The SPARC Data Initiative -

A multi-instrument comparison of stratospheric limb measurements

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and the SPARC Data Initiative Team

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Motivation

Knowledge of quality of different satellite data sets needs to be improved for different applications:

- Tracer scenario validation (Montreal Protocol, Cl_y)
- Model validation projects (CCMI, IPCC)
- Trend analyses (e.g., stratospheric water vapour)
- Empirical studies of stratospheric climate and variability

Objectives

Inter-comparison of vertically resolved climatologies of 25 chemical tracers and aerosol from 18 multi-national satellite instruments

- Will be published as **a peer-reviewed SPARC report**, as well as in journal publications
- Will summarize useful information and highlight differences between data sets
- Will provide guidance to space agencies about required improvements in existing data sets and future observations

Team:

- ✓ HALOE (UARS): **John Anderson**
- ✓ MLS (Aura/UARS): **Lucien Froidevaux, Ryan Fuller**
- ✓ TES (Aura): **Jessica Neu**
- ✓ ACE-FTS (SCISAT-1): **Kaley Walker, Ashley Jones**
- ✓ MAESTRO: **Kaley Walker**
- ✓ OSIRIS (Odin): **Doug Degenstein, Adam Bourassa**
- ✓ SMR (Odin): **Joachim Urban**
- ✓ MIPAS (ENVISAT): **Thomas von Clarmann, Bernd Funke**
- ✓ SCIAMACHY (ENVISAT): **Alexei Rozanov**
- ✓ GOMOS (ENVISAT): **Erkki Kyröla**
- ✓ SAGE I / II / III: **Ray Wang**
- ✓ HIRDLS (AURA): **John Gille, Lesley Smith**
- ✓ SMILES (ISS): **Yasuko Kasai**
- ✓ LIMS (NIMBUS-7): **Ellis Remsberg, Gretchen Lingenfelser**
- ✓ POAM II / III: **Jerry Lumpe**
- ✓ **Matthew Toohey**

Co-leads:

Michaela Hegglin

Susann Tegtmeier

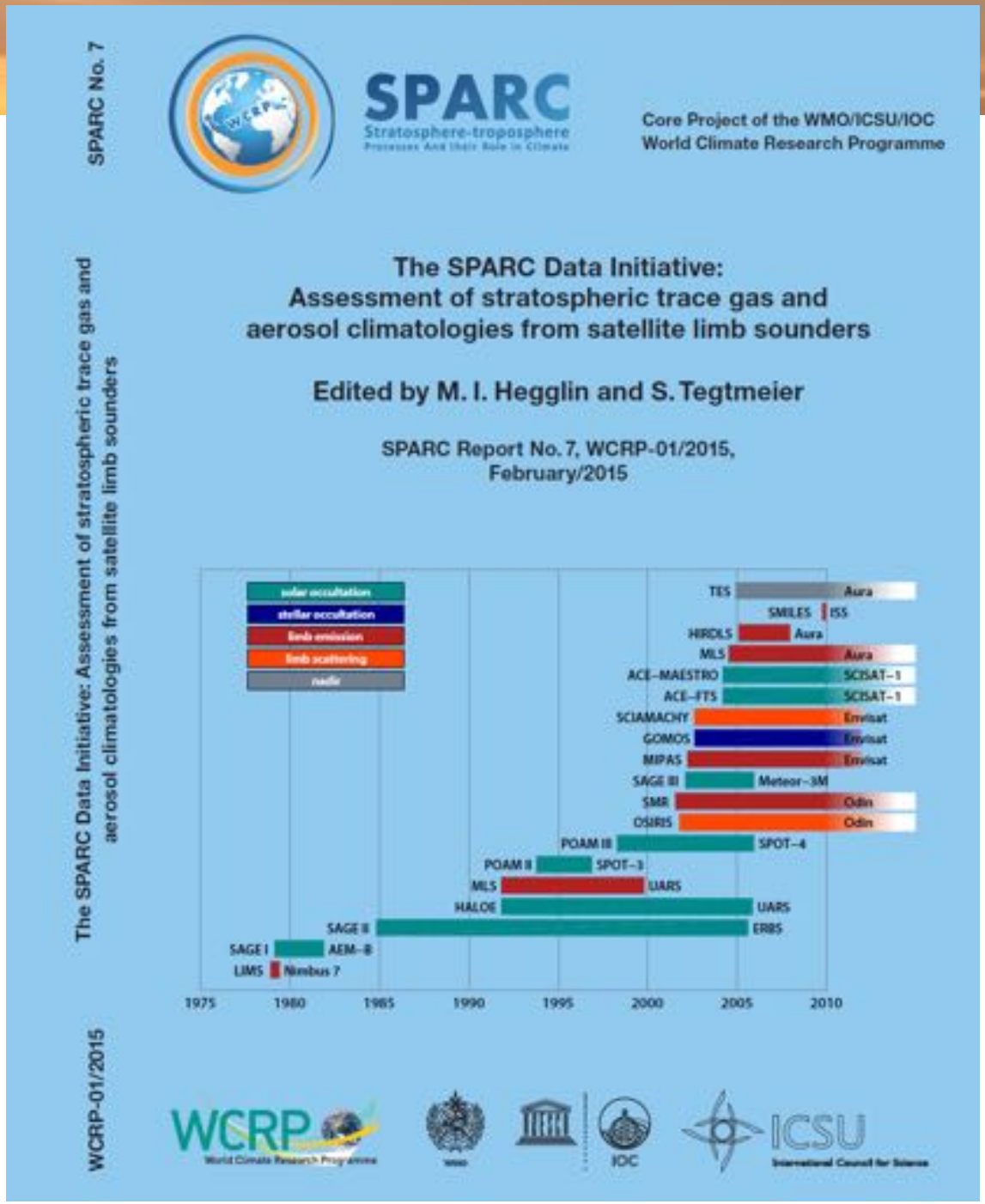
SPARC Data Initiative	O_3	H_2O	CH_4	N_2O	CCl_3F	CCl_2F_2	CO	HF	SF_6	NO	NO_2	NO_x	HNO_3	HNO_4	N_2O_5	$ClONO_2$	NO_y	HCl	ClO	HOCl	BrO	OH	HO_2	CH_2O	CH_3CN	aerosol
ACE-FTS	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x						x		
Aura-MLS	x	x		x			x						x					x	x	x		x	x			
GOMOS	x										x															x
HALOE	x	x	x					x		x	x	x						x								
HIRDLS	x				x	x					x		x													
LIMS	x	x									x		x													
MAESTRO	x																									
MIPAS	x	x	x	x	x	x	x		x	x	x	x	x	x	x	x	x		x	x				x		
OSIRIS	x										x	x_d					x_m				x					x
POAM II	x										x															x
POAM III	x	x									x															x
SAGE I	x																									
SAGE II	x	x									x															x
SAGE III	x	x									x															x
SCIAMACHY	x	x									x	x_d									x					x
SMILES	x												x					x	x	x	x				x	
Odin/SMR	x	x		x			x			x			x				x_m		x				x_{lc}			
UARS-MLS	x	x											x						x							
TES	x_t																									

'Climatologies'

- Monthly mean zonal mean time series
  - **VMR or aerosol extinction coefficients**,
  - 1σ standard deviation,
  - number of measurements per grid box,
  - mean, min, and max local solar time,
  - average day of month and latitude.
- Range: upper troposphere to the lower mesosphere
- Time period covered: 1978 - 2010
- Grid: 5° latitude bins on the CCMVal-2 pressure grid (28 levels)
- Data sets are provided in a common format (netcdf) easily useable by the atmospheric science community

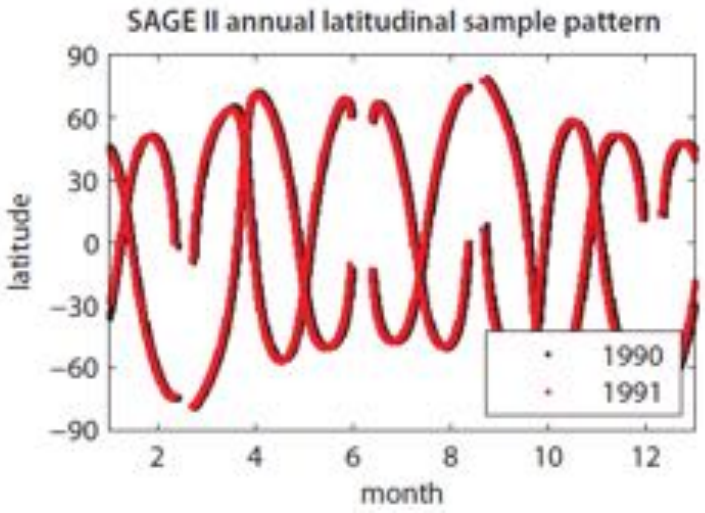
SDI report

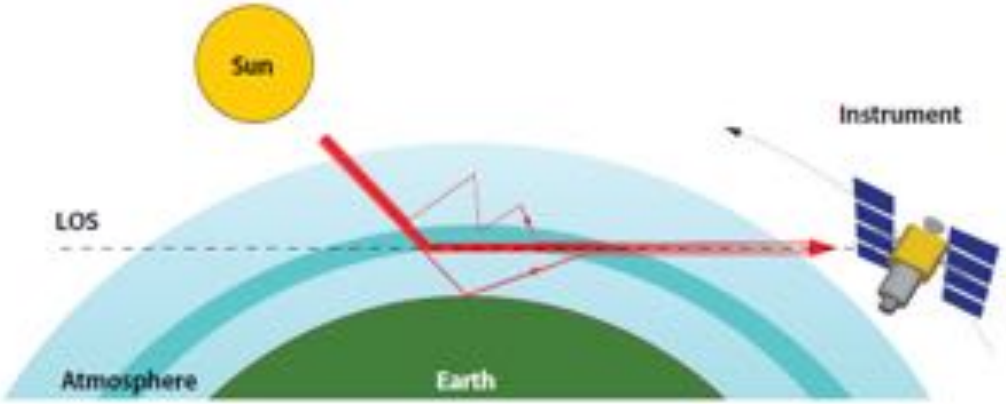
- SPARC report no. 7
- All chapters written, most typeset, some in proof read
- Publication in 2015/2016



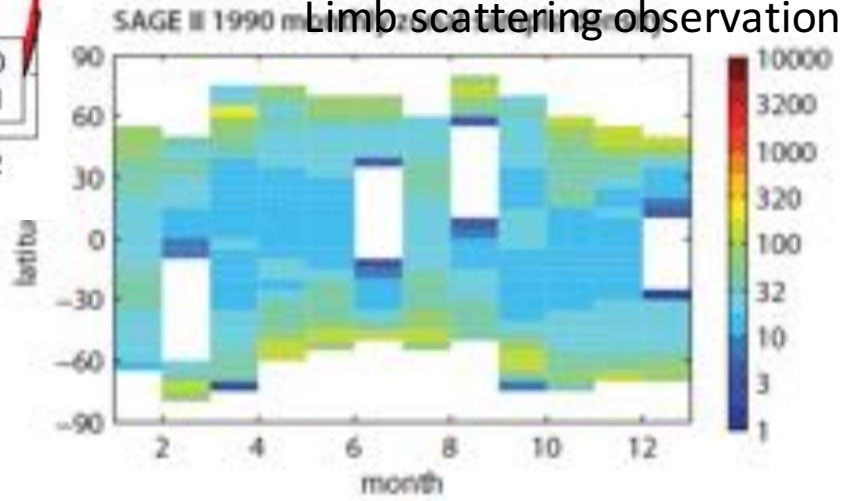
Chapter 2 - Satellite instruments and data sets

- Satellite measurement techniques (observation geometry, wavelengths, orbits)





Limb scattering observation geometry



Chapter 3 - Climatology framework

- Climatology construction (methodology, local time scaling, instrument-specific information)

Instrument	Latitudinal coverage	LT at equator[1]	LT of measure-ment[2]	Inc.[3]	Vert. Grid[4]	Alternate grid[5]	Meas.[6]	Conver-sion to VMR[7]	Data density per day
LIMS on Nimbus 7	64°S–84°N (daily)	a: 11:51 am d: 11:51 pm	a:1 pm d: 11 pm	99.3°	p	N/A	VMR	N/A	3000
SAGE I on AEM-B	75°S–75°N (~one month)	N/A	N/A	56°	z	NCEP	ND	NCEP	30
SAGE II on ERBS	75°S–75°N (~one month)	N/A	N/A	57°	z	NCEP	ND	NCEP	30
OSIRIS on Odin	82°S–82°N (daily, no winter hemisphere)	a: 6:30 pm d: 6:30 am	a: 6:30 pm d: 6:30 am	97.8°	z	ECMWF operation-al analysis	ND	ECMWF operation-al analysis	300 - 975
SMR on Odin	83°S–83°N (daily)	a: 6:30 pm d: 6:30 am	a: 6:30 pm d: 6:30 am	97.8°	p	N/A[8]	VMR	N/A	600-975
GOMOS on Envisat	90°S–90°N (daily, no summer poles for night)	a: 10:00 pm d: 10:00 am	a: 10-12 pm d: 8-10.30 am	98.55°	z	ECMWF operation-al analysis	ND	ECMWF operation-al analysis	100-300 (night mea-surments)
MIPAS	90°S–90°N	a: 10:00 pm	a: 10:00 pm	98.55°	z	MIPAS	VMR	N/A	1000 (1300

- Climatology uncertainties and diagnostics

'Climatological' validation approach based on binned/interpolated datasets

Advantages

- Consistent between all instruments
- Avoids sensitivity to arbitrary coincidence criteria
- Larger sample sizes (minimize the random sampling error)

Disadvantages

- Biased mean values due to non-uniformity of sampling
- Different resolutions in altitude (averaging kernels)

Evaluations

- Need for a reference that does not favor a certain instrument -> Use of the multi-instrument mean (MIM)
- But: MIM is not the best climatology available, can suffer from changes in time periods and set of available instruments

What can we learn from the SPARC Data Initiative?

1) **Sampling Bias Study**

2) **Study on the impact of the vertical resolution**

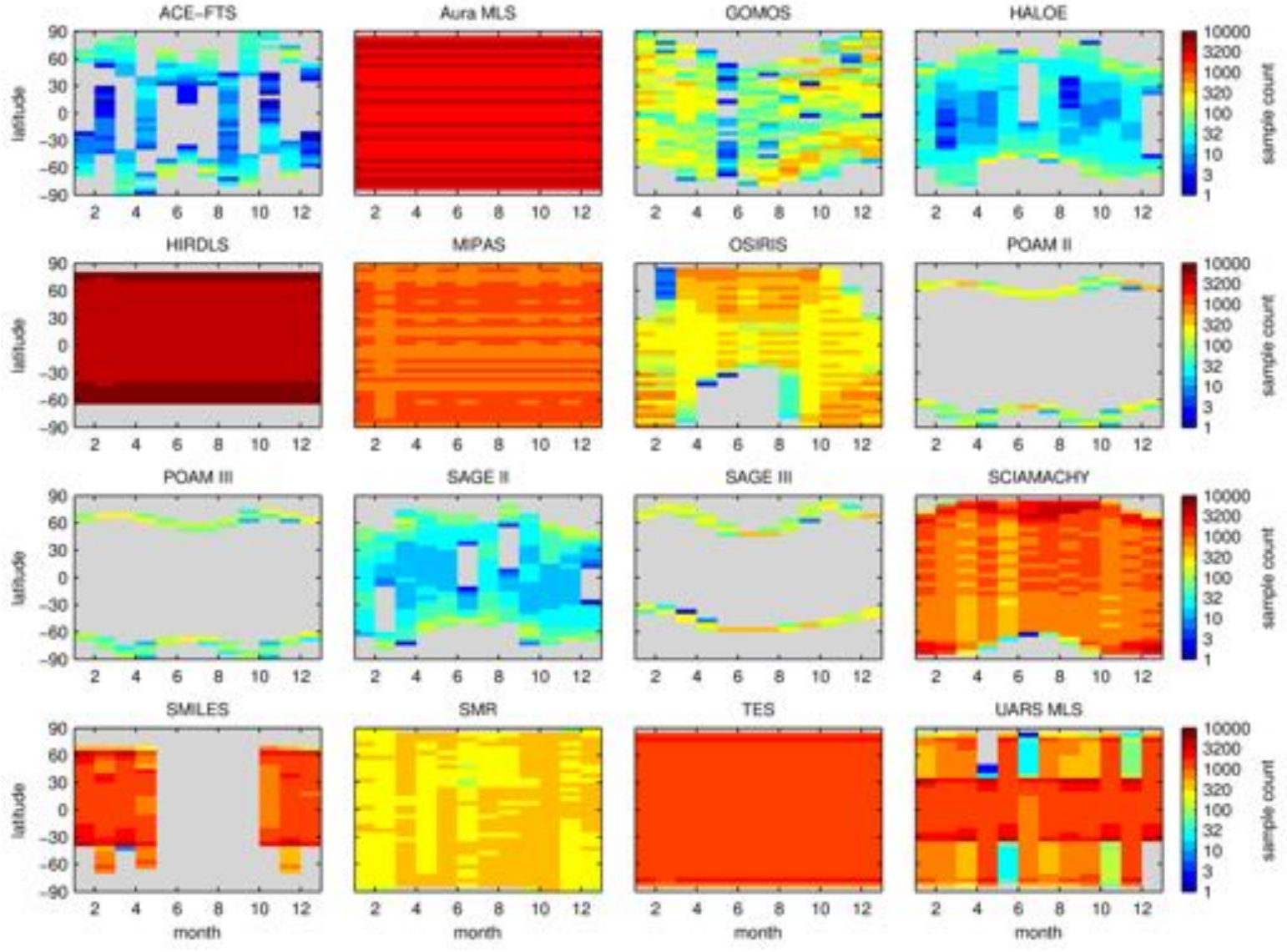
3) **Uncertainty in our knowledge of the atmospheric mean state**
   - Based on diagnostics of monthly /annual zonal mean cross-sections
   - Mean spread between data sets over maximum number of years

4) **Outliers and unphysical features**
   - Evaluation of variability and other physical features (e.g., seasonal cycle, QBO, tape recorder, Antarctic ozone , polar vortex dehydration, EPP NO_x)

5) **Implications for model-measurement intercomparison**

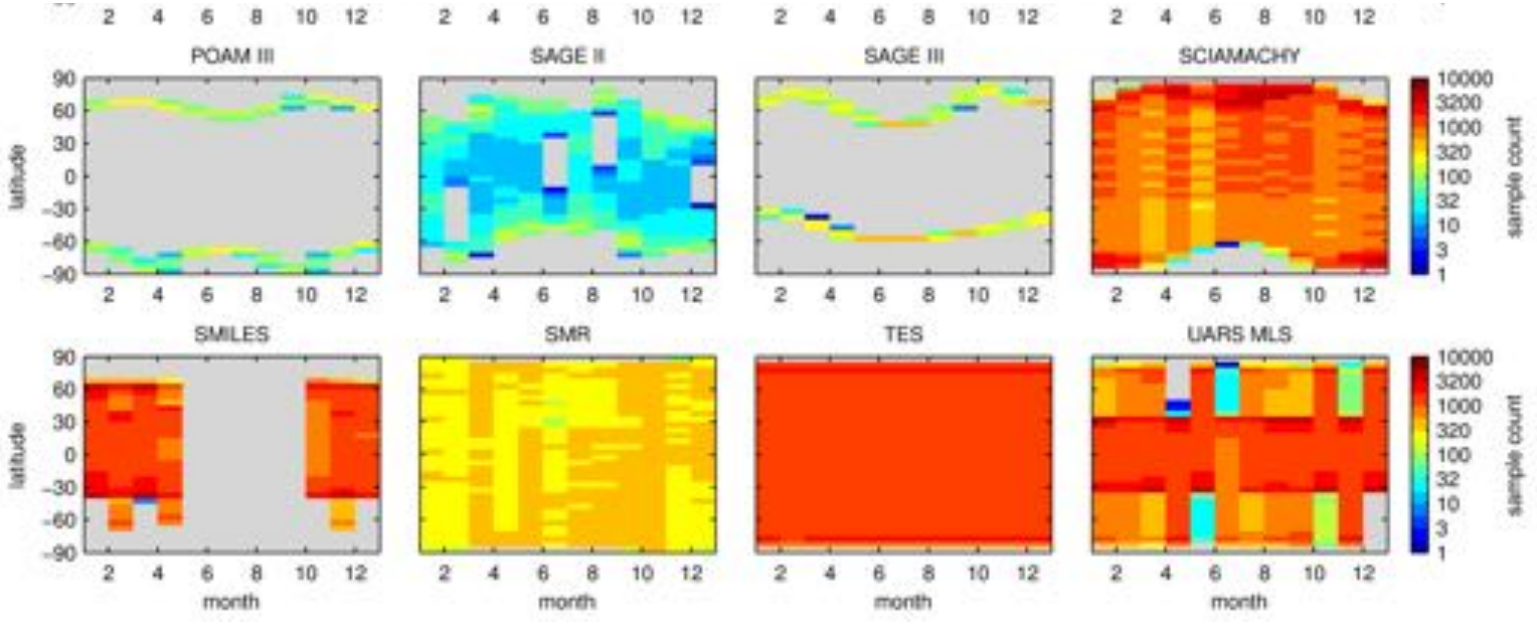
Sampling bias

Sampling patterns: sample counts



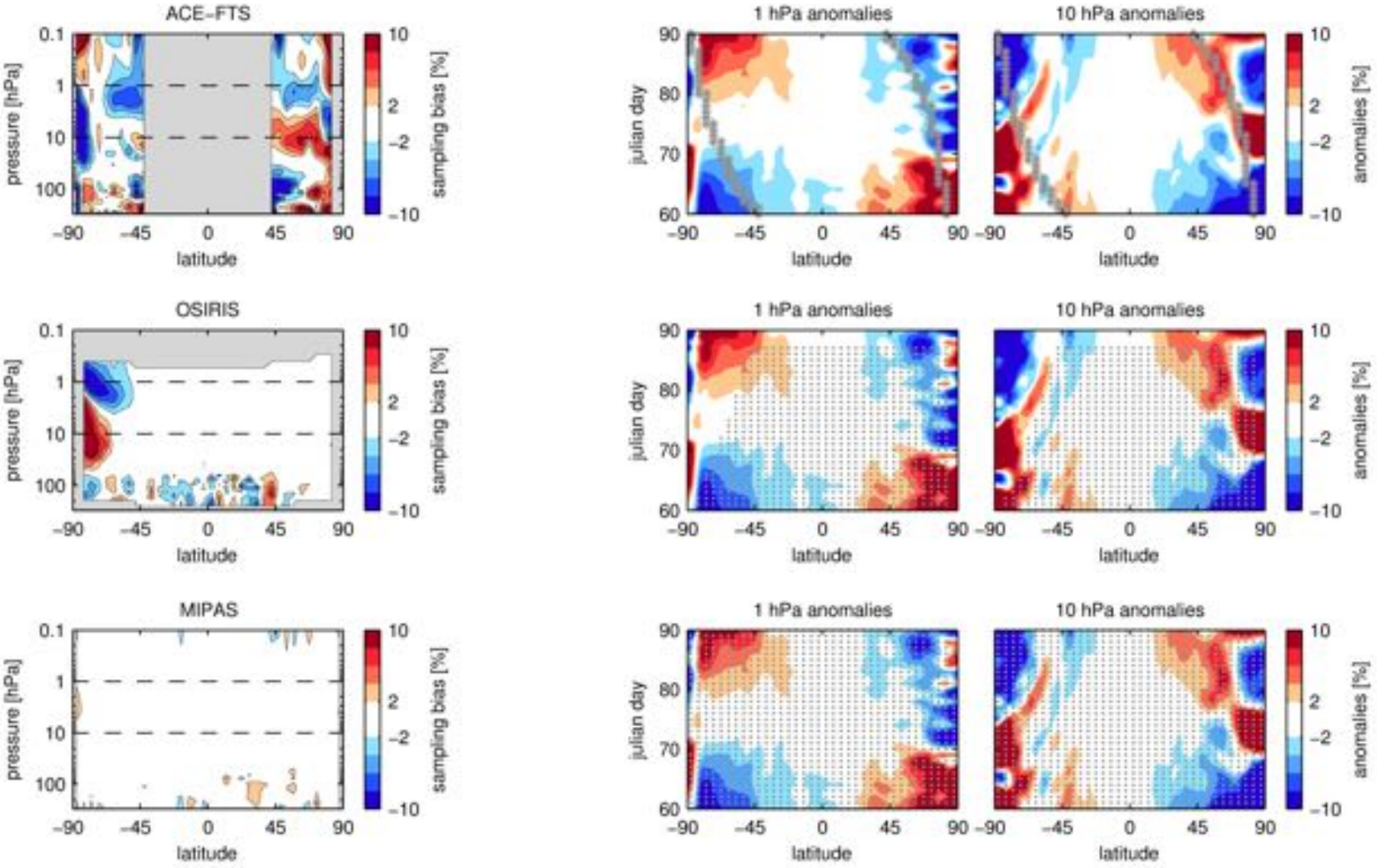
Sampling Bias Study

- Use chemical fields from a coupled chemistry model, (e.g., WACCM)
- Sample model fields based on space-time sampling patterns of specific instruments (“*satellite simulator*”)
- Difference of sample mean and population mean (with full resolution model fields) gives estimate of potential sample bias in climatologies.



Sampling bias

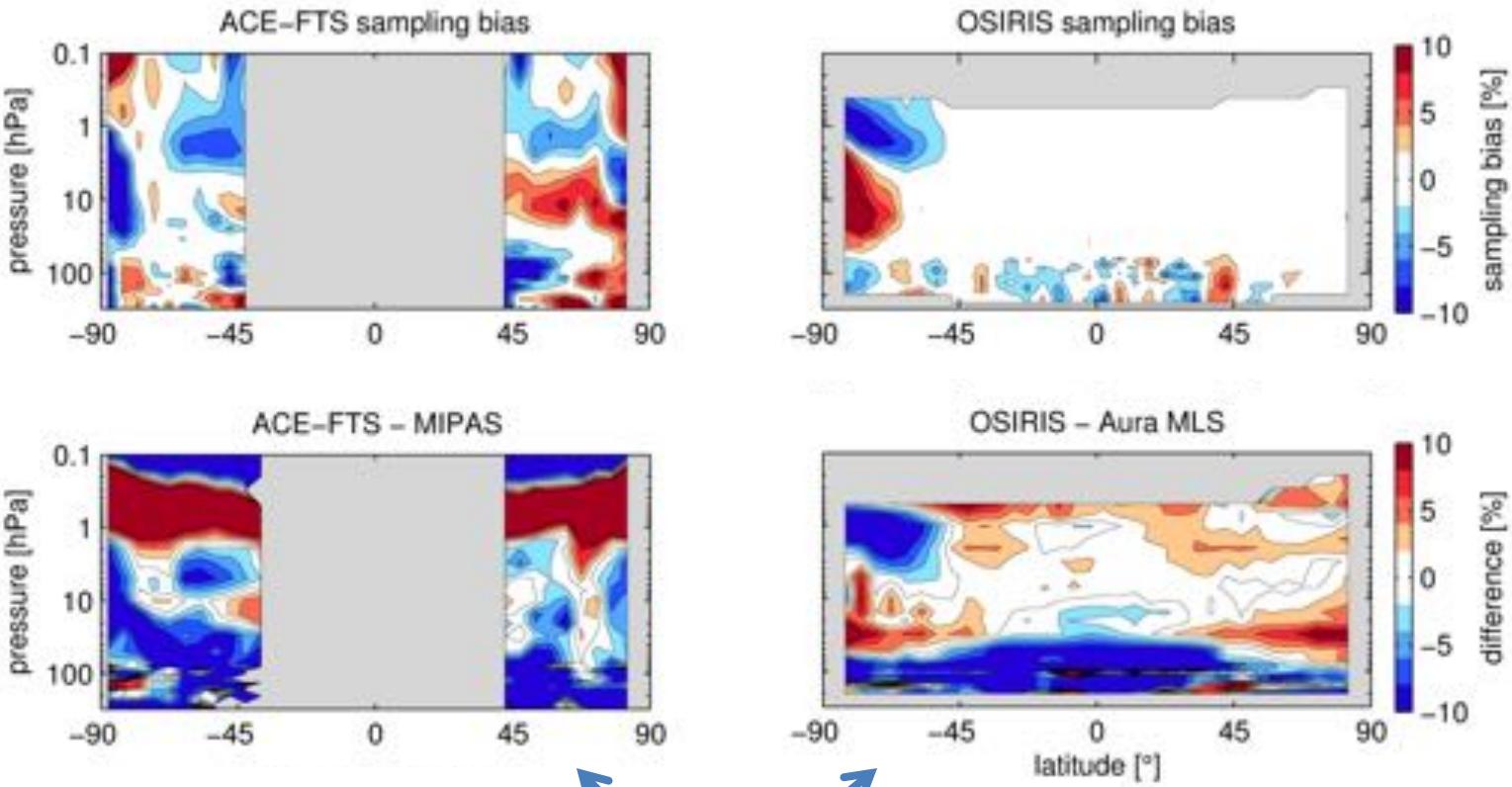
March O_3 case study: impact of temporal non-uniformity



Toohey et al., 2013

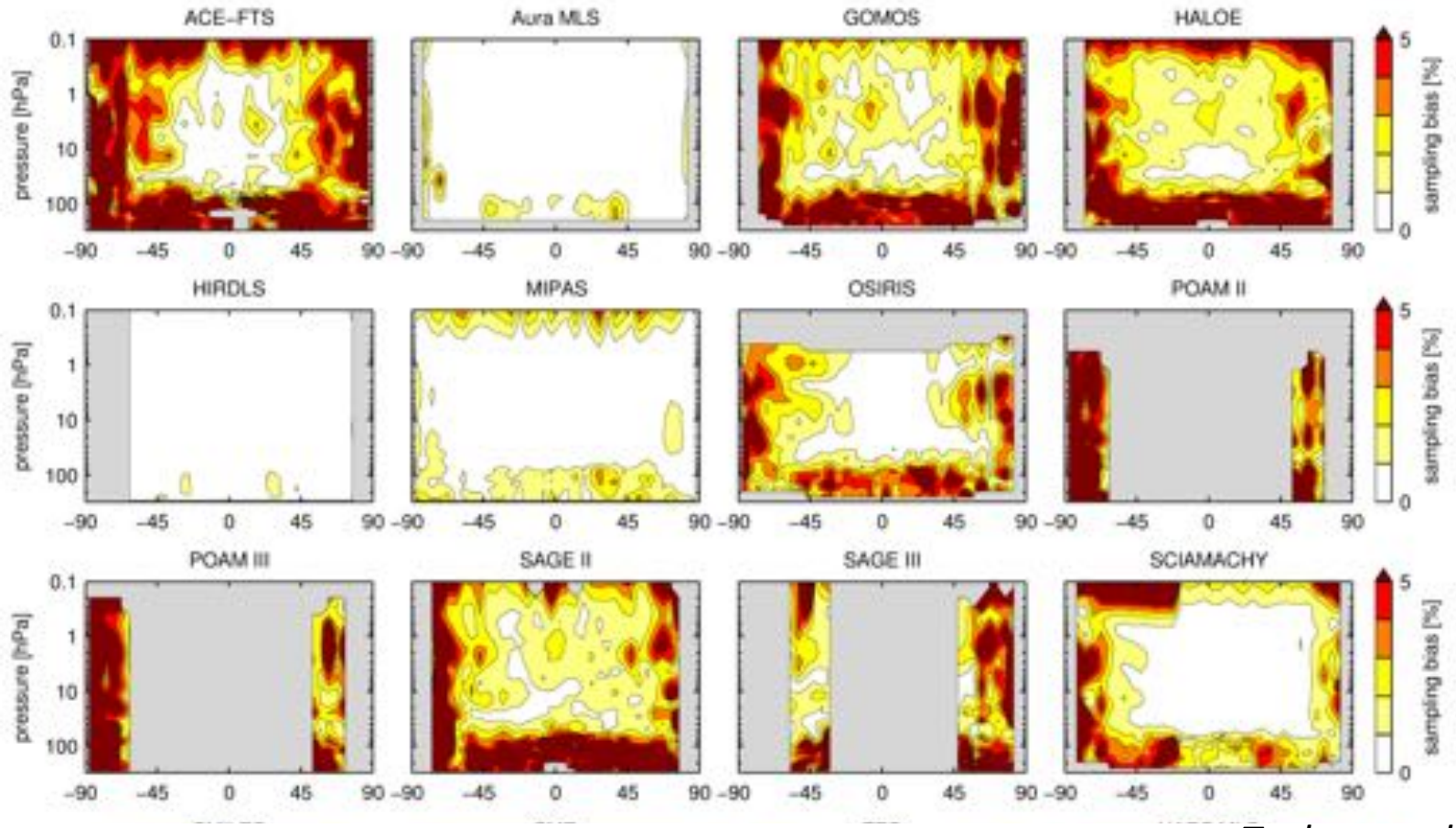
Sampling bias

March O_3 Case study: reality check



Real SPARC DI data!

Sampling bias



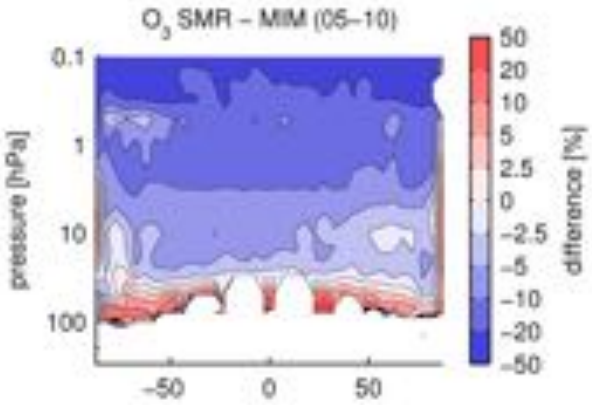
Toohey et al., 2013

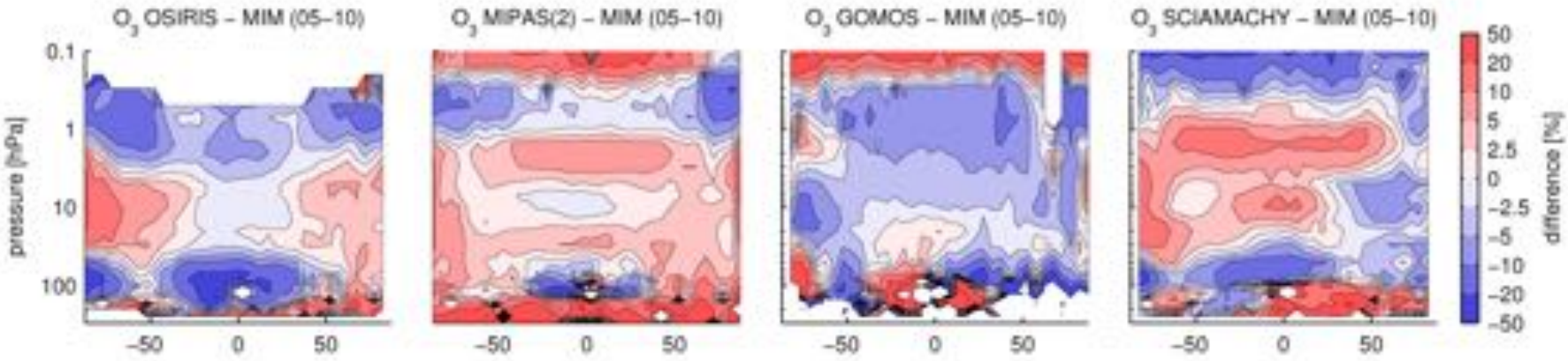
- Instruments with regular and uniform sampling patterns -> small sampling bias
- Instruments with varying latitudinal coverage -> strong sampling biases for certain months and locations
- Sampling biases for O_3 can be ≥ 10% (non-uniformity in day-of-month sampling)

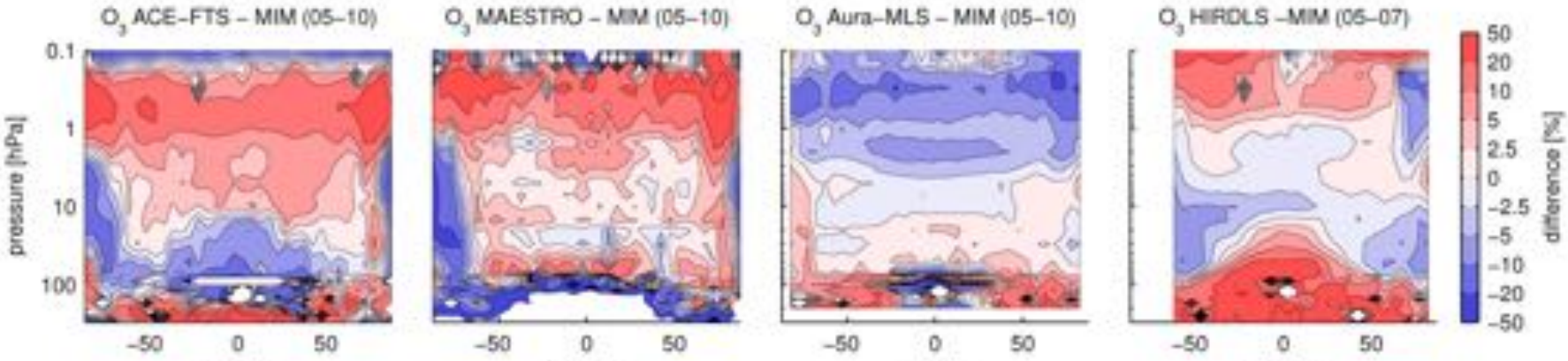
Ozone comparisons

Relative differences to the MIM 2005-2010

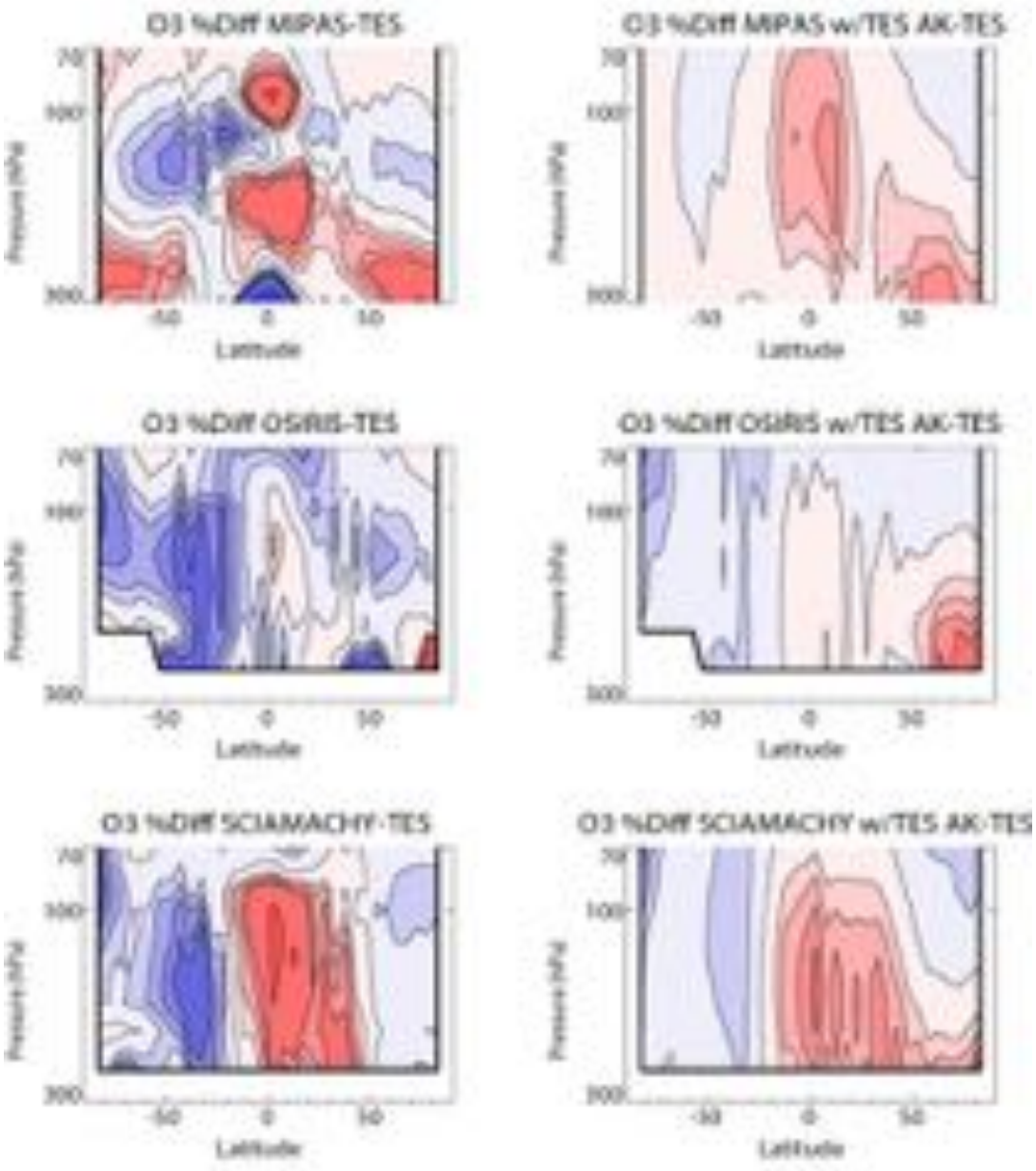
- Describe instrument performance on zonal mean annual mean basis
- Are used to derive climatological spread







Ozone comparisons



Application of TES observational operator to limb-viewing instruments

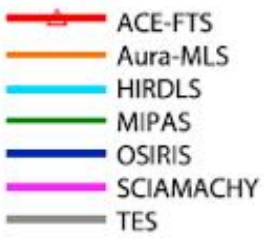
- Minimizes impact of vertical resolution
- Allows for identification of systematic difference
  e.g., positive bias of most instruments in tropical LS

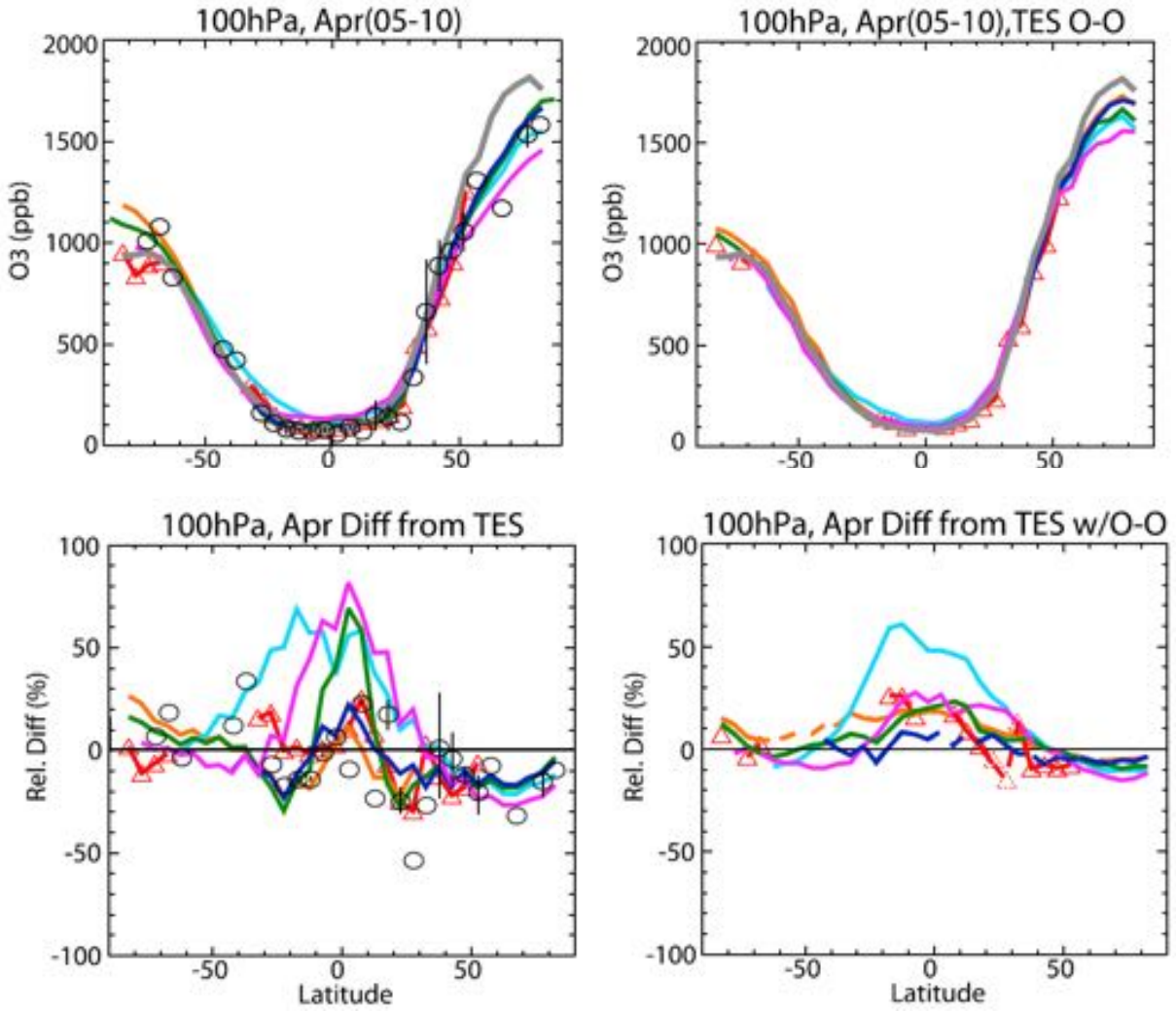
Neu et al., 2014

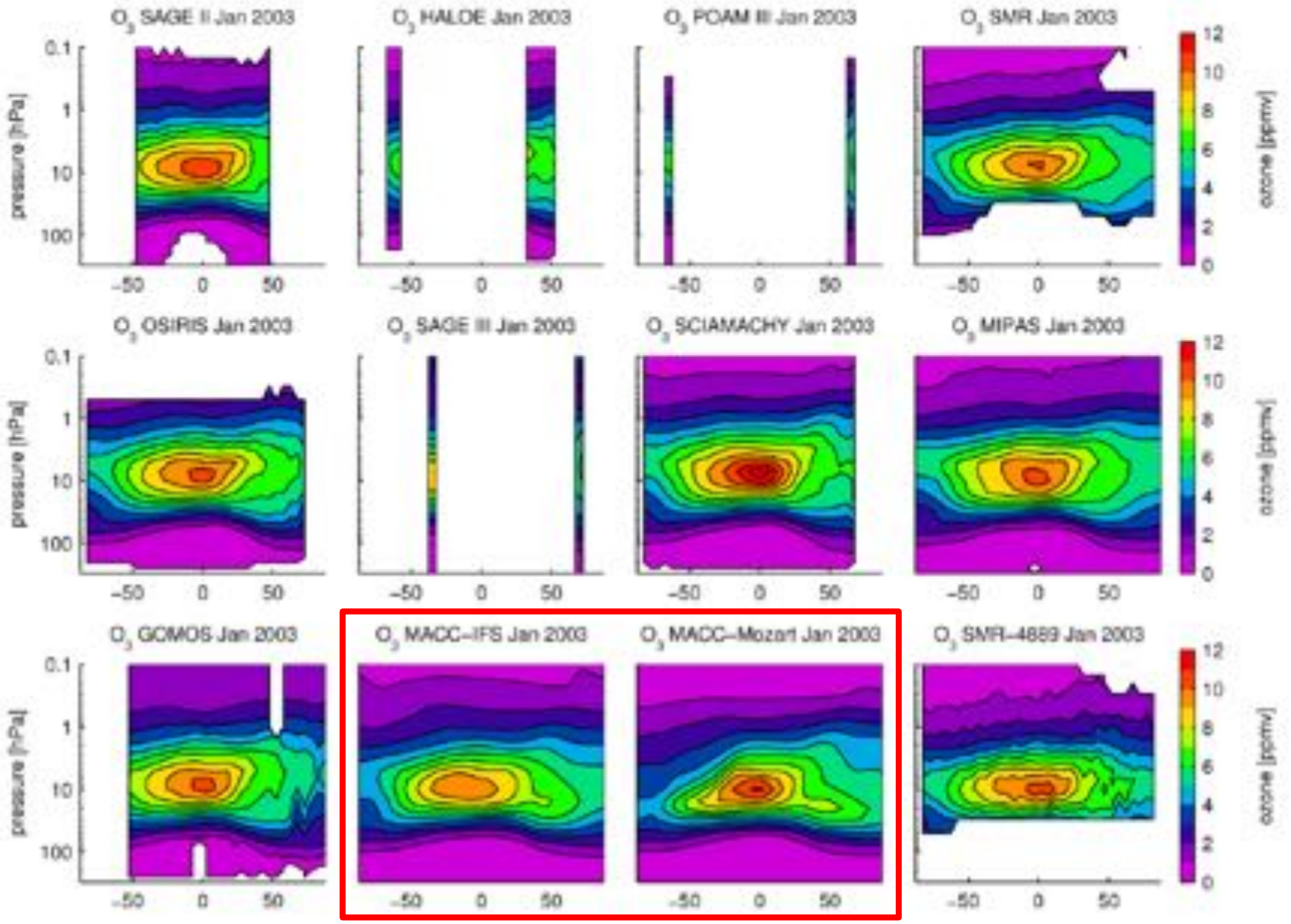
Impact of vertical resolution

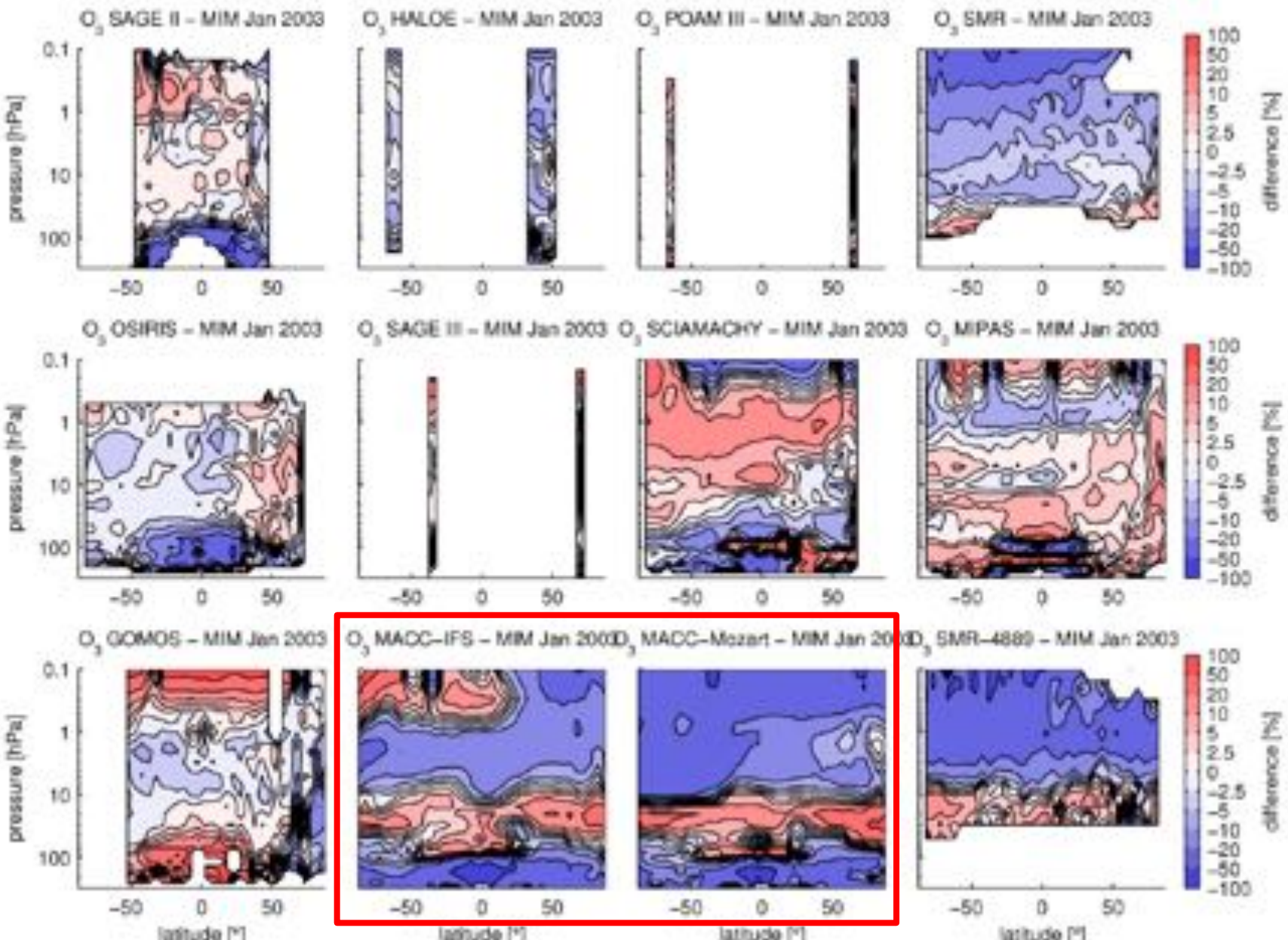
Application of TES observational operator to limb-viewing instruments

- Allows for identification of systematic difference e.g., positive bias of most instruments in tropical LS with respect to TES and ozone sondes





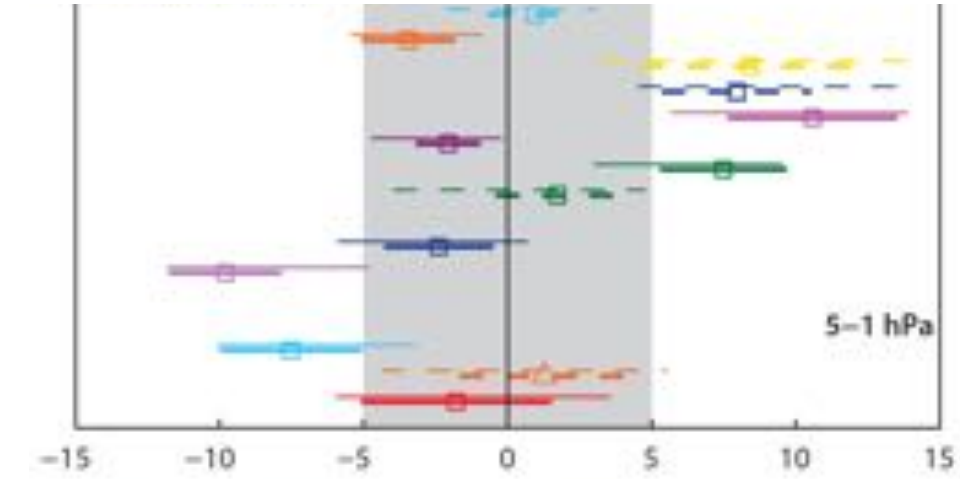

O3 SAGE II Jan 2003
O3 HALOE Jan 2003
O3 POAM III Jan 2003
O3 SMR Jan 2003
O3 OSIRIS Jan 2003
O3 SAGE III Jan 2003
O3 SCIAMACHY Jan 2003
O3 MIPAS Jan 2003
O3 GOMOS Jan 2003
O3 MACC-IFS Jan 2003
O3 MACC-Mozart Jan 2003
O3 SMR-4859 Jan 2003
pressure [hPa]
0.1
1
10
100
-50
0
50
ozone [ppmv]
12
10
8
6
4
2
0

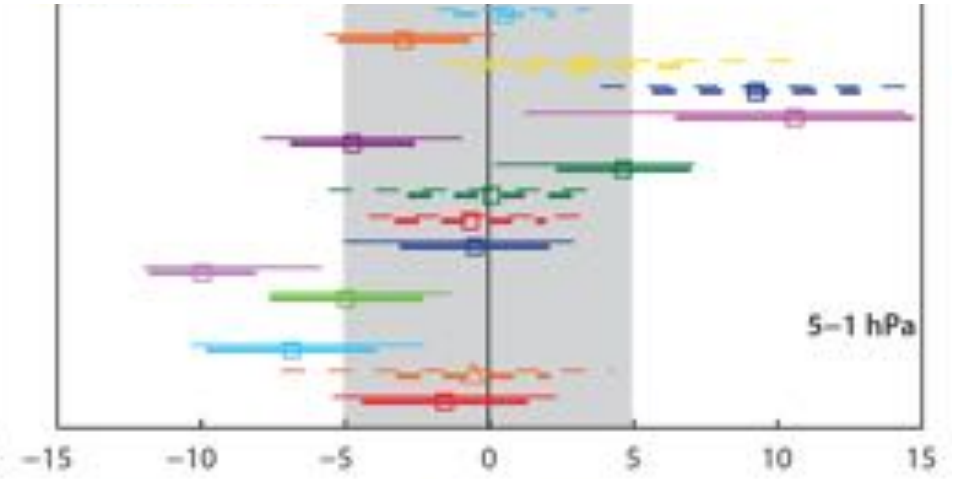

O3 SAGE II – MIM Jan 2003
O3 HALOE – MIM Jan 2003
O3 POAM III – MIM Jan 2003
O3 SMR – MIM Jan 2003
O3 OSIRIS – MIM Jan 2003
O3 SAGE III – MIM Jan 2003
O3 SCIAMACHY – MIM Jan 2003
O3 MIPAS – MIM Jan 2003
O3 GOMOS – MIM Jan 2003
O3 MACC–IFS – MIM Jan 2003
O3 MACC–Mozart – MIM Jan 2003
O3 SMR–4889 – MIM Jan 2003
pressure [hPa]
0.1
1
10
100
−50
0
50
latitude [°]
difference [%]
100
50
20
10
5
2.5
0
−2.5
−5
−10
−20
−50
−100

Ozone comparisons

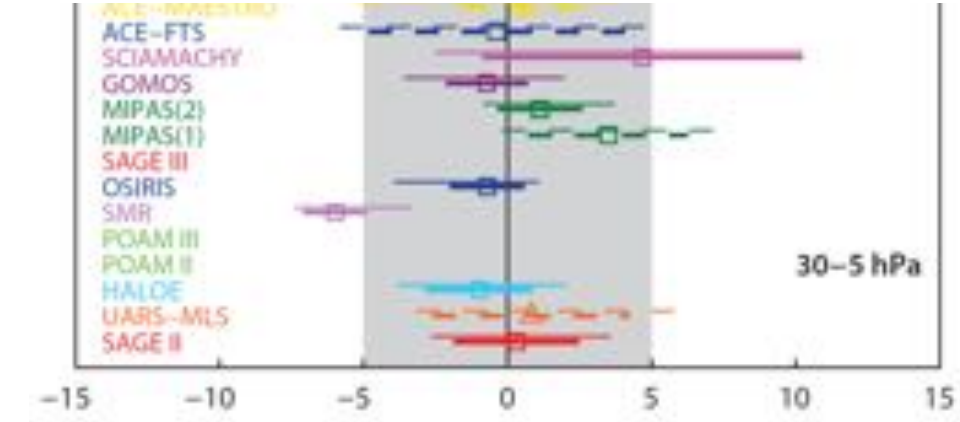
Evaluation of 18 ozone profile data sets [relative differences %]

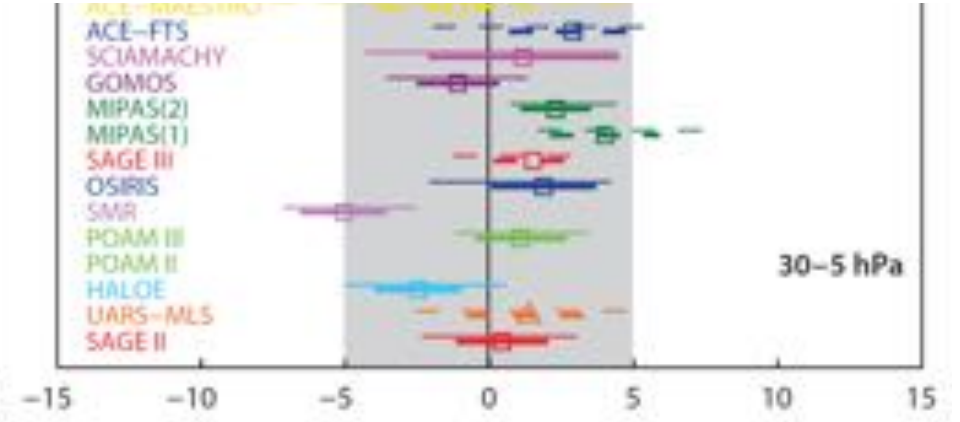
Upper stratosphere (5-1 hPa) - Good agreement: ±5% to **±10%.**



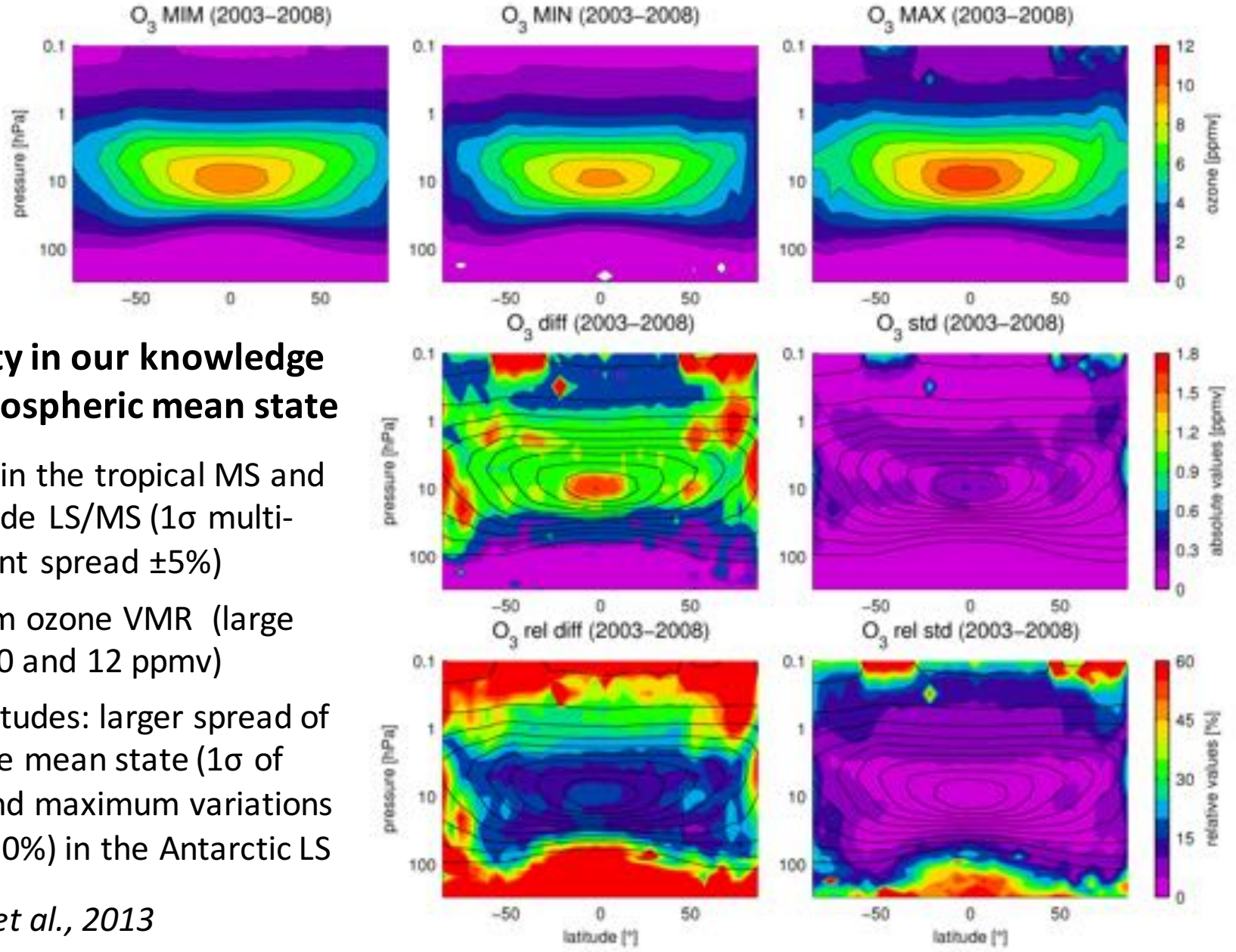


Middle stratosphere (30-5 hPa) - Lowest spread between the instrument data sets: **±5%**





O_3 atmospheric mean state



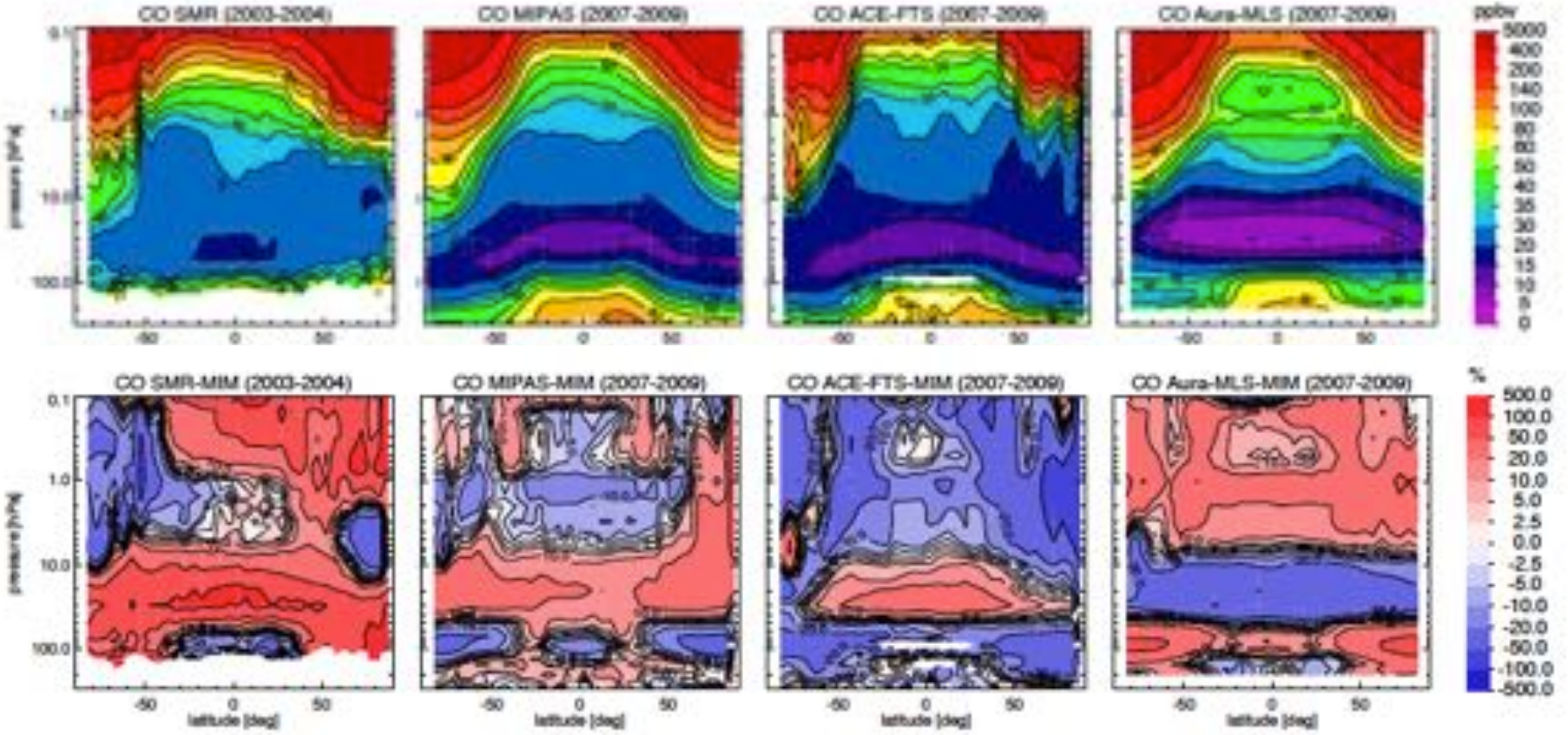
Uncertainty in our knowledge of the atmospheric mean state

- Smallest in the tropical MS and midlatitude LS/MS (1σ multi-instrument spread ±5%)
- Maximum ozone VMR (large spread 10 and 12 ppmv)
- Polar latitudes: larger spread of the ozone mean state (1σ of ±15%) and maximum variations (1σ of ±30%) in the Antarctic LS

Tegtmeier et al., 2013

CO comparisons

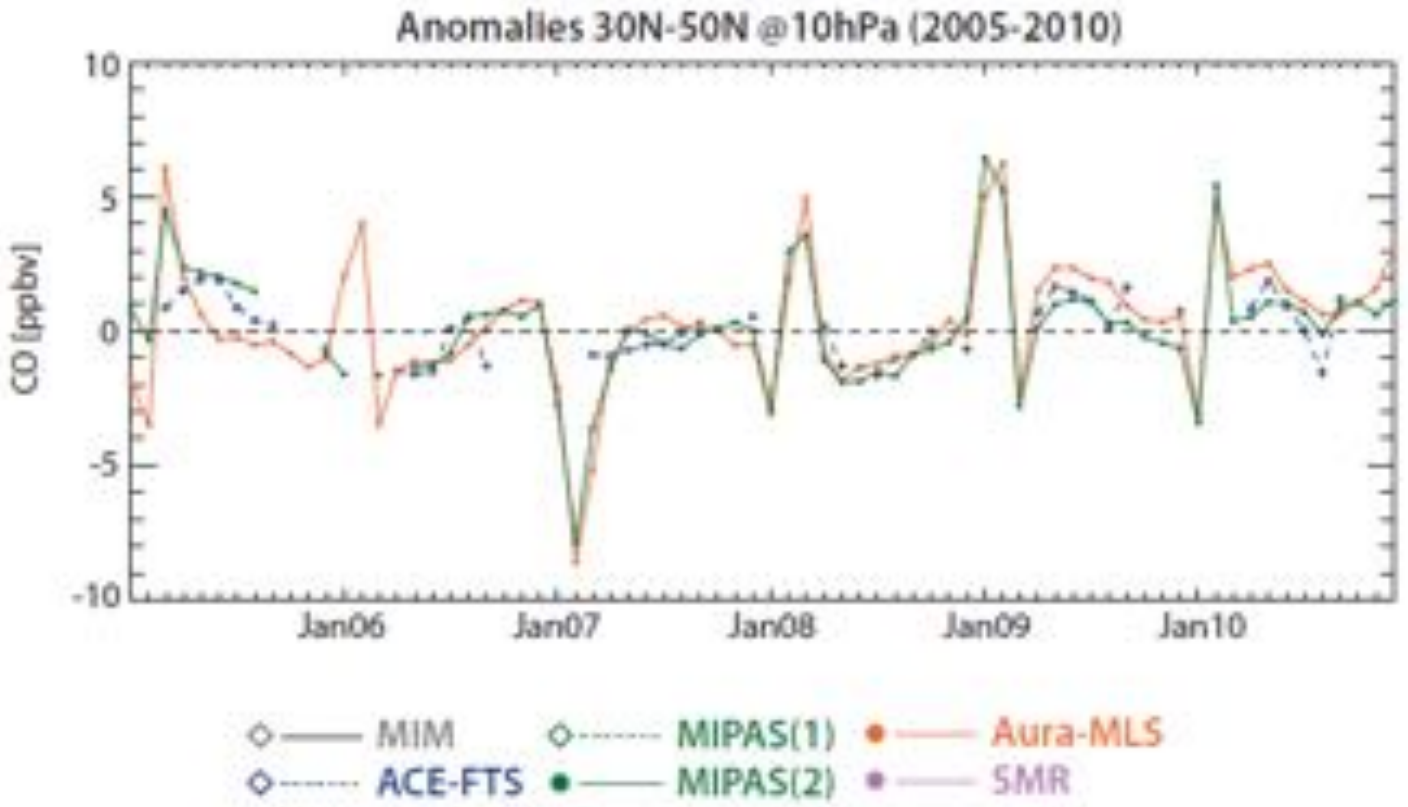
CO annual zonal mean cross sections



- **Large differences exist in some of the species in the annual zonal means.** Further retrieval studies are suggested to get at the cause of this discrepancy.

CO comparisons

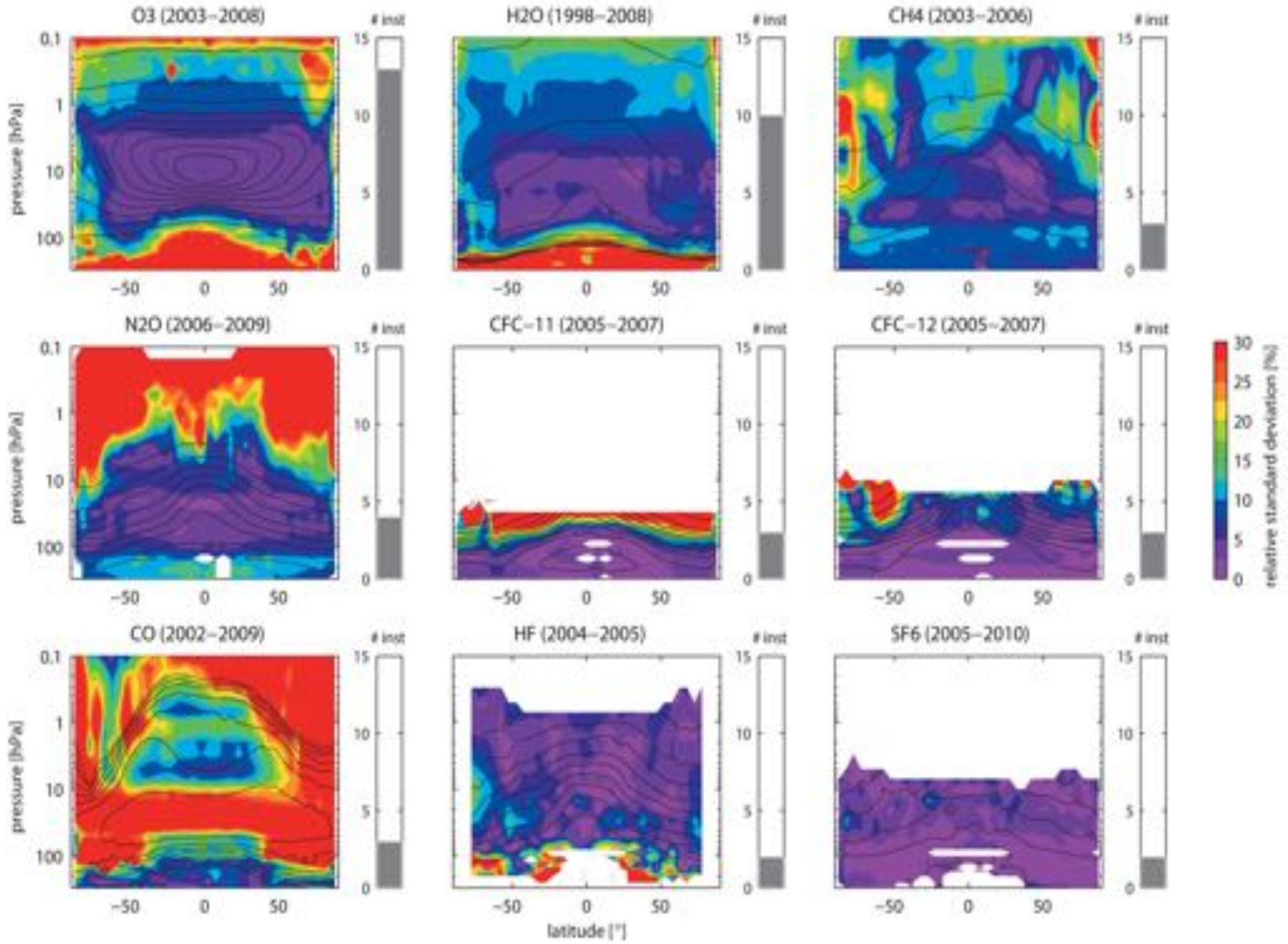
CO annual zonal mean cross sections

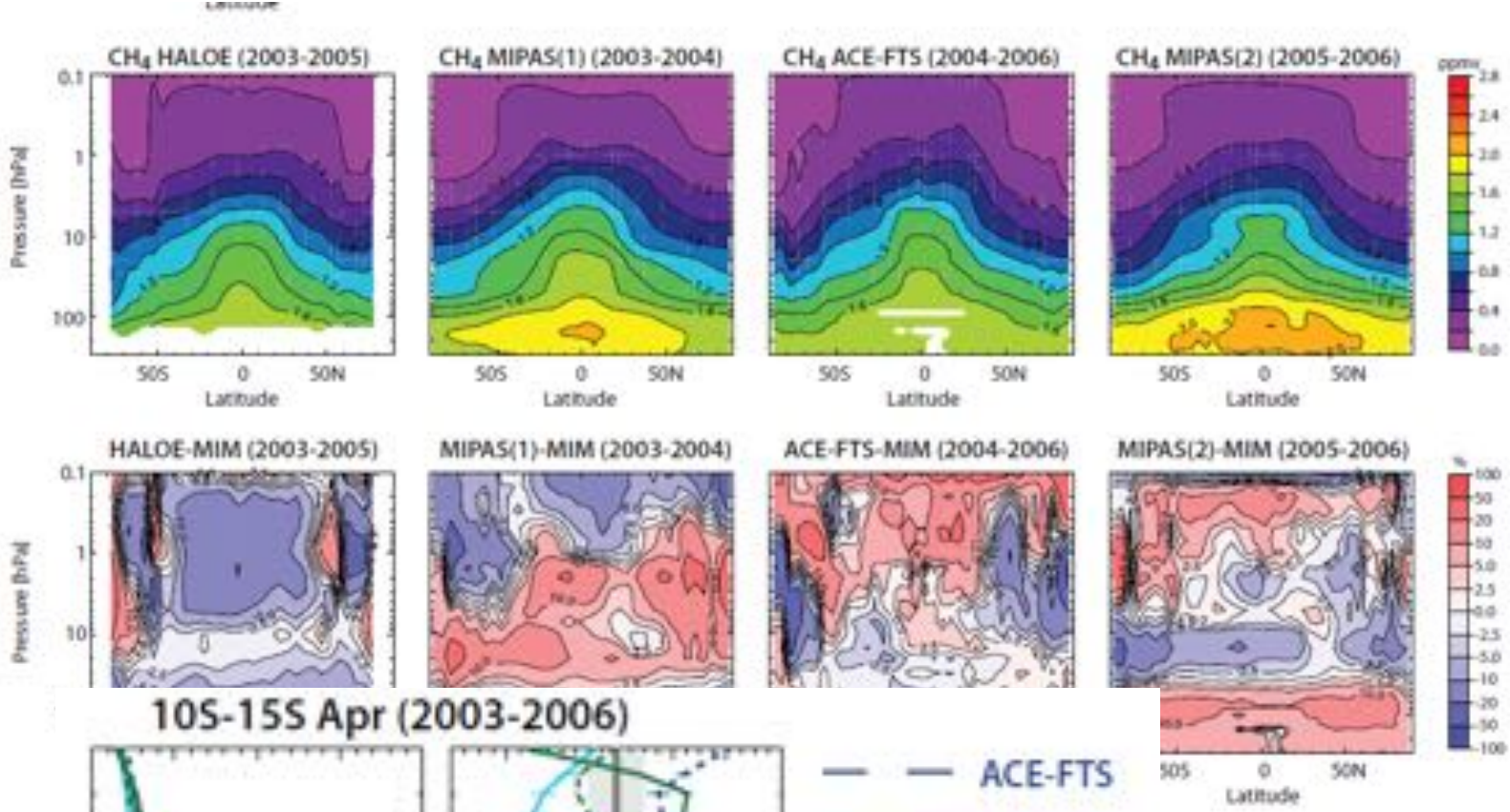


- **Large differences in the annual mean comparisons but very good agreement of the interannual variability.**

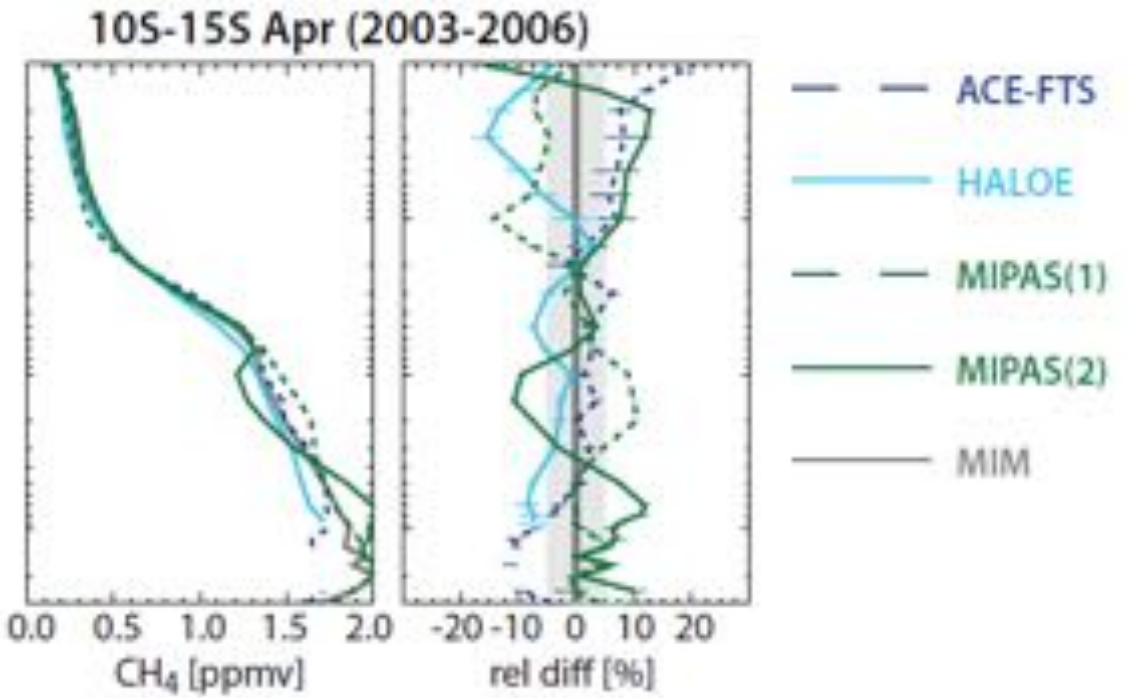
Atmospheric mean state

SPARC Data Assimilation workshop, Paris, 2015

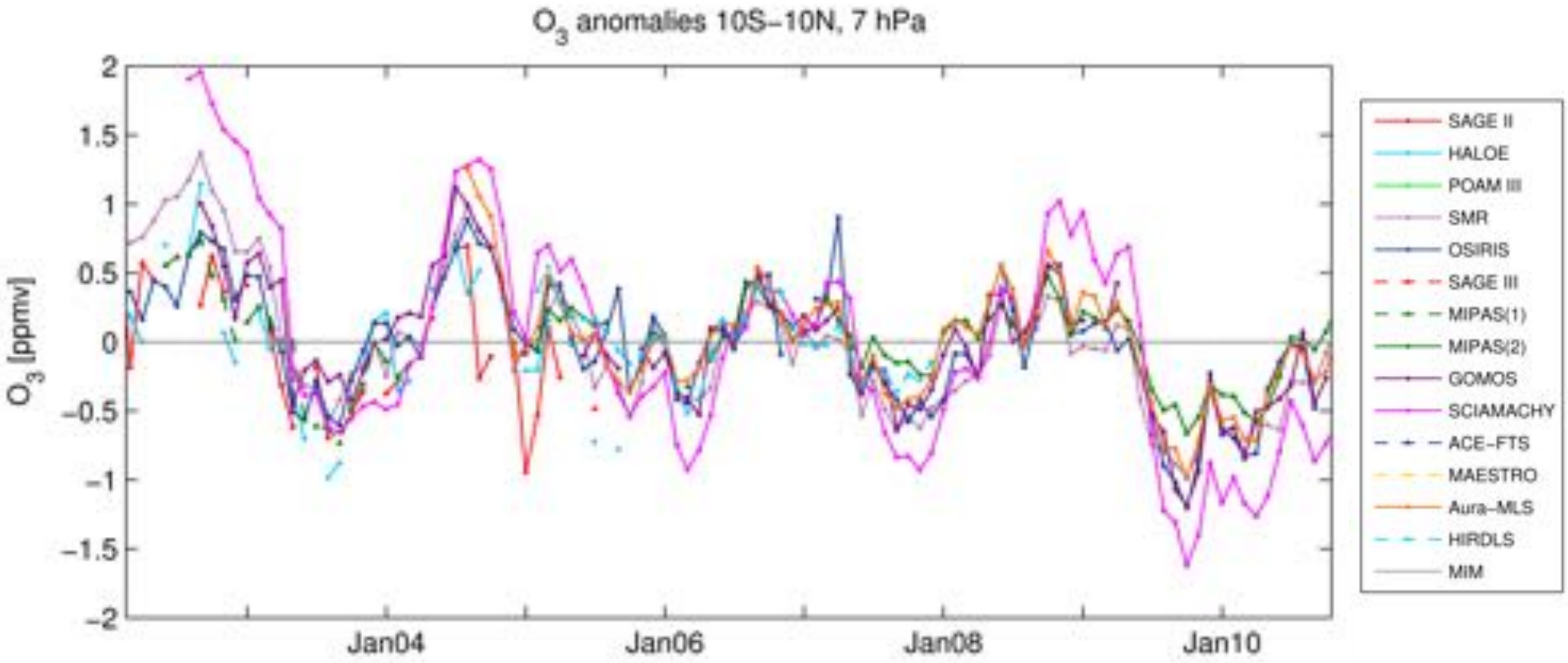



CH4 HALOE (2003-2005)
CH4 MIPAS(1) (2003-2004)
CH4 ACE-FTS (2004-2006)
CH4 MIPAS(2) (2005-2006)
Pressure [hPa]
Latitude
50S
0
50N
ppmv
HALOE-MIM (2003-2005)
MIPAS(1)-MIM (2003-2004)
ACE-FTS-MIM (2004-2006)
MIPAS(2)-MIM (2005-2006)
%

CH_4

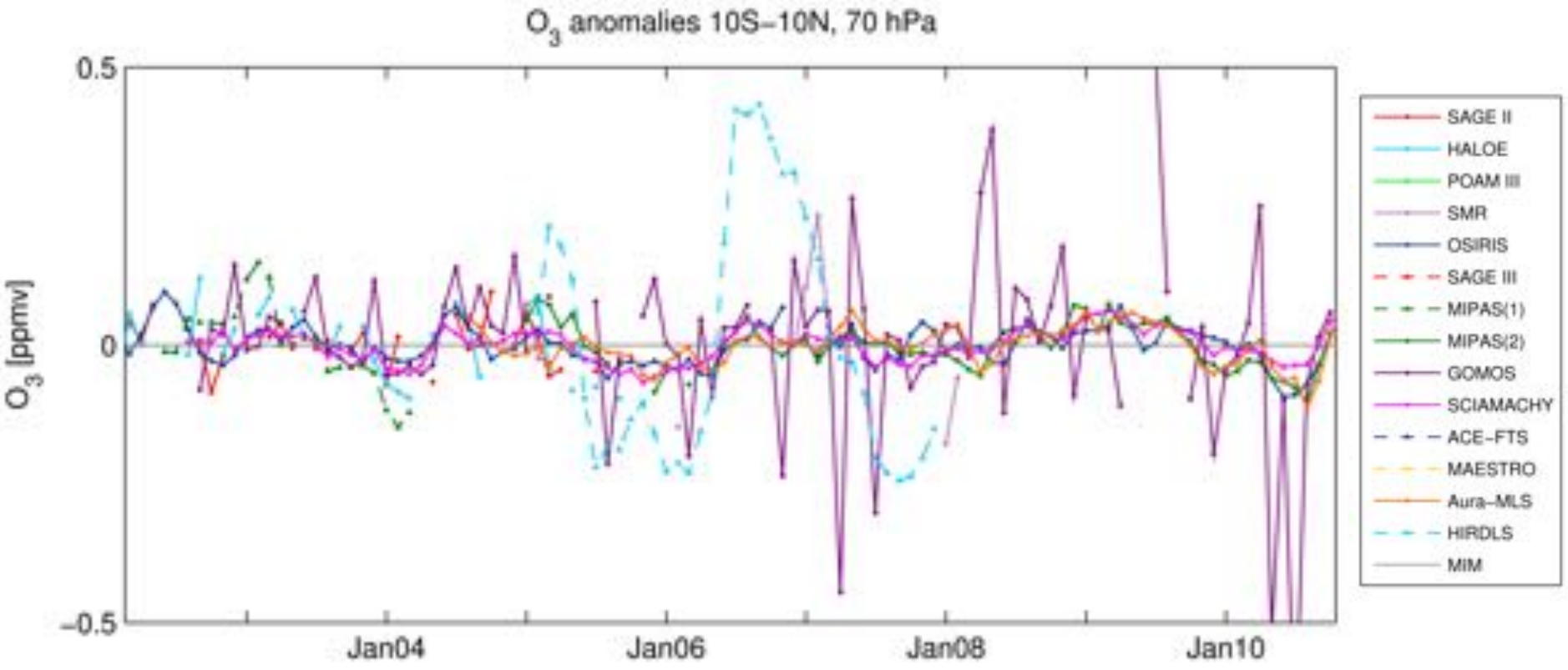

10S-15S Apr (2003-2006)
ACE-FTS
HALOE
MIPAS(1)
MIPAS(2)
MIM
0.0 0.5 1.0 1.5 2.0
CH4 [ppmv]
-20 -10 0 10 20
rel diff [%]

Ozone - Evaluation of interannual variability



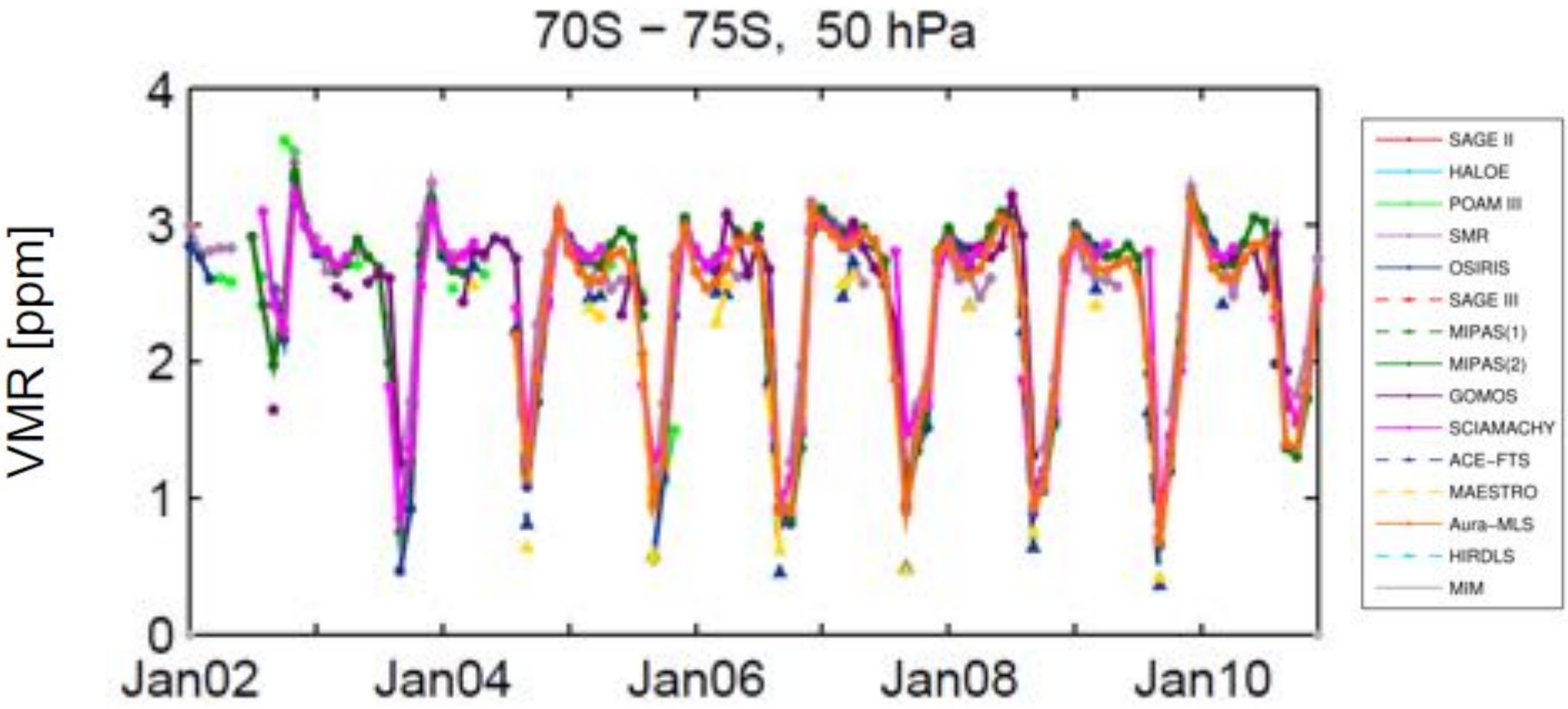
- Tropical **QBO signal in the middle stratosphere is captured well** by all instruments
- Slight deviations in displayed amplitude

Ozone - Evaluation of interannual variability



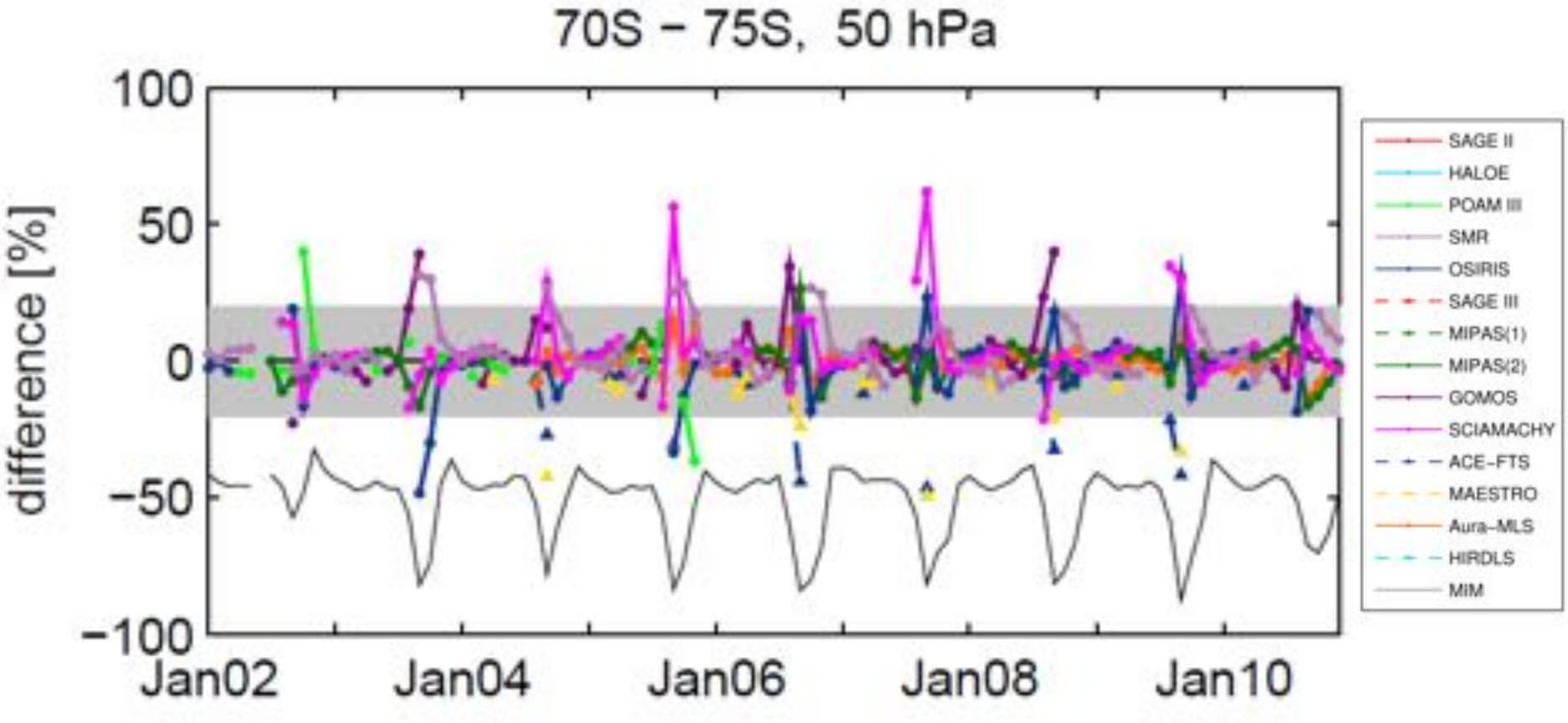
- **Larger difficulties in the lower stratosphere** where ozone abundances and inter-annual variations are small

Evaluation of Antarctic ozone



- **Large relative differences (to the MIM) in the Antarctic polar cap region** during the time of the ozone hole
- Spread between the monthly zonal mean fields of ±50%

Evaluation of Antarctic ozone



- **Large relative differences (to the MIM) in the Antarctic polar cap region** during the time of the ozone hole
- Spread between the monthly zonal mean fields of ±50%

Stratospheric satellite data for model evaluation

- Data Initiative: Provides the data and basic knowledge on data quality

- Mixed team of scientist
  - ✓ Generate list of diagnostics appropriate for model evaluations
  - ✓ Provide a 'best' estimate and its uncertainty range for ready use in model-measurement comparisons (CCMVal diagnostic tool)

- "Recipe" for deriving an observational uncertainty range
  - ✓ O_3 seasonal cycle at 200 hPa, mid-latitudes

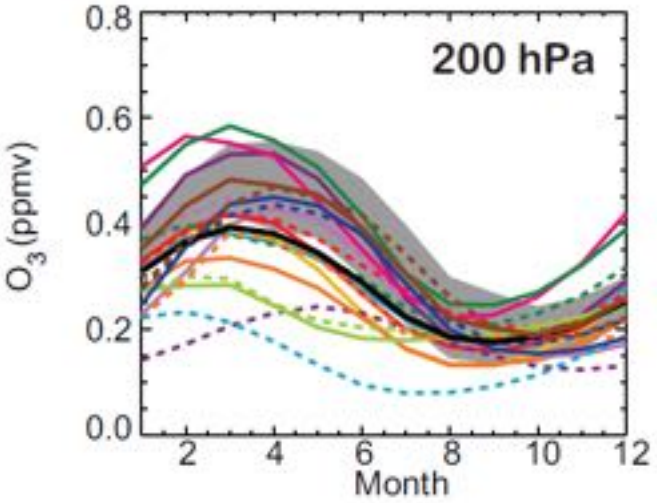
O_3 seasonal cycle, 40°N - 60°N, 200 hPa

Evaluate the representation of large-scale transport and mixing processes

CCMVal report, 2010

Observational data :

MIPAS 2004-2008

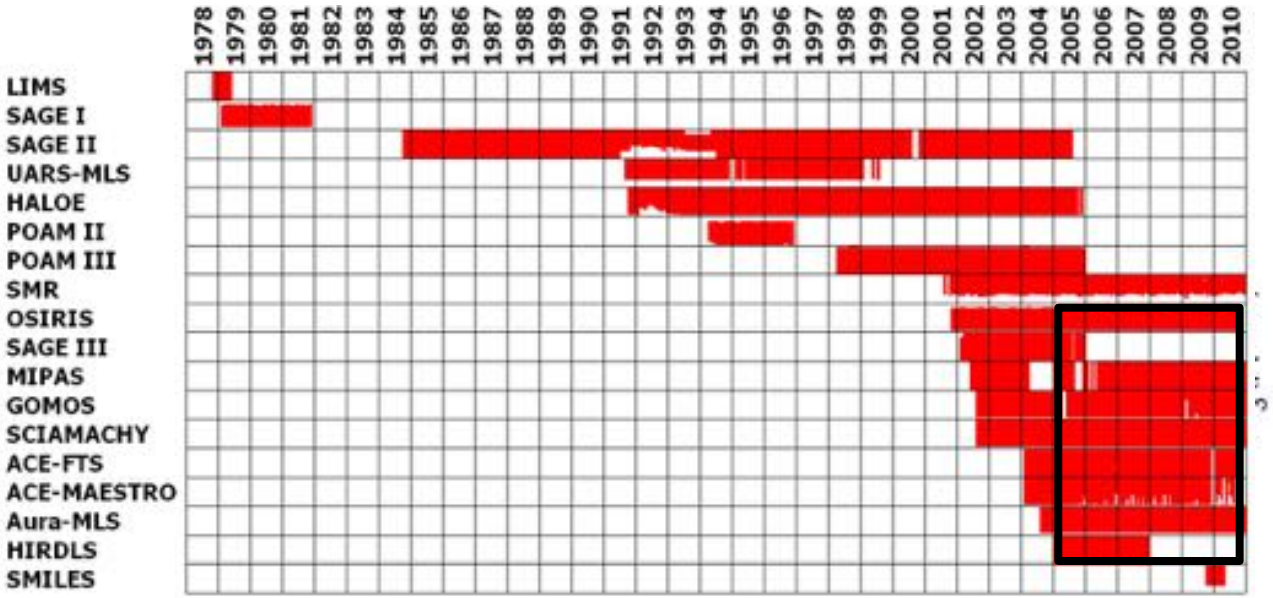


O_3 seasonal cycle, 40°N - 60°N, 200 hPa

Evaluate the representation of large-scale transport and mixing processes

Step 1: Define time period

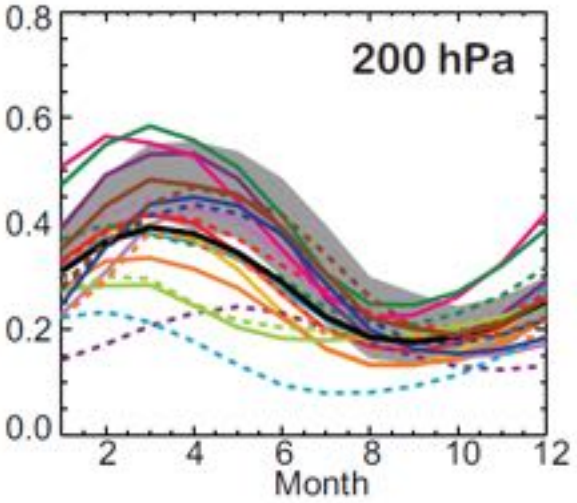
Find overlap period of maximum length including maximum number of instruments



CCMVal report, 2010

Observational data :

MIPAS 2004-2008



O_3 seasonal cycle, 40°N - 60°N, 200 hPa

Evaluate the representation of large-scale transport and mixing processes

Step 1: Define time period

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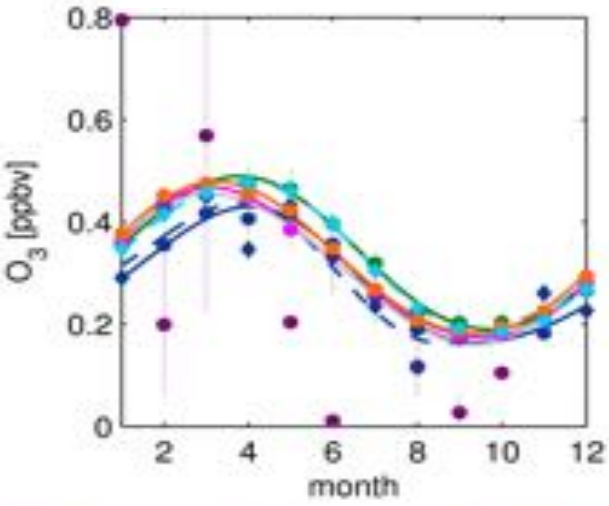
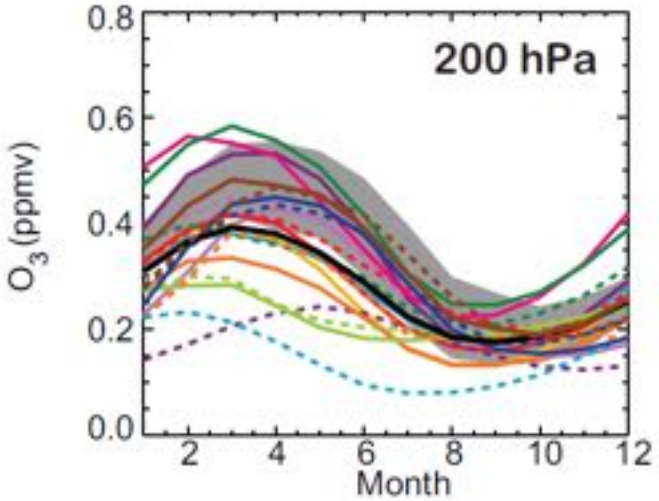
SPARC Data Initiative
Seven observational data sets, 2005-2010



CCMVal report, 2010
Observational data : MIPAS 2004-2008



OSIRIS — MIPAS(2) — GOMOS — SCIAMACHY - - - ACE-FTS — Aura-MLS - - - HIRDLS

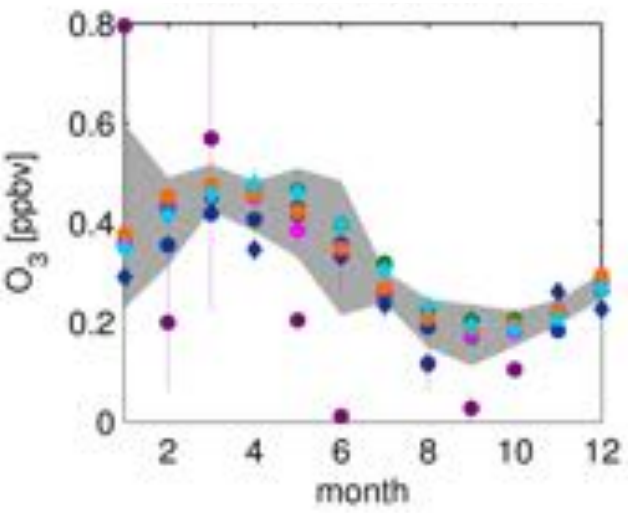
O_3 seasonal cycle, 40°N - 60°N, 200 hPa

Evaluate the representation of large-scale transport and mixing processes

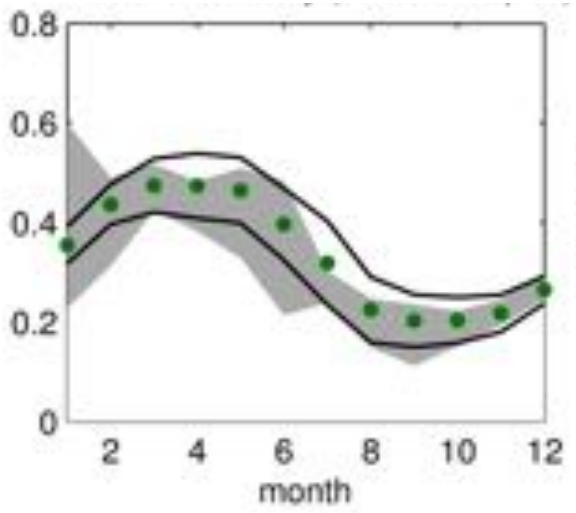
Step 2: Instrument spread

Calculate uncertainty range as the standard deviation over the instrument spread

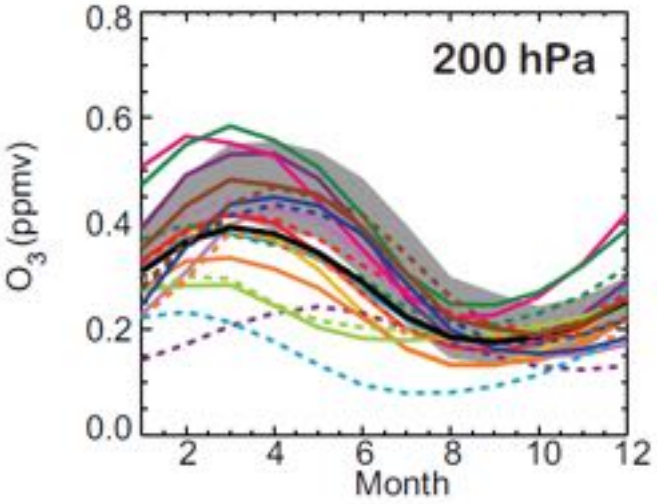
SPARC Data Initiative
Seven observational data sets, 2005-2010



SPARC Data Initiative *versus* ***CCMVal report***



CCMVal report, 2010
Observational data : MIPAS 2004-2008



OSIRIS — MIPAS(2) — GOMOS — SCIAMACHY - - - ACE-FTS — Aura-MLS - - - HIRDLS

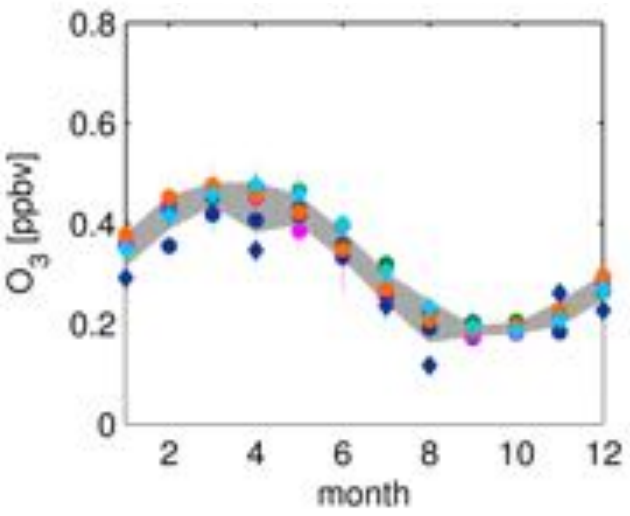
O_3 seasonal cycle, 40°N - 60°N, 200 hPa

Evaluate the representation of large-scale transport and mixing processes

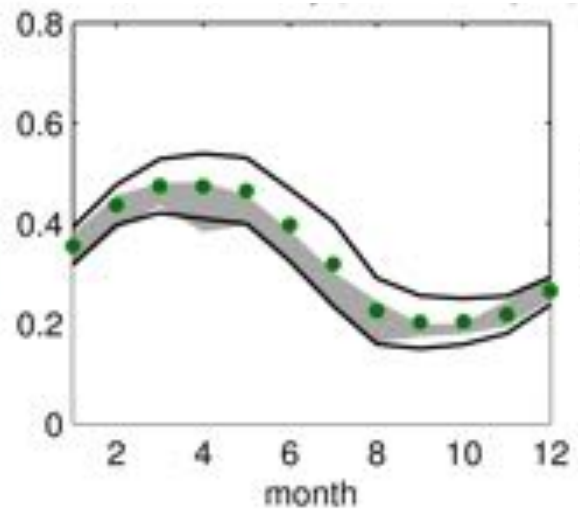
Step 3: Eliminate outliers

Remove all data points outside of the 3σ uncertainty range of all other instruments

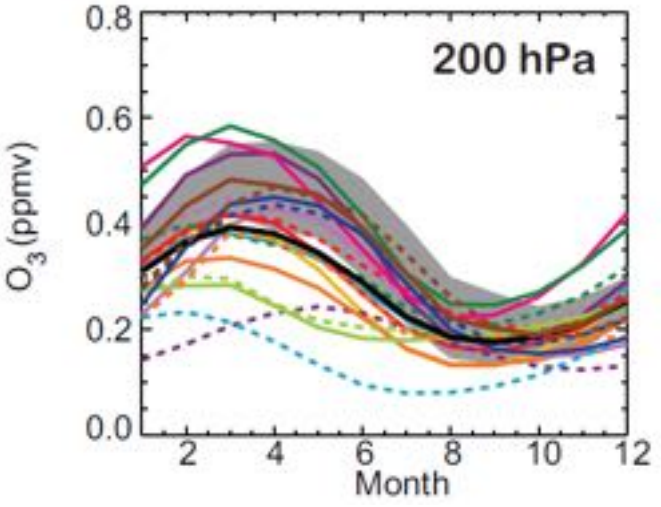
SPARC Data Initiative
Seven observational data sets, 2005-2010



SPARC Data Initiative versus ***CCMVal report***



CCMVal report, 2010
Observational data : MIPAS 2004-2008



OSIRIS — MIPAS(2) — SCIAMACHY - - - ACE-FTS — Aura-MLS - - - HIRDLS

Model evaluations

O_3 seasonal cycle, 40°N - 60°N, 200 hPa

Evaluate the representation of large-scale transport and mixing processes

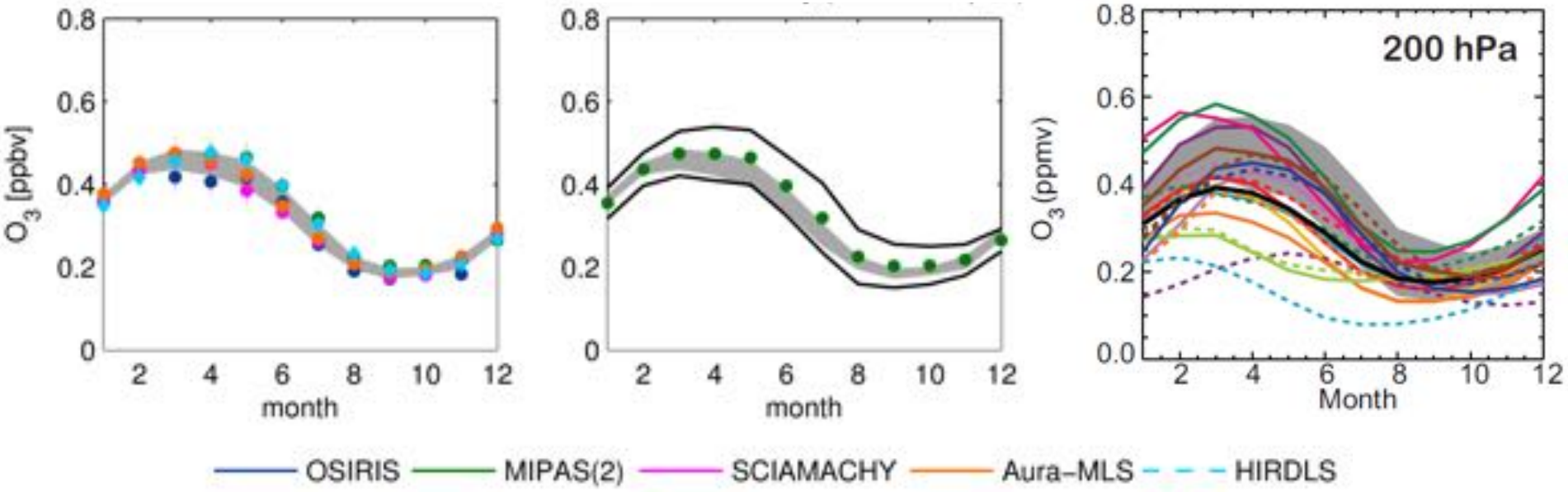
Step 4: Eliminate sampling bias

Remove data impacted by sparse sampling *(Toohey et al., 2013)*

SPARC Data Initiative
Seven observational data sets, 2005-2010

SPARC Data Initiative *versus* ***CCMVal report***

CCMVal report, 2010
Observational data : MIPAS 2004-2008



Model evaluations

O_3 seasonal cycle, 40°N - 60°N, 200 hPa

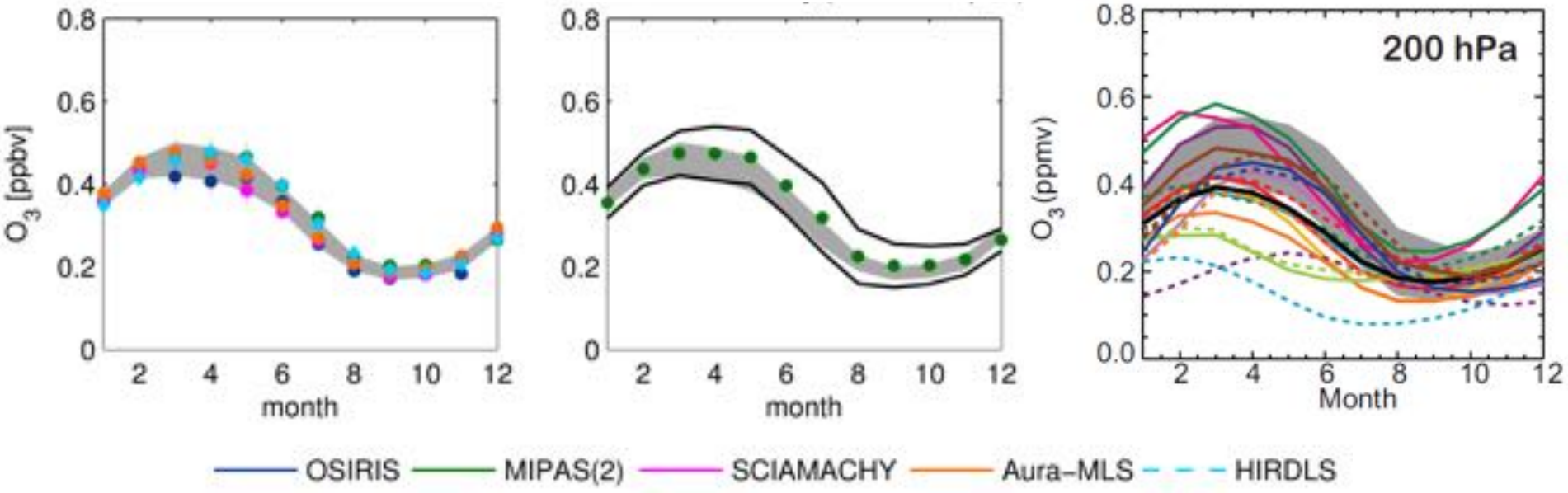
Evaluate the representation of large-scale transport and mixing processes

Step 5: Include interannual variability

SPARC Data Initiative
Seven observational data sets, 2005-2010

SPARC Data Initiative *versus* ***CCMVal report***

CCMVal report, 2010
Observational data : MIPAS 2004-2008

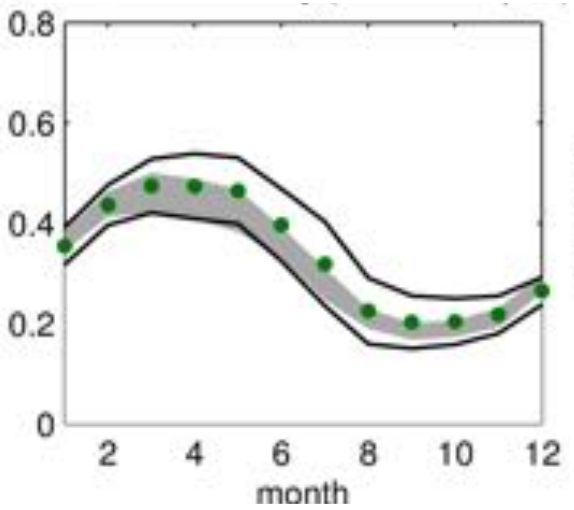


O_3 seasonal cycle, 40°N - 60°N, 200 hPa

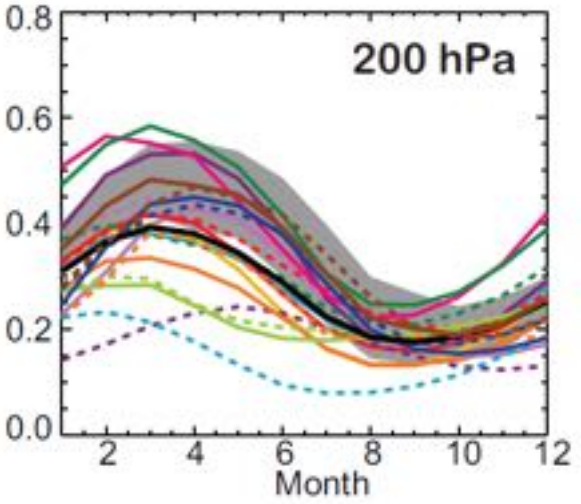
- **Reduced uncertainty range** → $g = 1 - \frac{1}{n_g} \frac{|\mu_{model} - \mu_{obs}|}{\sigma_{obs}}$
- **Observational range shifted to slightly lower values**
- **Shifted phase (earlier maximum)**

Douglass et al., 1998
Waugh and Eyring, 2008

SPARC Data Initiative *versus* ***CCMVal report***



CCMVal report, 2010
Observational data :
MIPAS 2004-2008



Implications for merging

Merging techniques

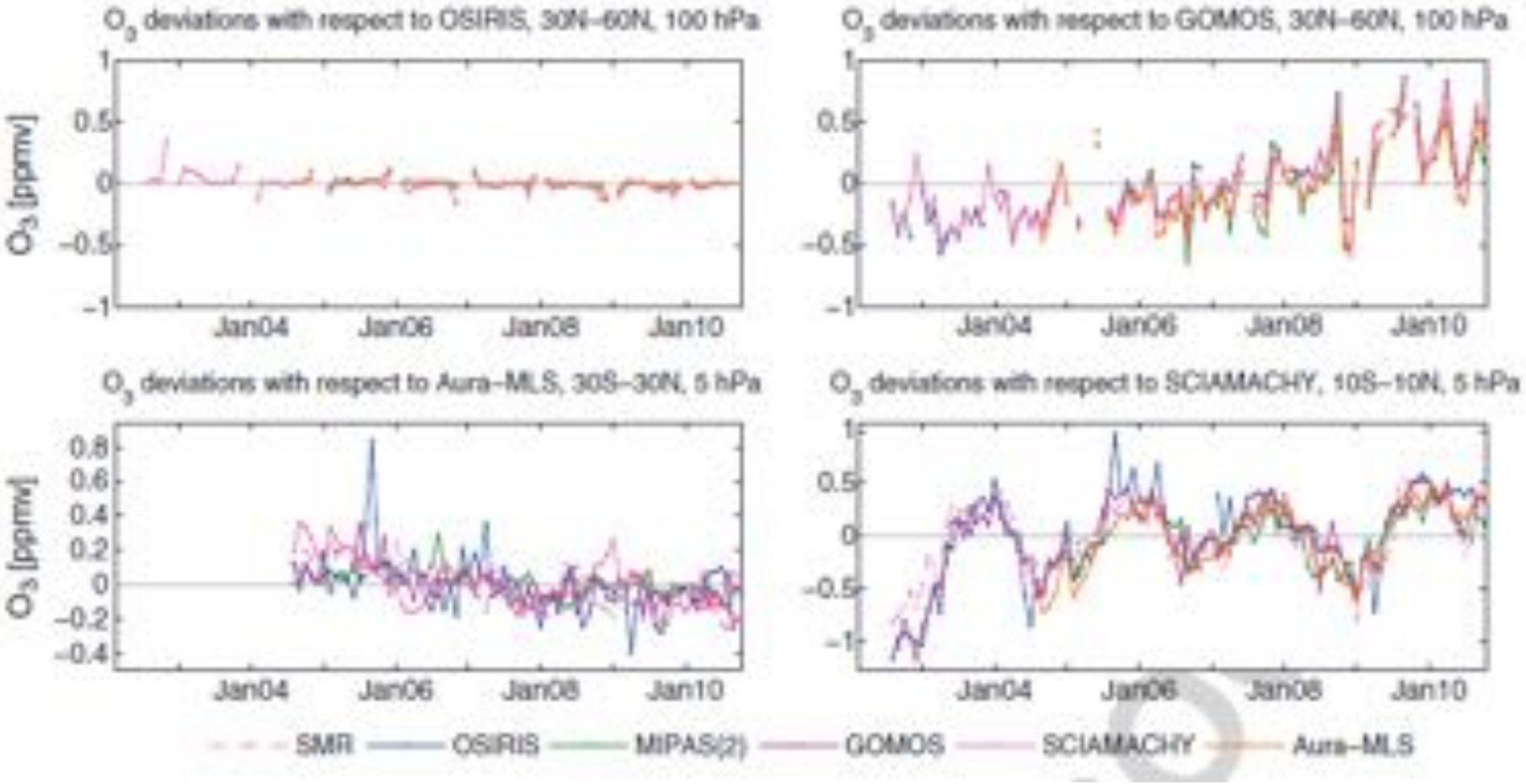
- Merging of two single datasets by accounting for an inter-instrument bias calculated over some overlap time period (SAGE/GOMOS)
- Merging of multiple datasets that uses detailed error characterization of instruments (Froidevaux GOZCARDS, Davis SWOOSH)
- Statistical methods to fill in observational gaps (BDPD)
- Nudged chemistry-climate model as transfer function between the instruments (Hegglin et al., 2014)

Problems

- Inverse estimated error (can differ between data sets, ideally instruments error covariances)
- Key problems: different altitude resolutions and different content of a priori information (application of the averaging kernel matrix)
- Drifts hard to identify (comparisons between two satellites non-conclusive, in situ measurements as reference often lead to lack of statistical significance)

Implications for merging

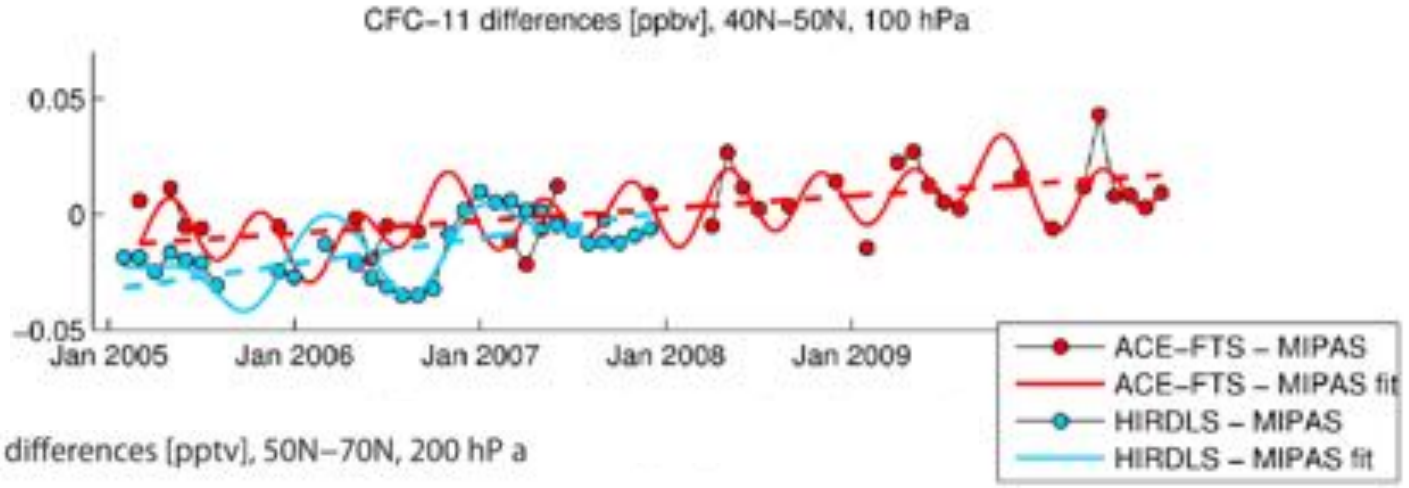
Drifts identified by comparison to all other available data sets

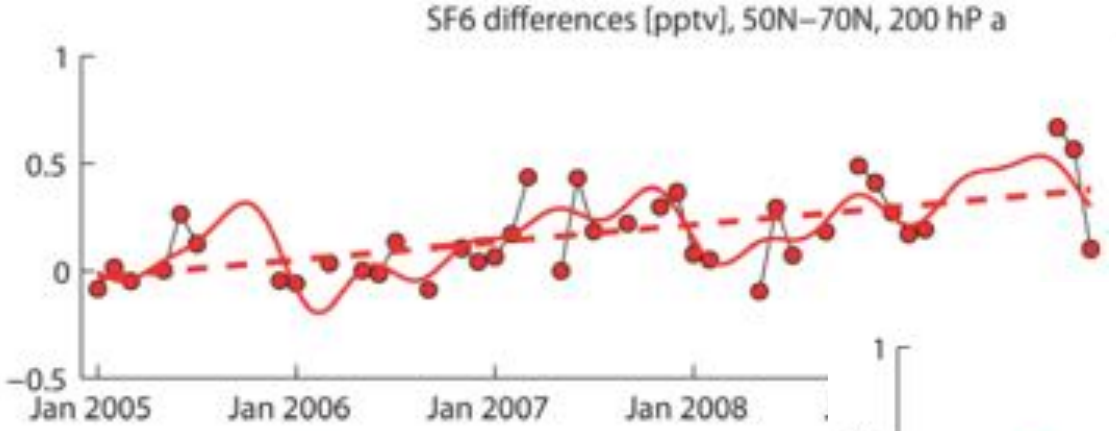


Implications for merging

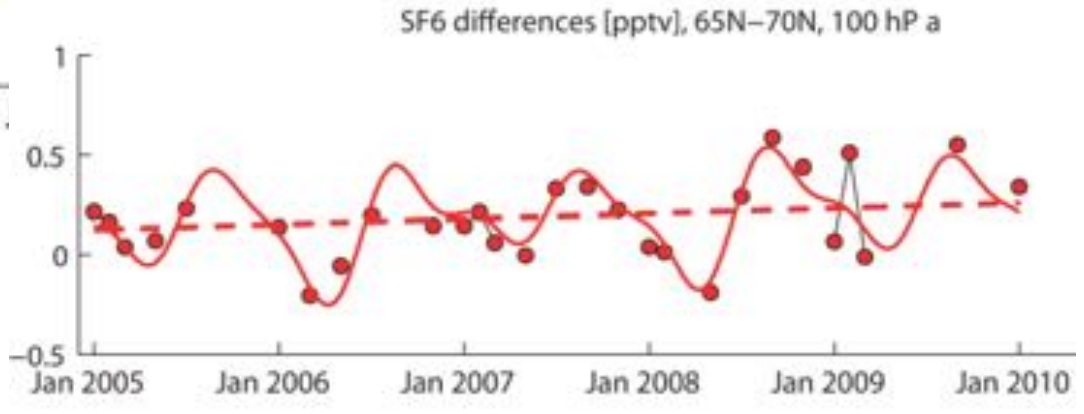
Multi-linear regression of time series of differences between pairs of instruments

CFC-11





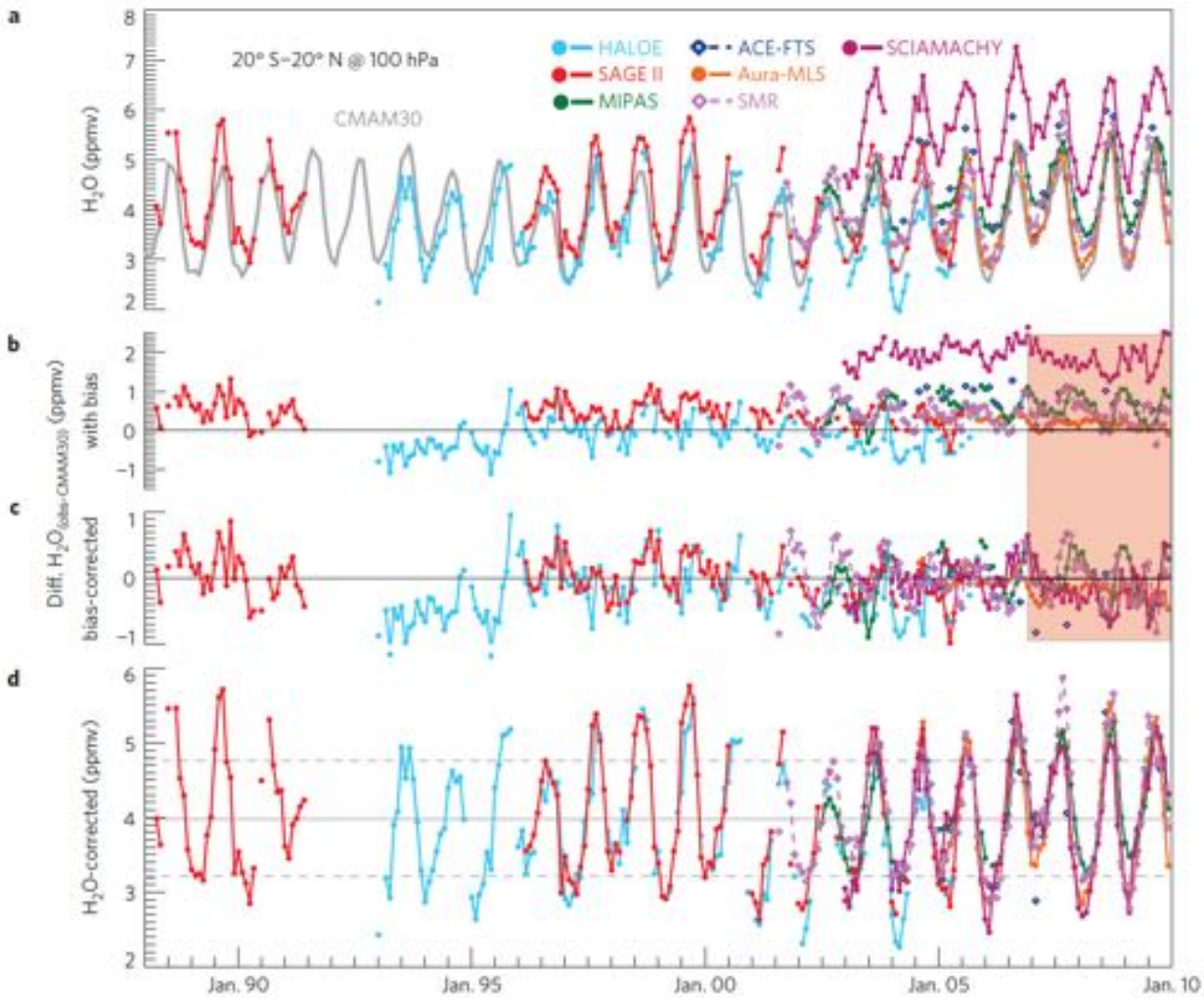
SF_6



Implications for merging

CCM nudged to observed meteorology is used as transfer function between observational data sets

- Long-term data record
- Instrumental drifts
- Representativeness of spatially limited data sets.
- Lower/mid stratospheric water vapour trends are negative
- Upper stratospheric water vapour trends are positive, (accelerated BDC in the lower stratosphere)



Hegglin et al, 2014

Summary

Comprehensive comparison of satellite instrument observations

- Better knowledge of the quality of available data products including information on where they are consistent and where they exhibit unphysical features or strong deviations
- Assessment of the range of measurements as an estimate of the systematic uncertainty in the measured field
- Need for further evaluation activities (e.g., in the UTLS and at high latitudes) identified
- Motivation for improvement of data products

Provide monthly zonal mean time series in a common format

- Will be published on the SPARC data archive website
- Will be updated in the future as soon as new time series are available)

Improve future model-measurement comparison activities

- Depending on the evaluation and trace gas, individual instruments may need to be excluded from the comparison (e.g., seasonal cycle in LS)

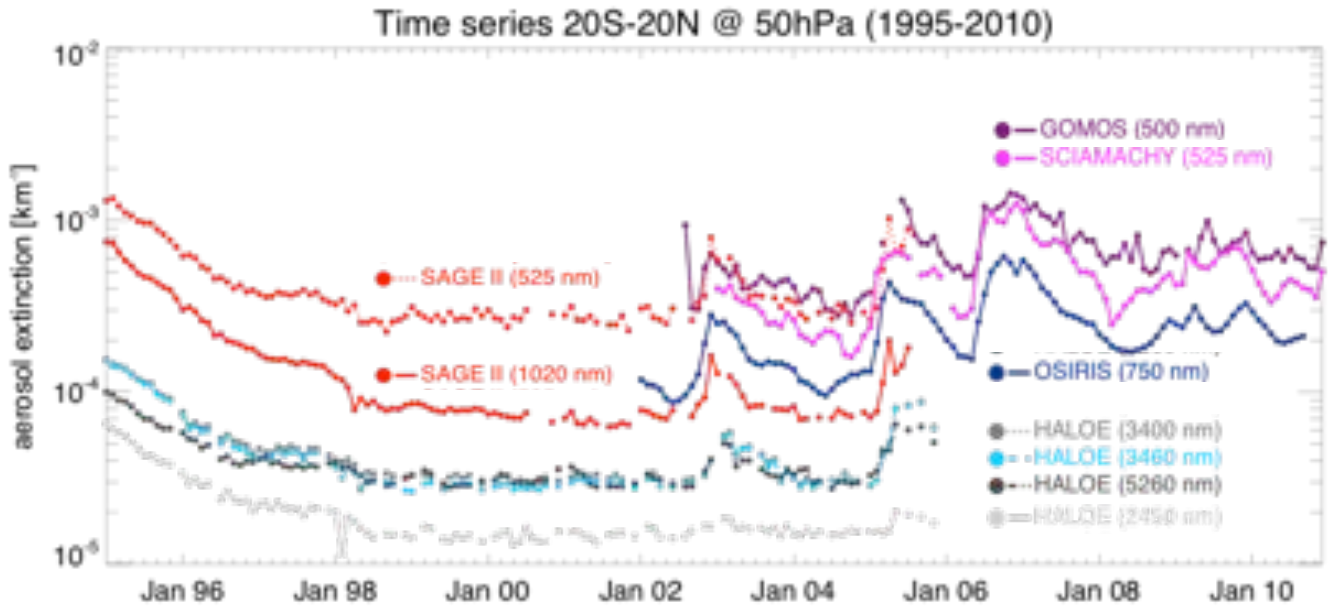
Aerosol anomaly evaluations

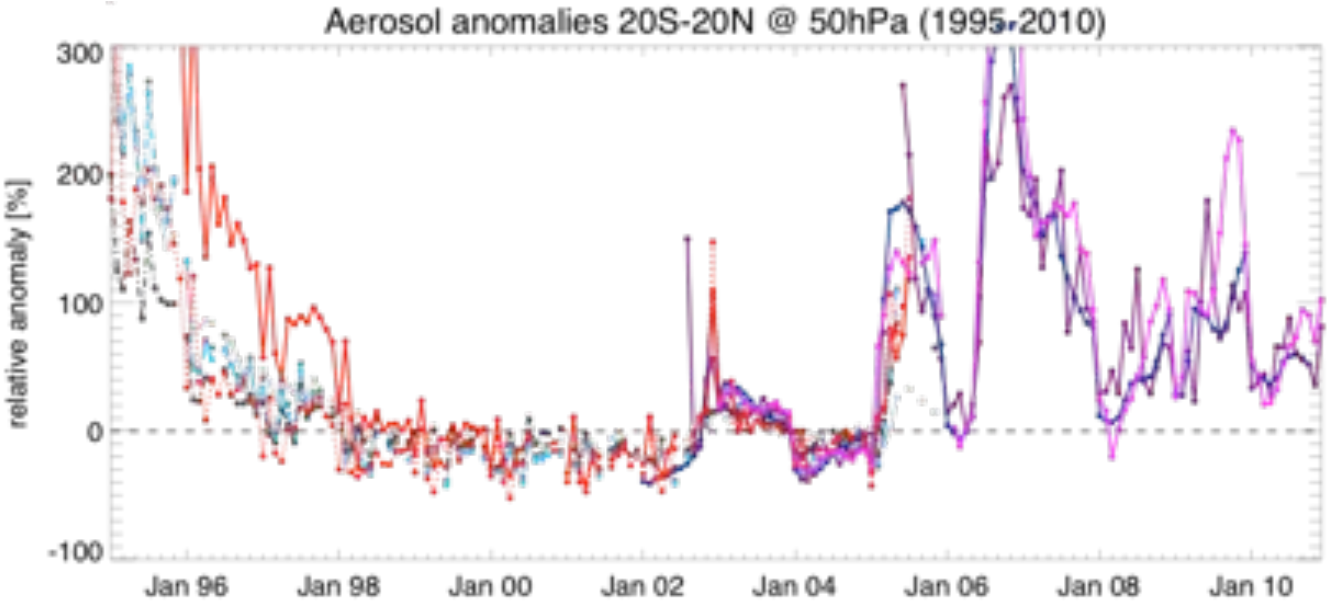
Aerosol time series between 1995 and 2010.

Aerosol anomalies are shown relative to 2003-2004 monthly means.

Relative anomalies compare well, with exception:

- SAGE II 1020 nm
- HALOE 5260 nm





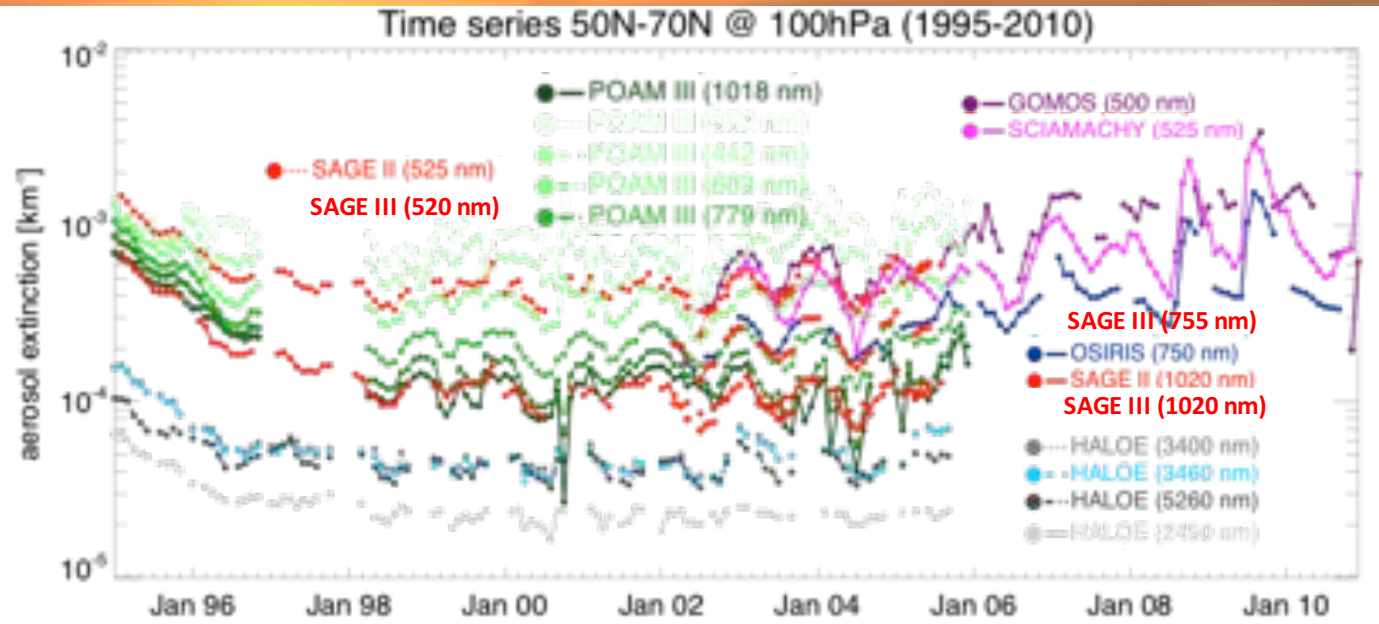
Aerosol anomaly evaluations

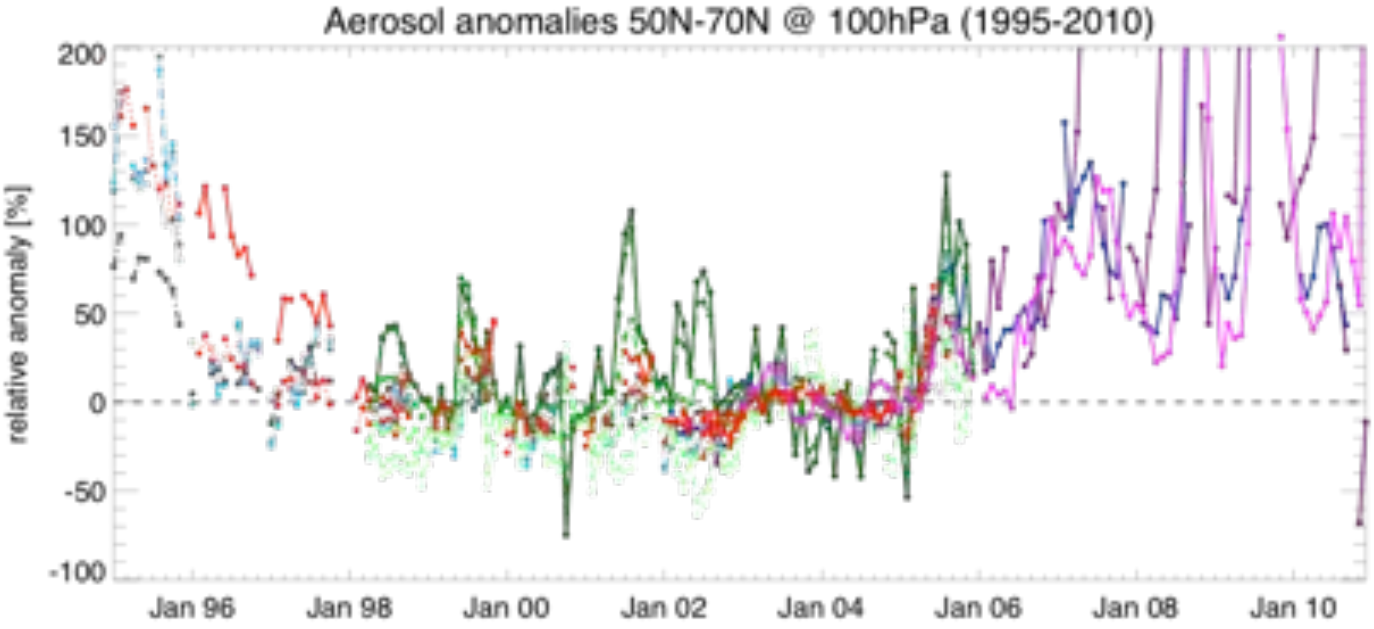
Aerosol time series between 1995 and 2010.

Aerosol anomalies are calculate using the 2003-2004 monthly means.

Extra-tropical lower stratosphere 'outliers':

- SAGE II 1020 nm
- POAM III 779 nm

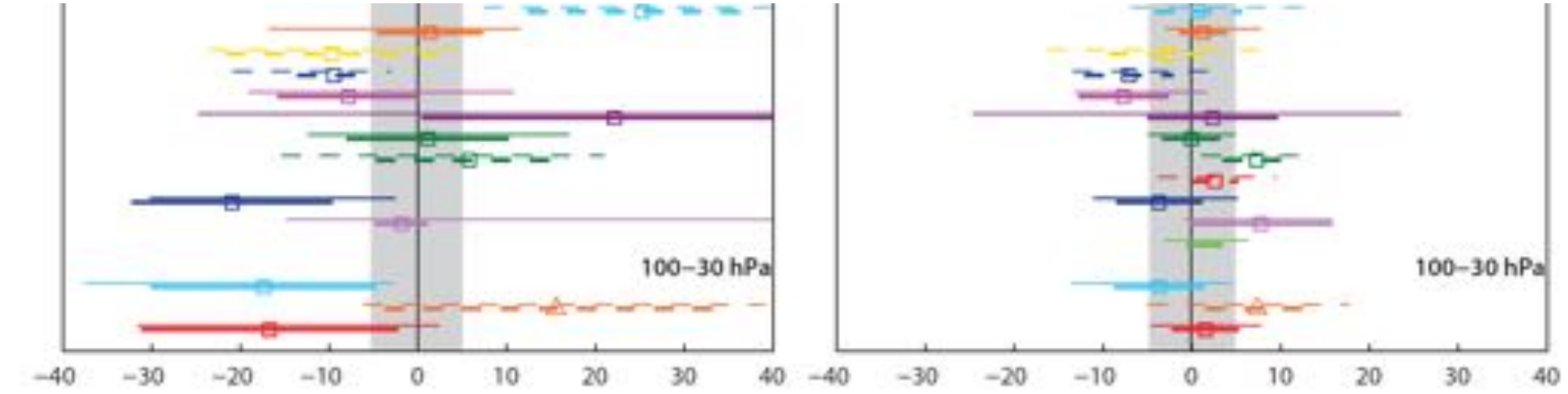
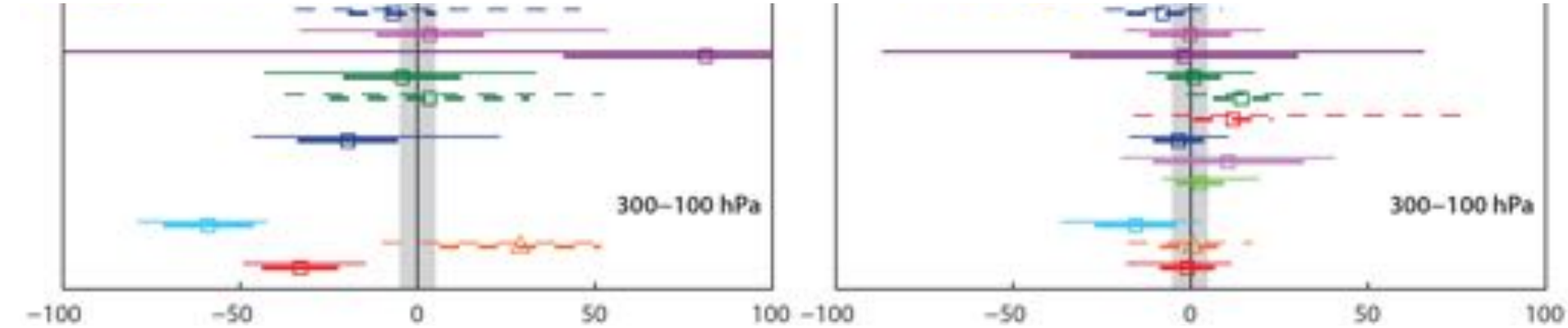




Ozone comparisons

Evaluation of 18 ozone profile data sets

Lower stratosphere (100-30 hPa) - Tropics: **±20%** and Mid-latitudes: **±10%**



Upper troposphere (300-100 hPa) - Tropics: ±20% to **±50%** and Mid-latitudes: mostly **±10%**