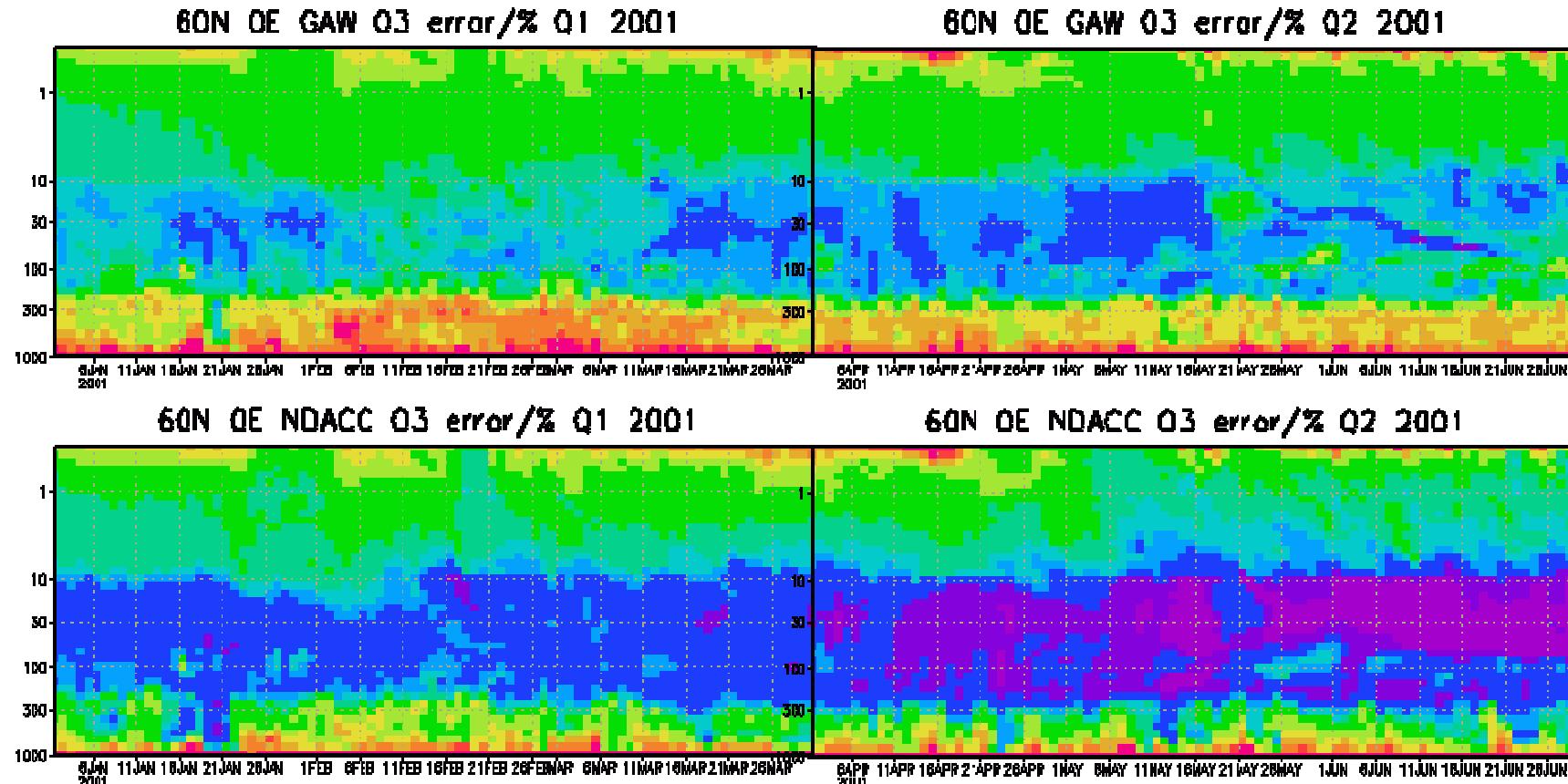
  

	WOUDC Q3			
	#	mean	bias	rms
SH	12468	3.83	5.61	15.49
TP	1314	3.84	3.69	16.90
NH	6986	3.00	-1.99	11.18

# PDF analysis Q2: Reference/WOUCD - HALOE



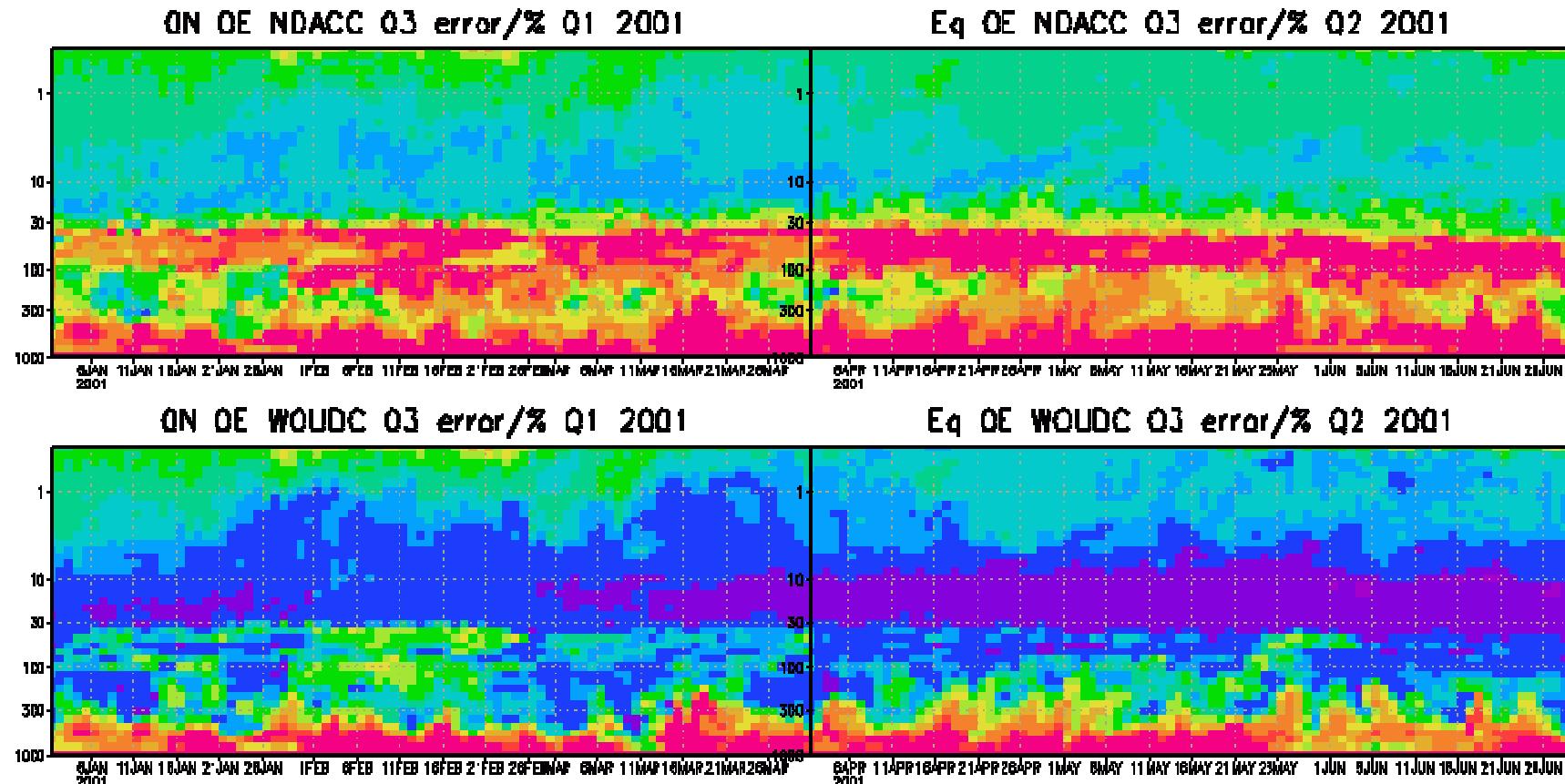
# Analysis error GAW/NDACC Q1, Q2 60°N



# Analysis error NDACC/WOUDC

Q1, Q2

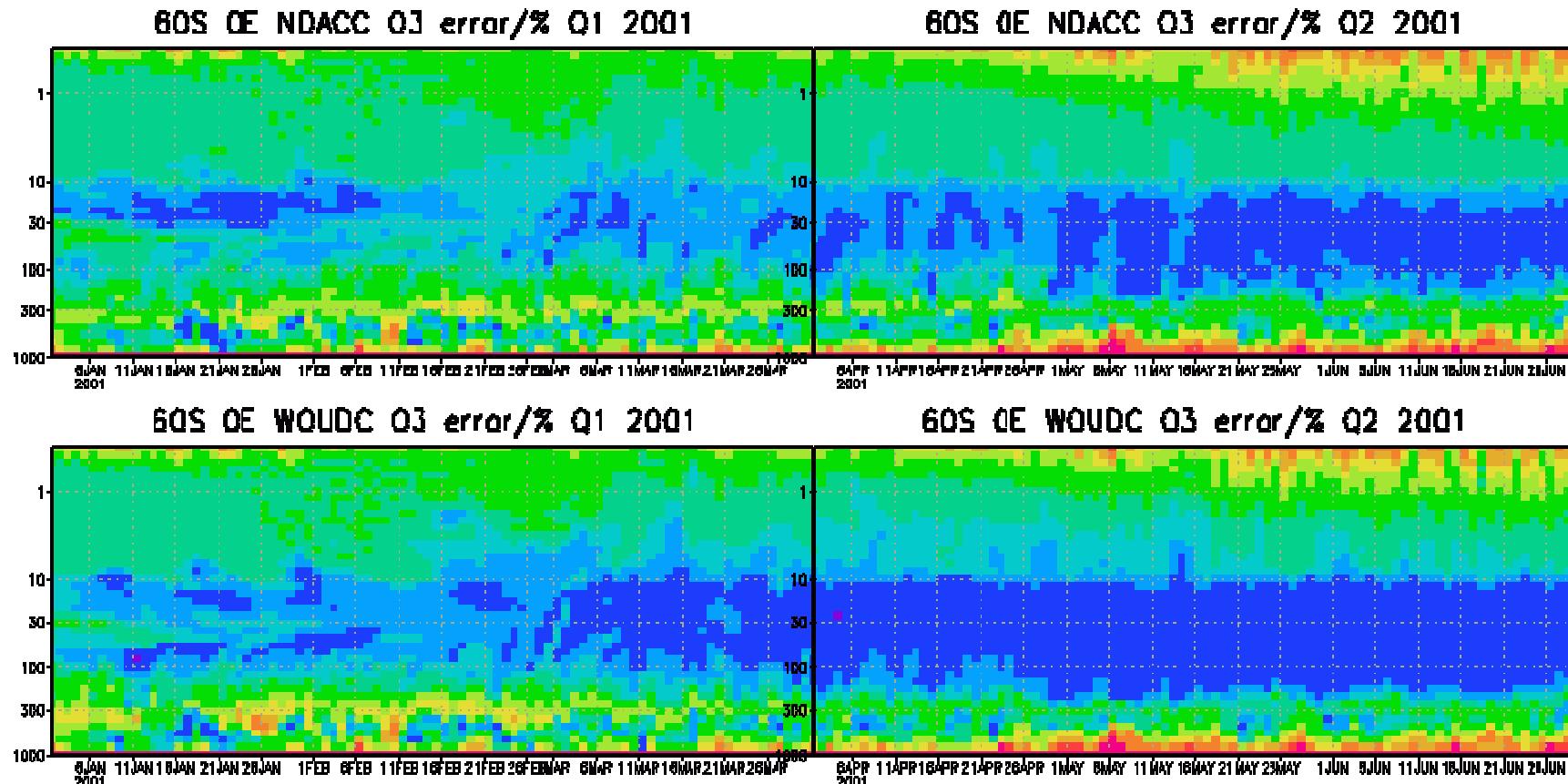
Eq



# Analysis error NDACC/WOUDC

Q1, Q2

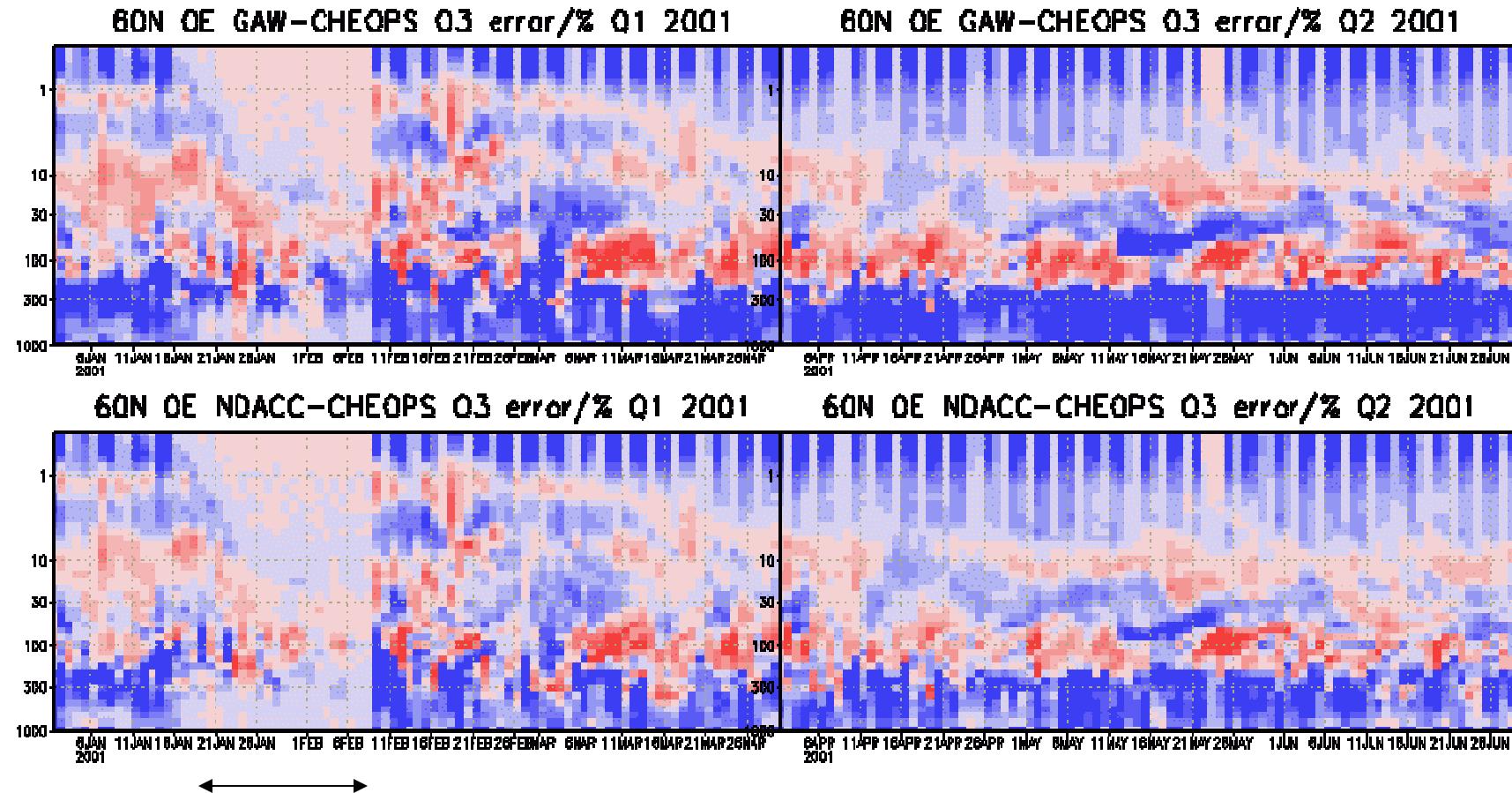
60 °S



# FMO errors GAW/NDACC

Q1, Q2

60 °N



GOME data gap



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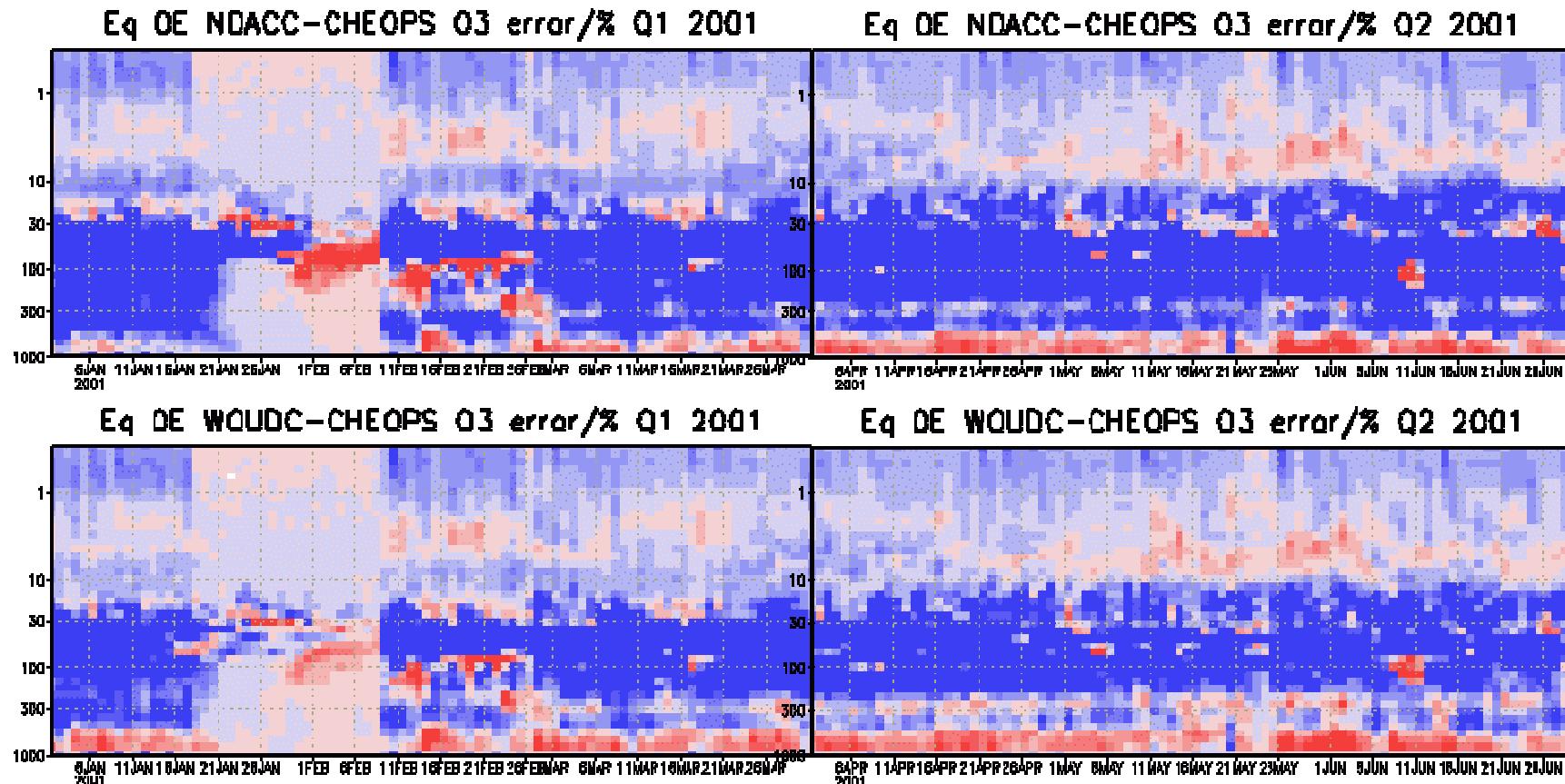
slide 24

Baier et al., Impact of ozone sondes

# FMO errors NDACC/WOUDC

Q1, Q2

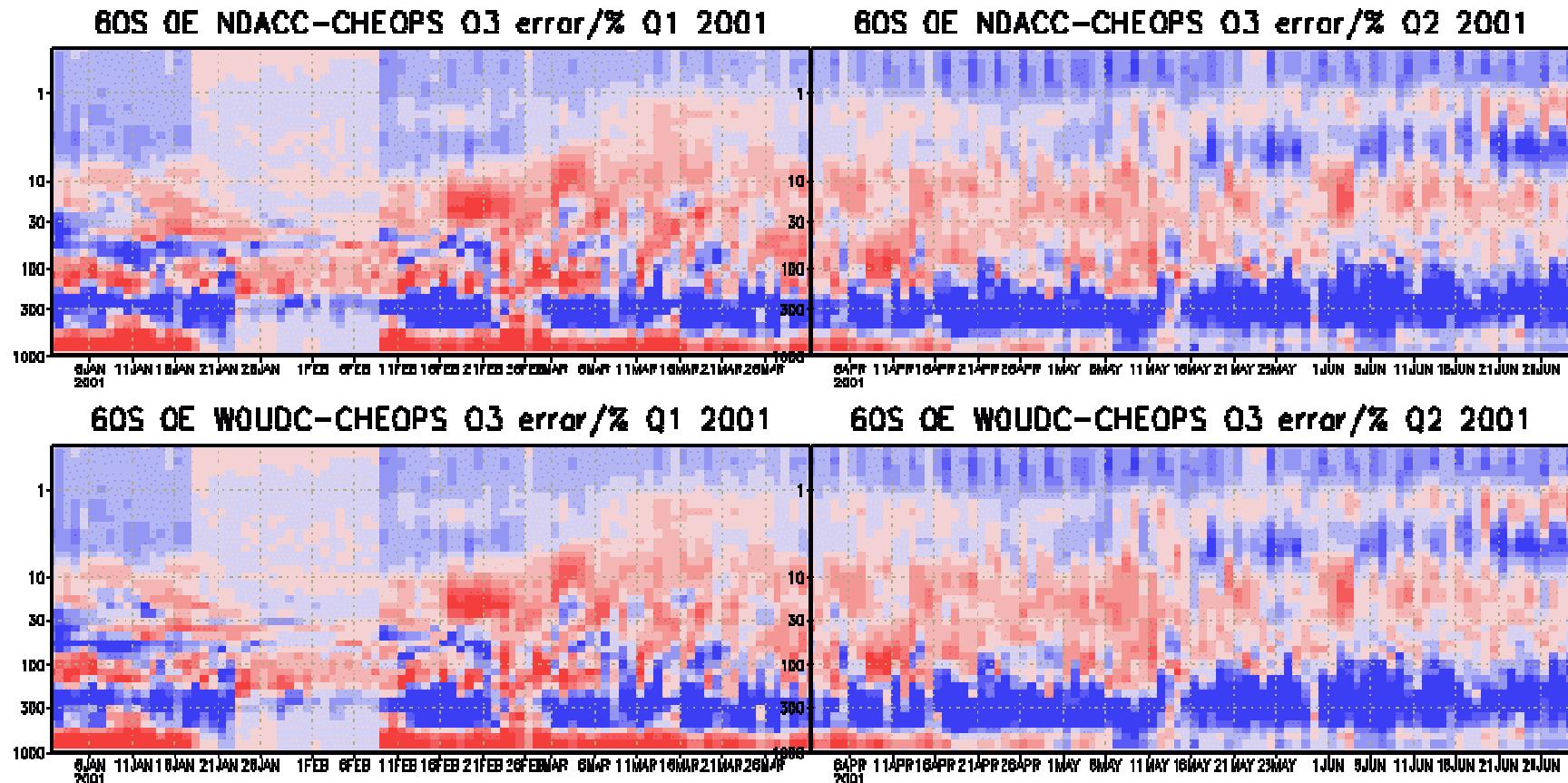
Eq



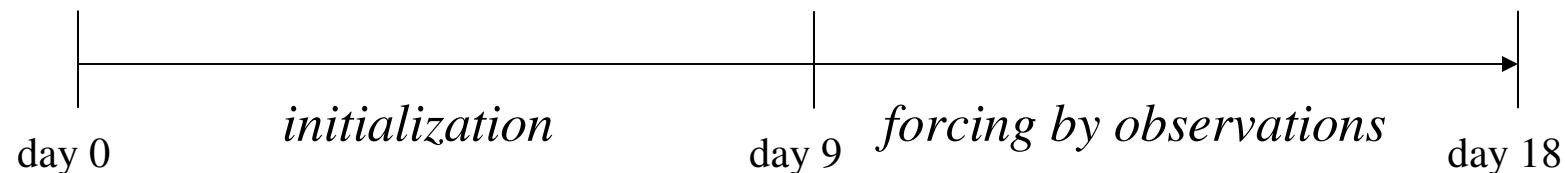
# FMO errors NDACC/WOUDC

Q1, Q2

60 °S



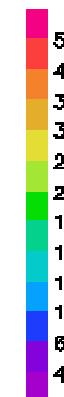
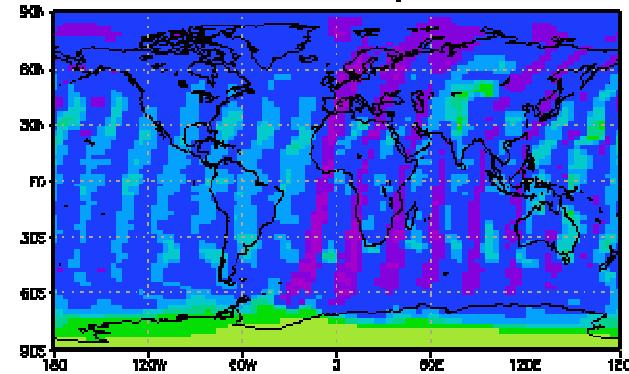
# ‘short-term’ experiments: 1997 APR 01-18, 1998 FEB 01-18, 2002 SEP 11-28



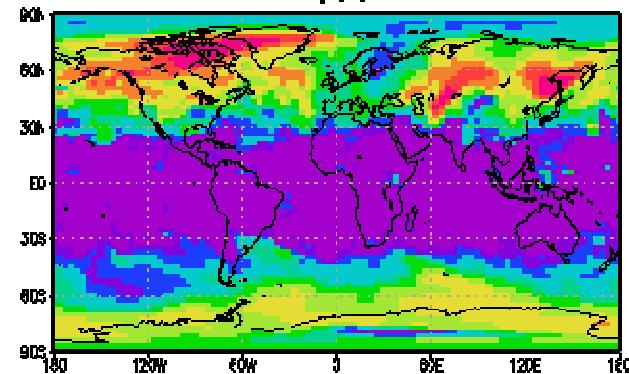
1997 April 01-18th:	network WOUDC	1/day	>30 °N
1998 Febr. 01-18th:	WOUDC	1/day	<30 °NS
2002 Sept. 11-28th:	WOUDC	1/day	>30 °S

# CHEOPS ozone record 1997 April 9-12th

58hPa CHEOPS O3 error/% APR 1997 12



56hPa CHEOPS O3/ppmv APR 1997 12



northern intrusion  
event

O3O5: NOV/1998



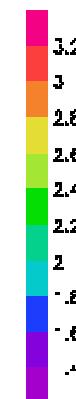
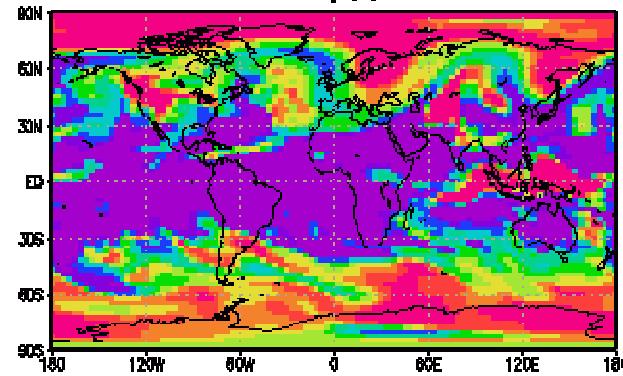
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slide 28

Baier et al., Impact of ozone sondes

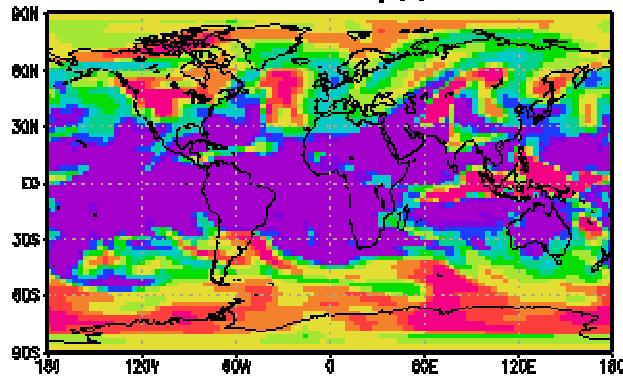
# WOUDC/Reference 1997 April 12th

56hPa Reference O3/ppmv APR 1997 12



ozone bias >60°N

56hPa CHEOPS-WOUDC O3/ppmv APR 1997 13



SADS: COLA/122

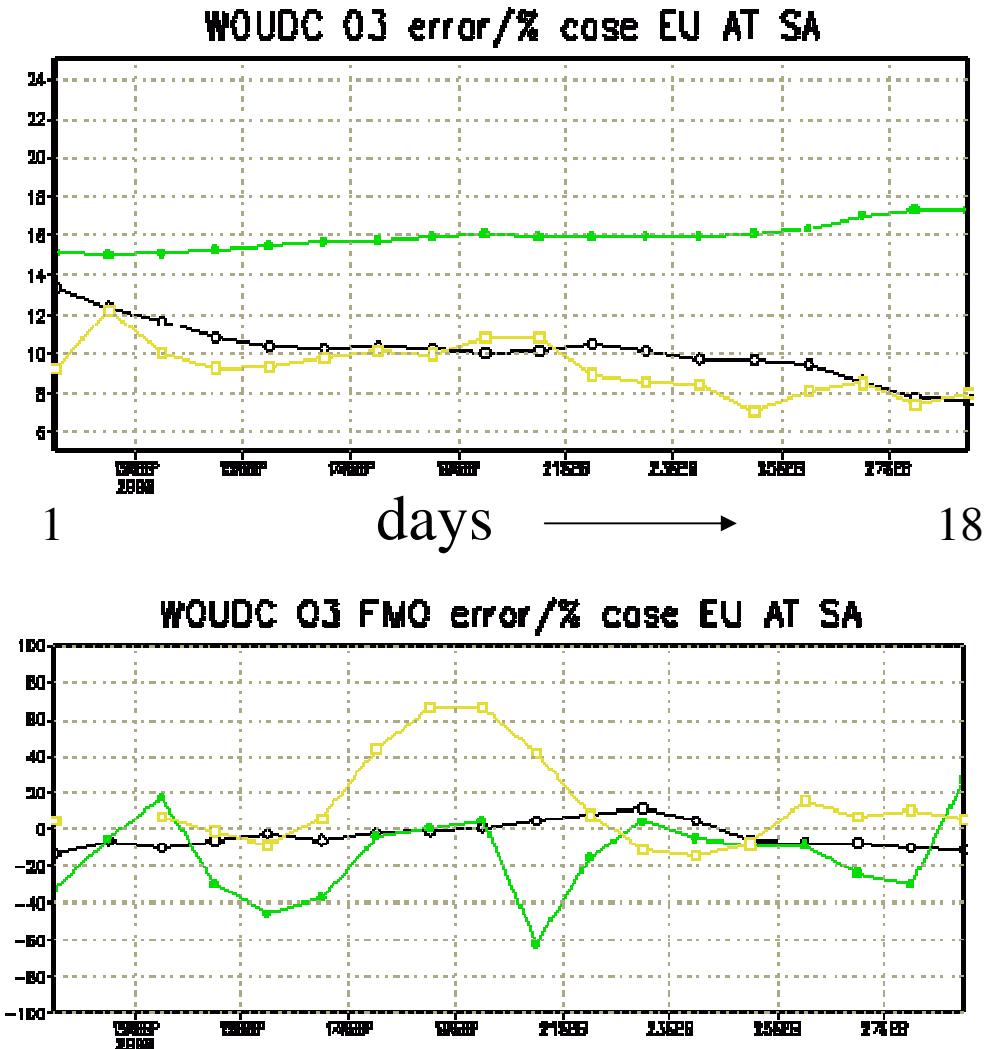


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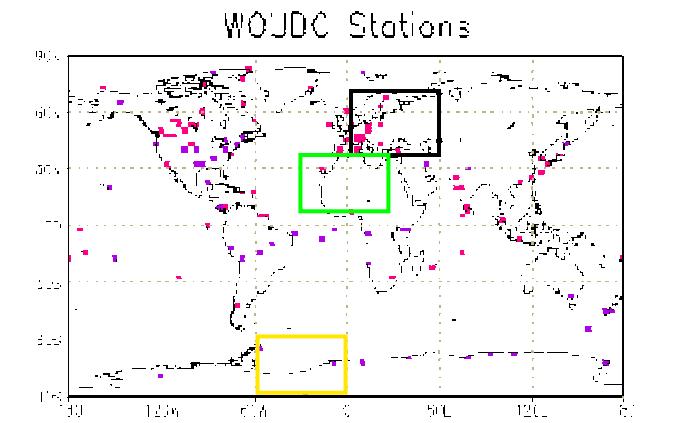
slide 29

Baier et al., Impact of ozone sondes

# 'short-term' aggregated results: three test areas



EU      40-70°N/0°E-60°E  
AT      10-40°N/30°W-30°E  
SA      60-90°S/60°W-0°E



# CHEOPS/SACADA adjoint receptor analysis

Resolution = 250km (icosaeder), 43 sigma levels (top at 65 km)

ECMWF analysis as init for GME multi-day forecasts

Semi-Lagrange transport scheme

Non-QSSA chemistry, NAT, ICE PSCs (not this study) and aerosols

4Dvar: incremental with isotropic background covariances (Courtier, 1997)

Instantaneous ‘observations’ using CHEOPS data at 7 LT up to 10 hPa



# CHEOPS/SACADA adjoint receptor analysis

Resolution = 250km (icosaeder), 43 sigma levels (top at 65 km)

ECMWF analysis as init for GME multi-day forecasts

Semi-Lagrange transport scheme

Non-QSSA chemistry, NAT, ICE PSCs (not this study) and aerosols

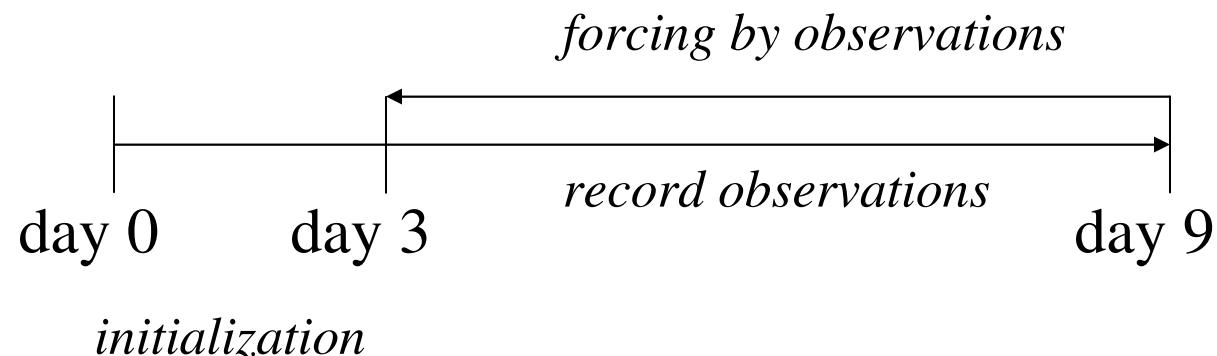
4Dvar: incremental with isotropic background covariances (Courtier, 1997)

This study: assess impact of observations via gradient of cost function

$$J(x_N) = \frac{1}{2} \sum \delta x_i \frac{1}{O} M \delta x_o \rightarrow \frac{\partial J}{\partial x_o} = M^T \frac{1}{O} \delta x_N \text{ with } O = \sigma^2 \text{ (obs. error)}$$

  
observation inc.    adjoint variable

# CHEOPS/SACADA adjoint receptor analysis

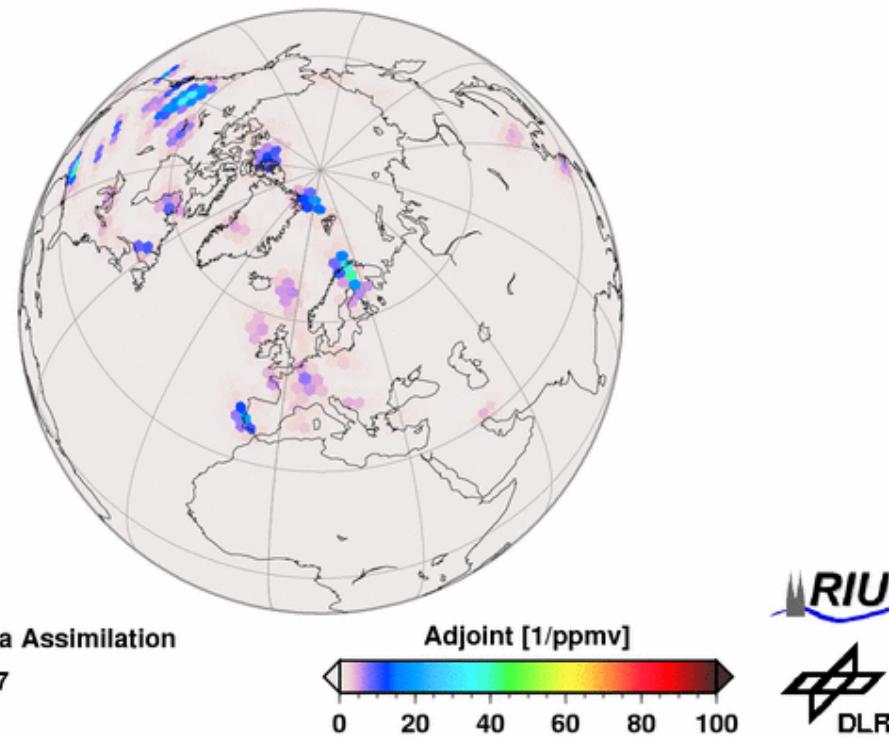


WOUDC:  
one sounding per day

# CHEOPS/SACADA adjoint receptor analysis

GOME-2 / MetOp – 4DVar Analysis  
 $O_3$ ad at 55.4 hPa

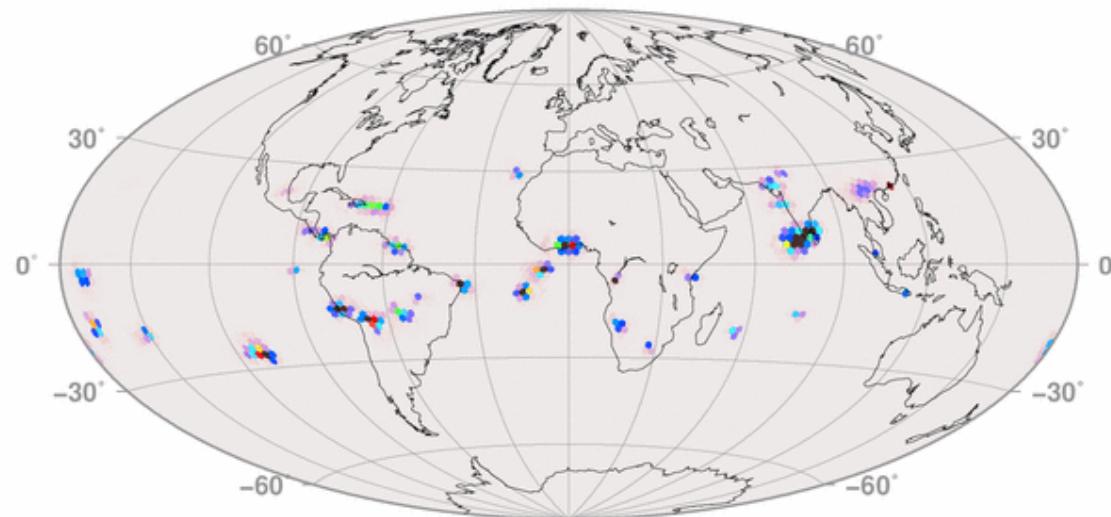
h 120 Apr 08, 1997  
Northern Hemisphere



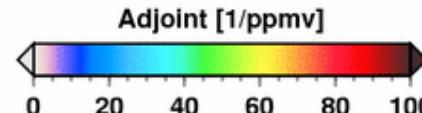
# CHEOPS/SACADA adjoint receptor analysis

GOME-2 / MetOp – 4DVar Analysis  
 $O_3$ ad at 55.4 hPa

h 120 Feb 08, 1998



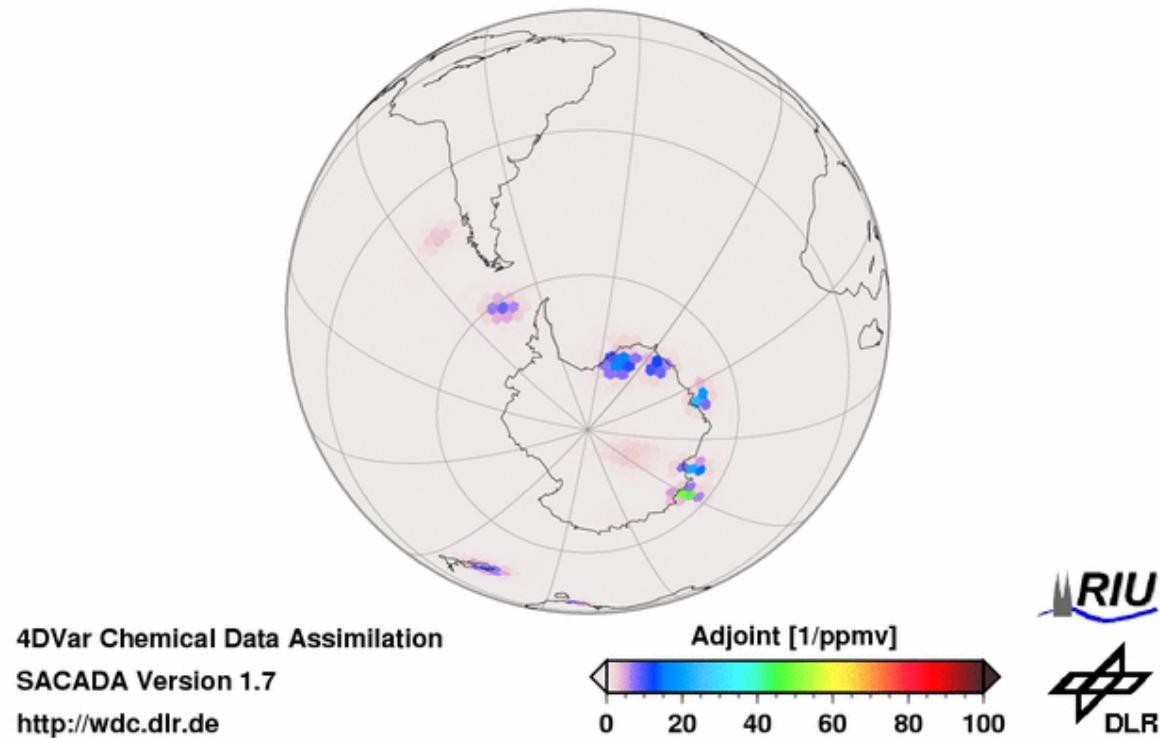
4DVar Chemical Data Assimilation  
SACADA Version 1.7  
<http://wdc.dlr.de>



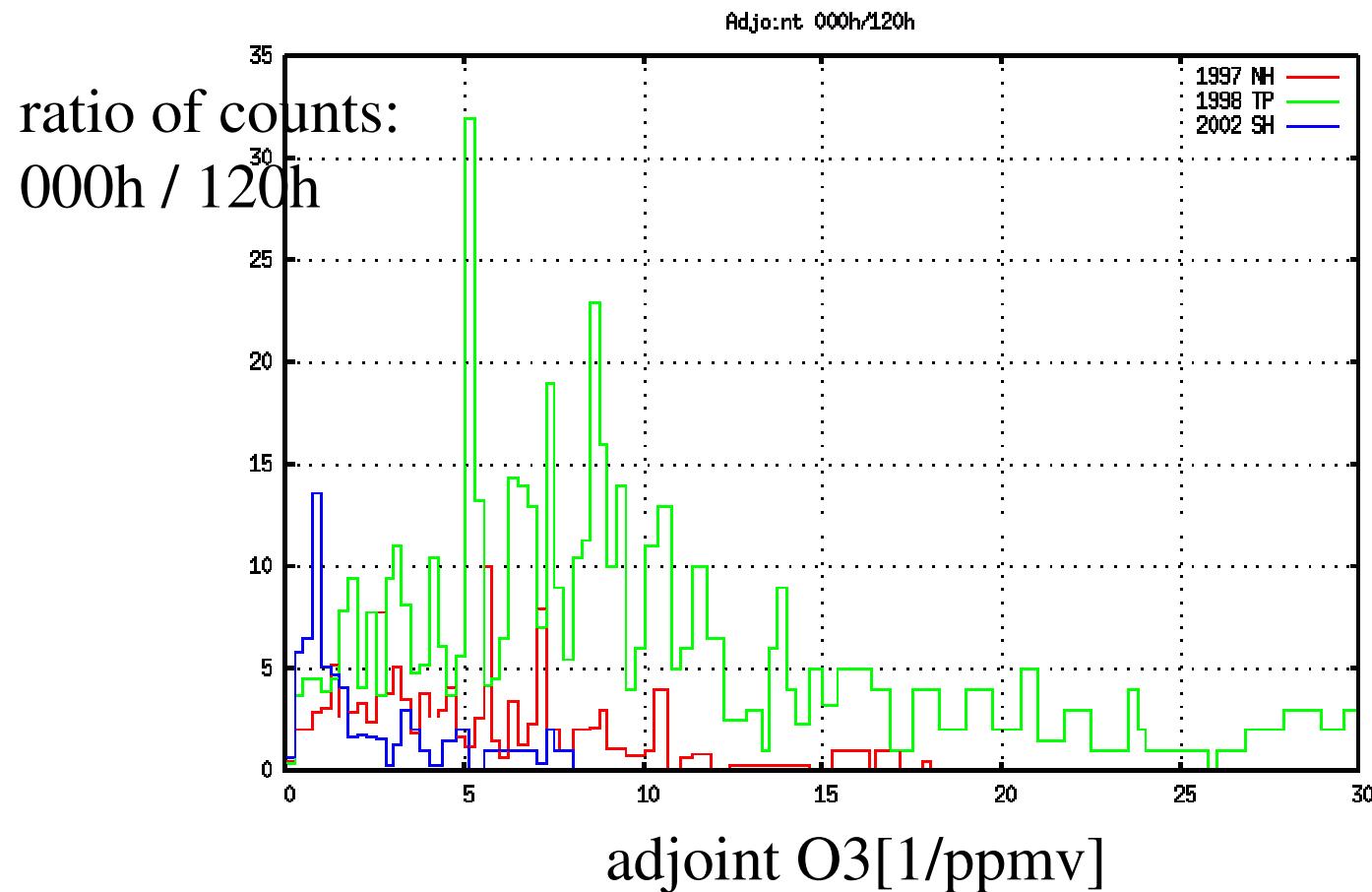
# CHEOPS/SACADA adjoint receptor analysis

GOME-2 / MetOp – 4DVar Analysis  
 $O_3$ ad at 55.4 hPa

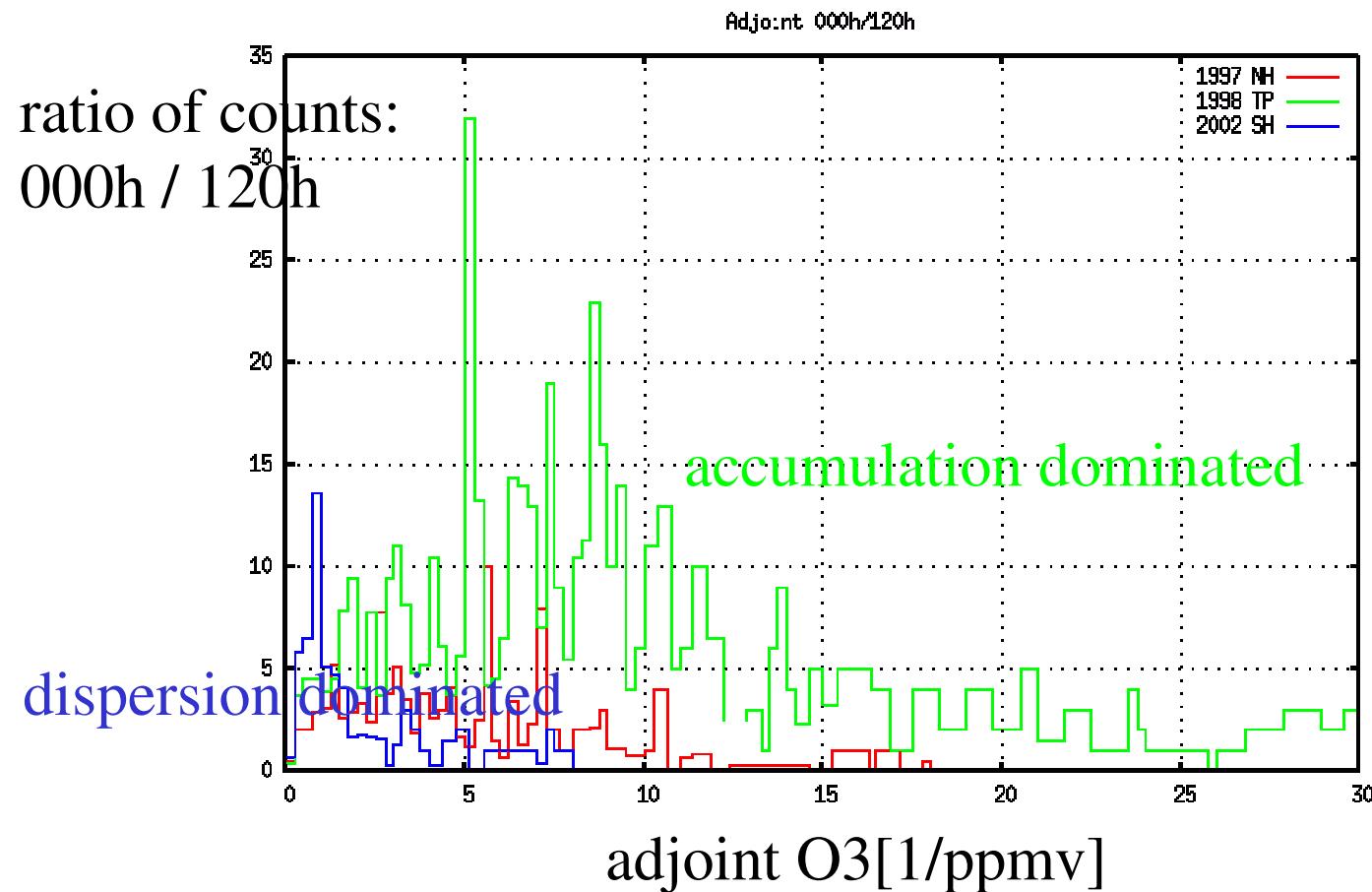
h 120 Sep 18, 2002  
Southern Hemisphere



# CHEOPS/SACADA adjoint receptor analysis



# CHEOPS/SACADA adjoint receptor analysis



# Summary

- ↗ OSSE experiments using CHEOPS ozone profile analyses
- ↗ Test of different ozone sonde networks and sounding frequencies
- ↗ Multi-day adjoint analysis of sounding sensitivity

## Long-term experiment 2001

- ↗ Up to 25% rms error reduction c.t. HALOE for tropics and SH
- ↗ Increase of soundings per stations does not compensate for lack of cover.
- ↗ Model results without observations already at 15% level for NH
- ↗ Tropics: results obstructed by poor model performance - noisy wind fields

## Short-term experiments '97 '98 '02

- ↗ NH: model bias reduced: improved streamer forecast
- ↗ Tropics: weak dispersion of observations, resulting in poor coverage
- ↗ SH: current network layout not adequate during dynamic events (v-split)

# Recommendations

- ↗ Increase number of regular soundings at base stations
- ↗ Better distributed soundings in tropics to improve coverage
- ↗ Use Umkehr/satellites etc. to reduce model bias
- ↗ Coordinated measurements to better capture dynamic events

Many thanks to:

NCAR (National Center for Atmospheric Research)

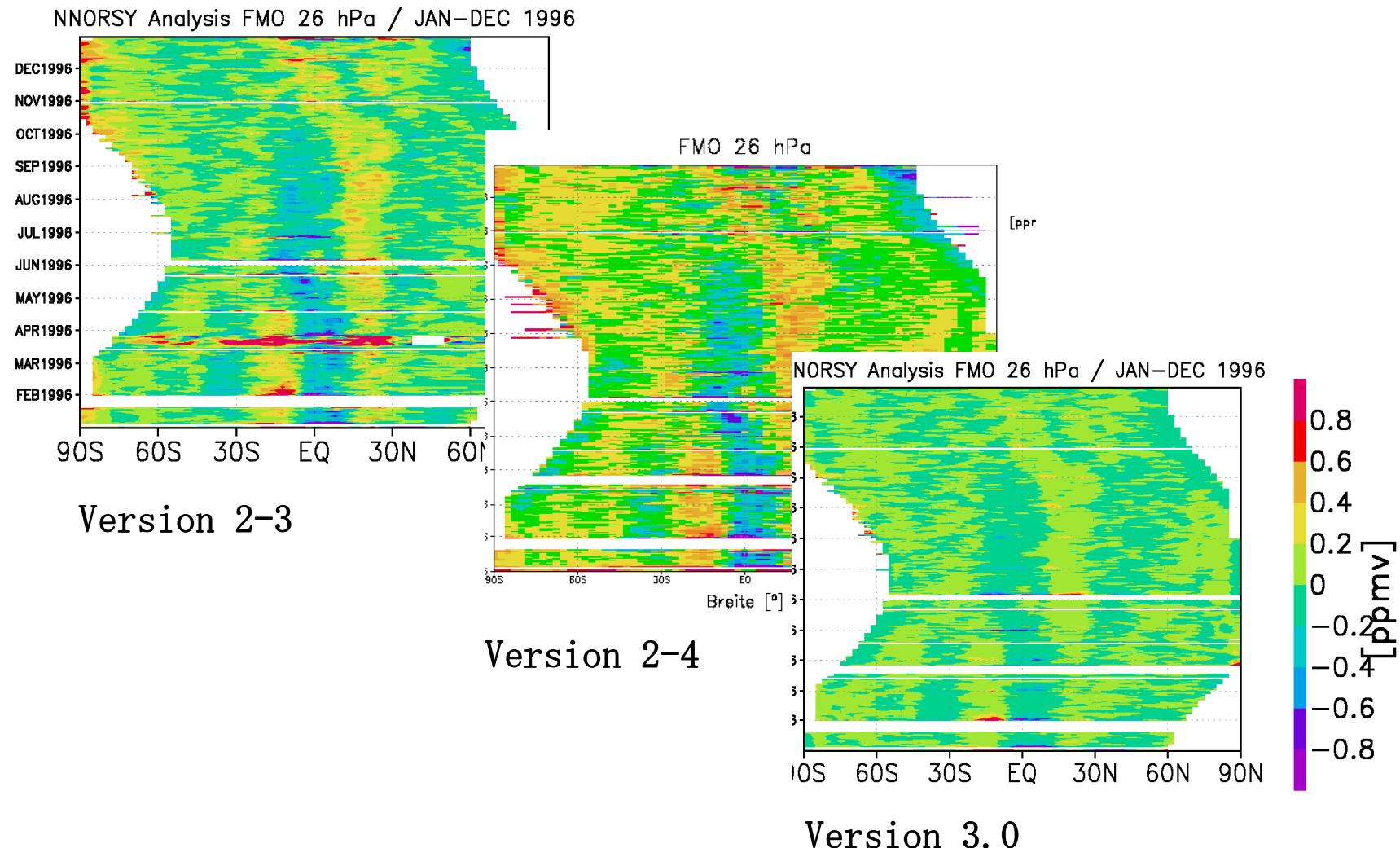
WMO/IGACO (Integrated Global Atmospheric Chemistry Observations)

GAW/ (Global Atmospheric Watch)

NDACC (Network for the. Detection of. Atmospheric Change)

WOUDC (World Data Center for Ozone and UV)

# First-guess minus observation (FMO) errors: Improvements of GOME/NNORSY from v2.3 to 3.0



# HALOE 2003/2004 comparison results

<b>ROSE-UKMO c.t. HALOE (100-2 hPa)</b>				
obs	mean	bias/%	rms/%	
O3	48776	5.10	0.29	13.71
H2O	48778	5.05	4.29	9.30
Nox	41478	7.79	0.97	26.30
CH4	48576	4.26	7.77	15.19
HCl	41484	1.82	-9.02	19.61

<b>SACADA c.t. HALOE (100–2 hPa)</b>				
obs	mean	bias/%	rms/%	
O3	65582	4.99	-0.43	13.09
H2O	65584	5.11	4.47	10.00
Nox	55761	6.85	-11.75	24.25
CH4	65452	4.05	6.49	12.45
HCl	55768	1.27	-59.36	75.64

<b>ROSE-GME c.t. HALOE (100-2 hPa)</b>				
obs	mean	bias/%	rms/%	
O3	54252	5.16	1.64	8.81
H2O	54254	5.09	5.01	9.14
Nox	46137	7.99	2.73	24.86
CH4	54050	4.21	7.49	13.56
HCl	46142	1.92	-4.28	15.23

