The Importance of Validation in establishing atmospheric ECVs

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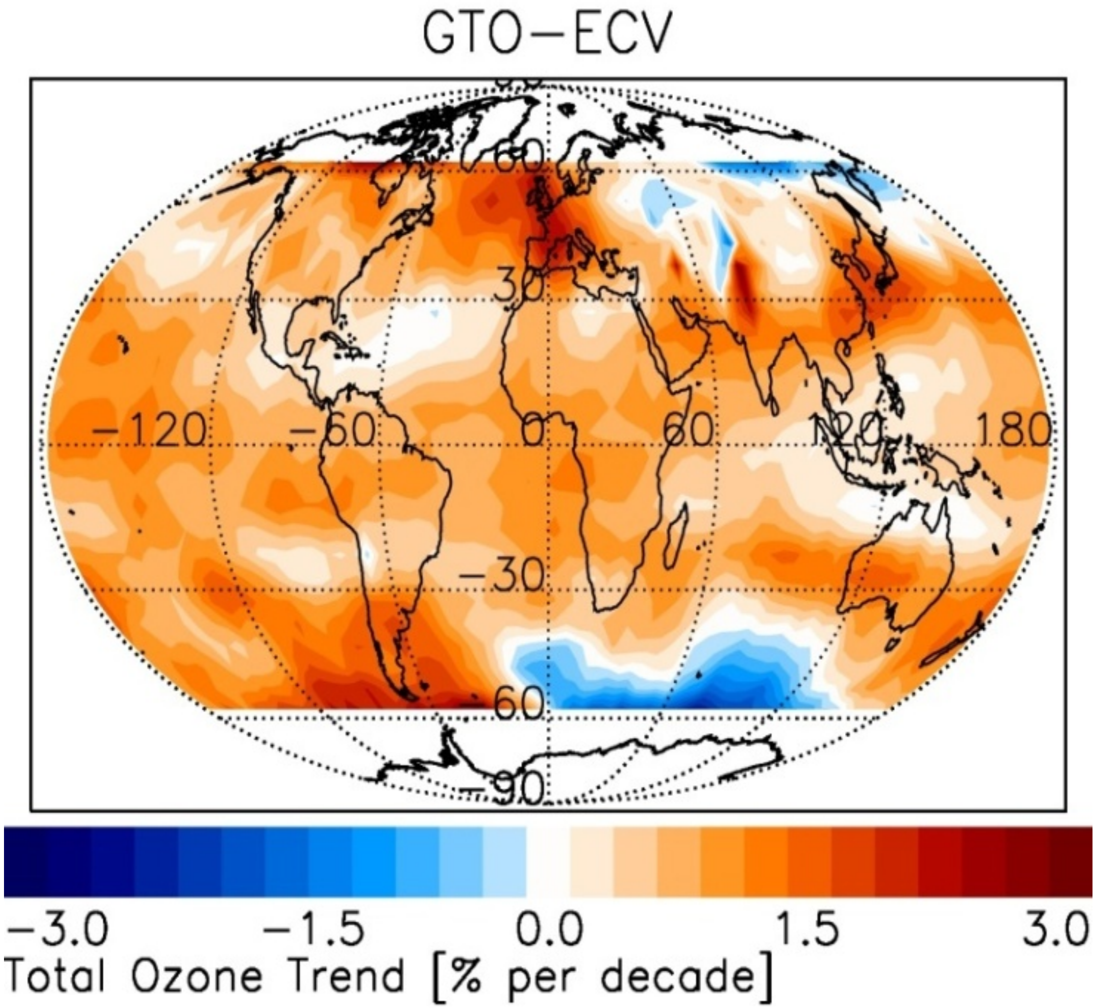

03/1996 – 06/2011

OVERVIEW

- ESA Climate Change Initiative Programme/Ozone
- User Requirements/Users
- Validation – Uncertainty Characterisation
- Observations confronted with Chemistry-Climate Models
- Algorithm Selection (Round Robin) via Data Assimilation
- Fitness for Purpose?
- Lessons Learned

Objectives of the CCI

Realise the full potential of the long-term global EO archives that ESA, together with its Member states, has established over the last thirty years …

… as a significant and timely contribution to the Essential Climate Variables (ECV) databases required by the United Nations Framework Convention on Climate Change.

START: 2010 with a 6 years duration, budget of about 90 Meuro, 2 project phases each of 3 years

13 ECV Projects, 1 Project on ECV Assessment by Climate Modellers (CMUG)

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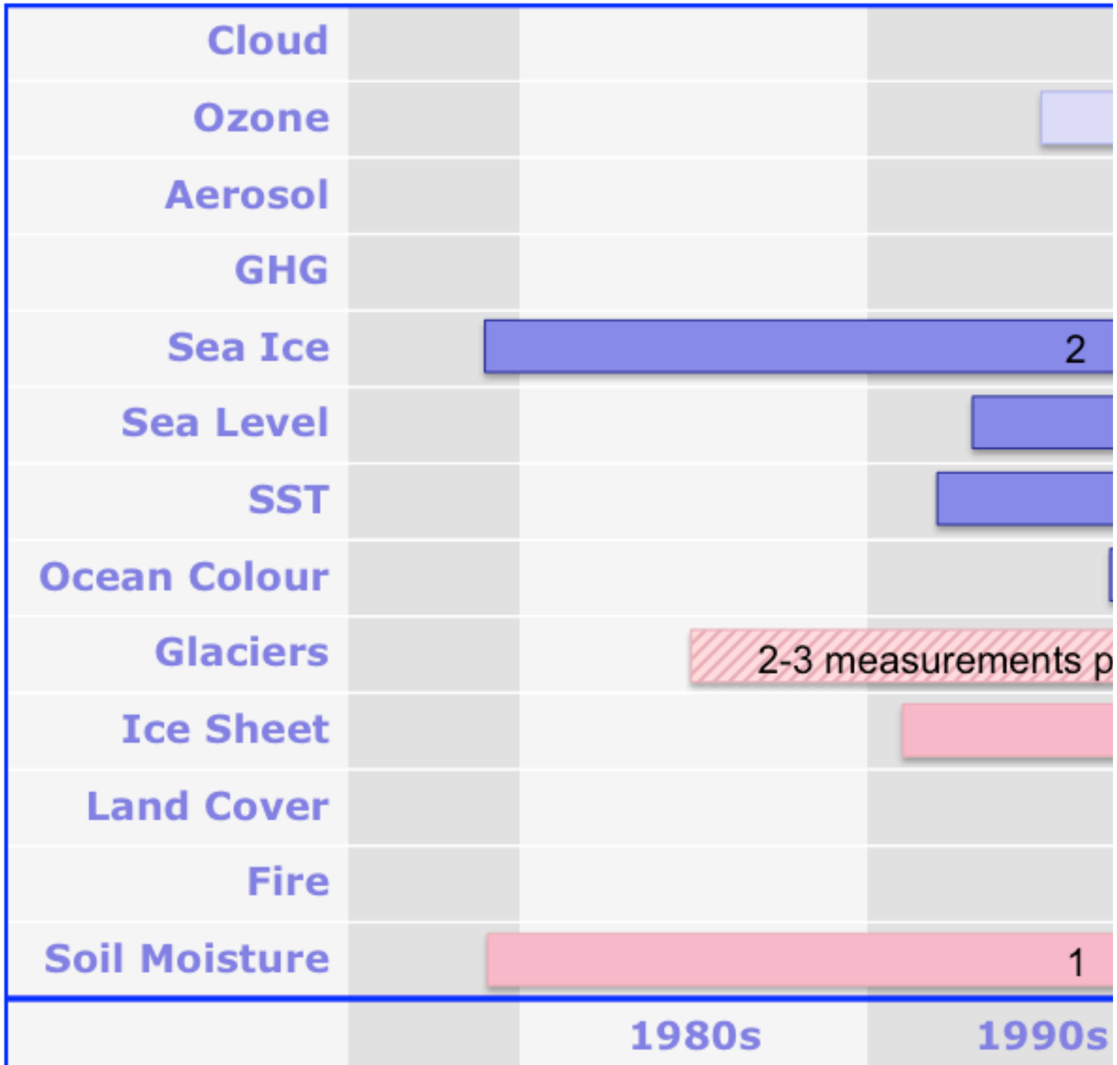
CCI Products Time Coverage

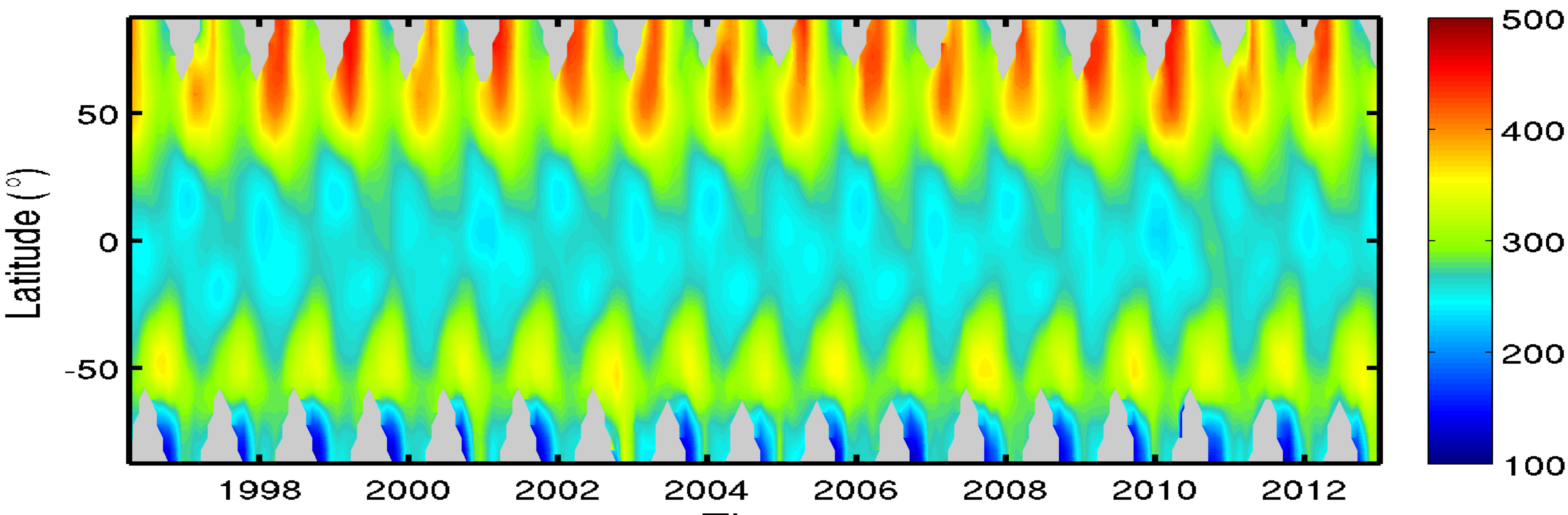


Objectives of the CCI

- Starting from GCOS Requirements for satellite ECVs
- Key European Experts involved (including climate modellers)
- Algorithm Selection (Round Robin exercise)
- Validation/Uncertainty characterisation
- Long Term Data Generation (easy access)
- ECV Evaluation by Climate Modellers
- Ozone: http://www.esa-ozone-cci.org - logos: institutions involved in O3_cci - lead by BIRA/IASB

Phase 1: Total Ozone

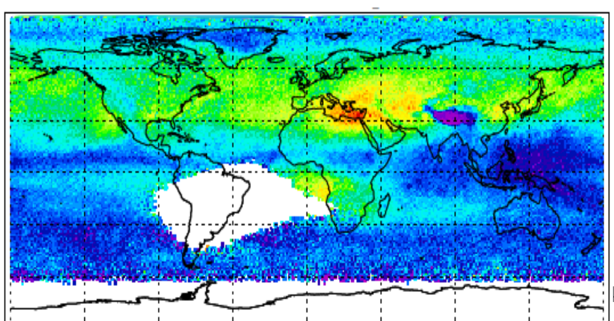
Total ozone		
Level-2	Full reprocessing using GODFIT multi-sensor prototype algorithm	GOME (1996-2011) SCIAMACHY (2002-2012) GOME-2 (2007-2012)
Level-3	Monthly-averaged data set, residual inter-sensor bias corrected using GOME as a reference	GOME, SCIAMACHY, GOME-2 (1996-2011)



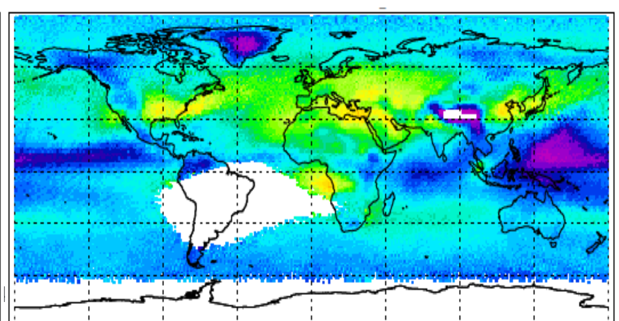
Phase 1: Nadir Ozone Profiles

Nadir Ozone Profiles		
Level-2	Demonstration CCI algorithm, with profiles on fixed pressure levels common to limb products – RAL algorithm selected (best performance in troposphere)	GOME (1997) GOME-2 (2007-2008)
Level-3	Monthly mean gridded data	GOME (1997) GOME-2 (2007-2008)
Level-4	Assimilated ozone profiles on 6 hourly global fields	GOME (1997) GOME-2 (2007-2008)

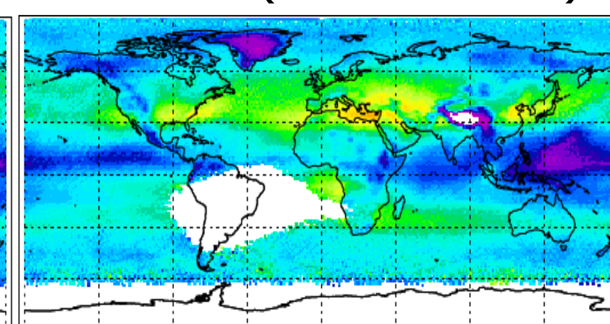
GOME2



TOMCAT

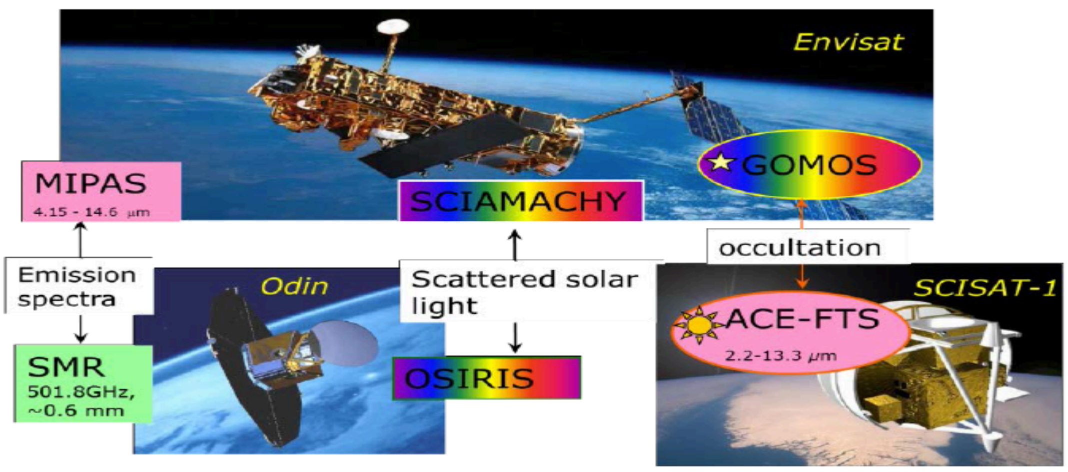


TOMCAT (GOME2 AKs)



Phase1: Limb Ozone Profiles

Limb Ozone Profiles		
Level-2	Harmonized Single Instrument (HARMOZ): individual profiles with a common pressure grid and concentration unit, MIPAS Round Robin: selection of KIT algorithm	SCIAMACHY, GOMOS, MIPAS, OSIRIS, SMR, ACE (all lifetime)
Level-3	Single Instrument Monthly Mean Zonal Mean (MZM) – 10º latitude bin	SCIAMACHY, GOMOS, MIPAS, OSIRIS, SMR, ACE (all lifetime)
	Merged Mean (MMZM) – including monthly zonal mean and bi-weekly mean (20º long. 10º lat.)	SCIAMACHY, GOMOS, MIPAS, OSIRIS, SMR, ACE (2007-2008 demonstration),



GCOS Requirements for Ozone

Target Requirements					
Variable/ Parameter	**Horizontal Resolution**	**Vertical Resolution**	**Temporal Resolution**	**Accuracy**	**Stability**
Ozone profile in upper stratosphere and mesosphere	100-200km	3km	daily	5-20%	<1%
Ozone profile in upper troposphere and lower stratosphere	100-200km	1-2km	4h	10%	1%
Total ozone	20-50km	N/A	4h	Max (2%; 5 DU)	<1%
Tropospheric ozone	20-50km	5km	4h	10-15%	1%

Terminology

Accuracy: concept – closeness of agreement between a quantity value obtained by measurements and the true value of the measurand - word not really used anymore within CCI projects

Uncertainty Characterisation: systematic and random components

Users

Network of Remote Sensing Ground-Based Observations for the GMES Atmospheric Service

Climate Research Group: Users of **Chemistry-Climate Models** (CCMs) with particular focus on long-term numerical simulations using CCMs for the detailed investigation of model feedbacks between ozone chemistry, ozone depleting substance (ODS) trends, and climate.

- P. Dameris (DLR)
- P. Braesicke (KIT)
- M. van Weele (KNMI)

Climate Modelling User Group: CMUG is a consortium comprising the Met Office Hadley Centre, the Max Planck Institute for Meteorology, ECMWF and Météo-France who confronts models with observations with the following aims:

1. To interpret the observations and explain the causes of observed variability and change;
2. To develop, constrain and validate climate models, thus gaining confidence in projections of future change;
3. To initialise models for seasonal and decadal timescale predictability.

- R. Dragani (ECMWF)

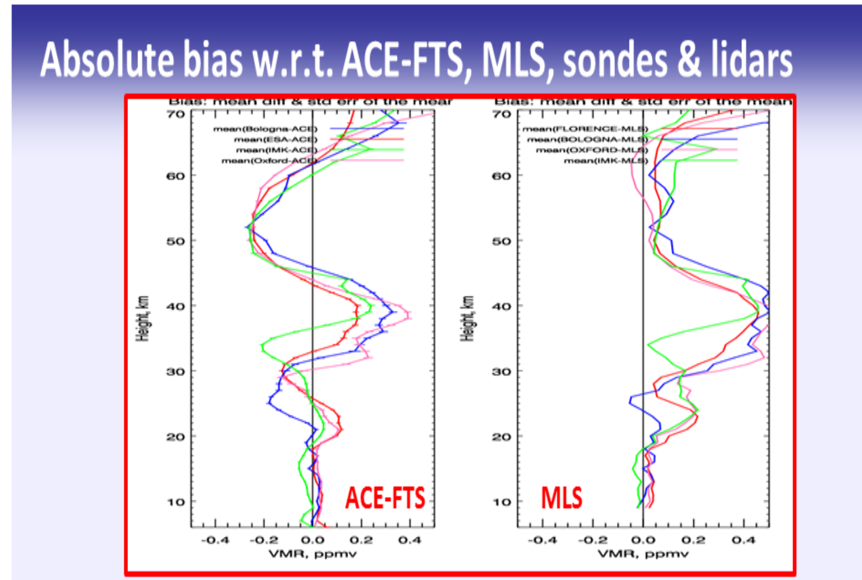
MIPAS Round Robin

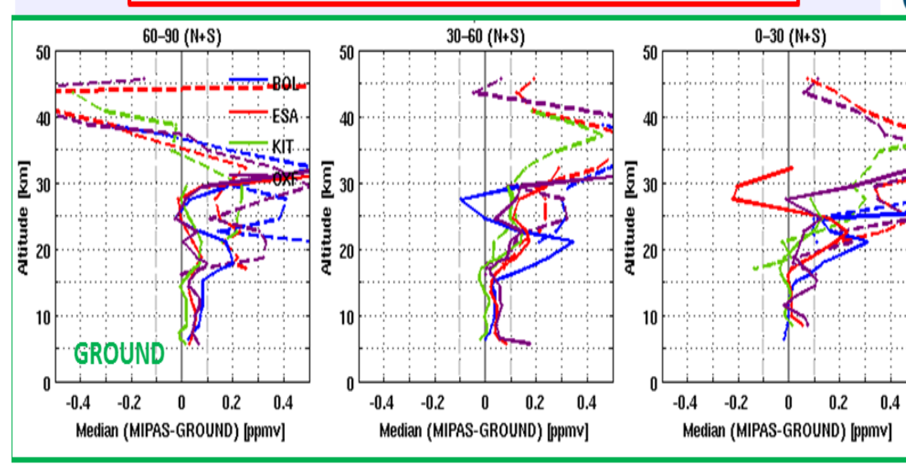
Selection from four MIPAS algorithms: Bologna, Firenze (ESA prototype), KIT-IMK, and Oxford

In the troposphere clear biases are found in all four products. The lowest bias at these Altitudes is observed for the KIT product

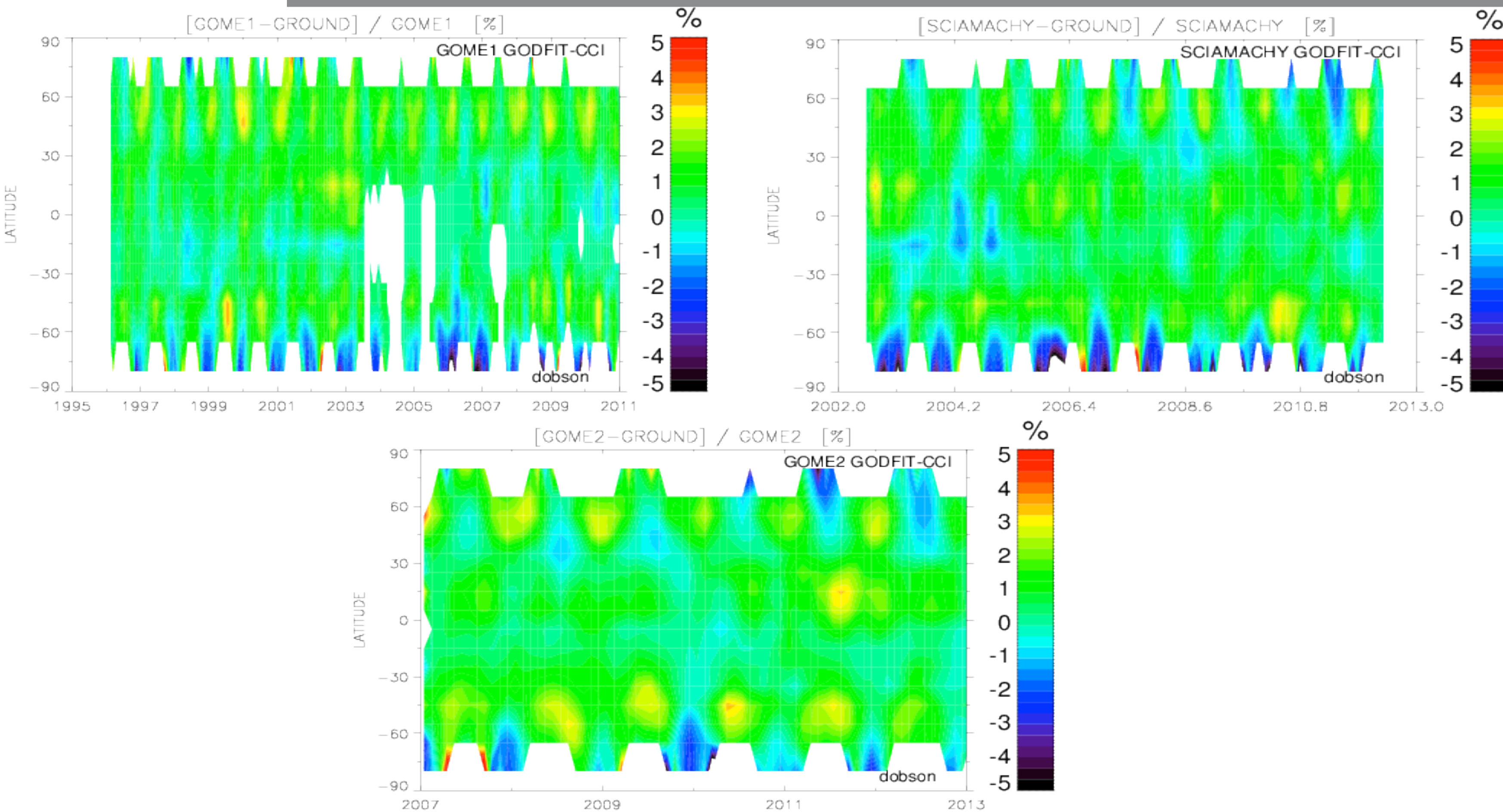
In the stratosphere, all four products are positively biased, by 2-5%. KIT only above 35 km.

The profile–to-profile spread of the KIT profiles is smallest and KIT has the largest fraction of valid profiles passing the applicable filter criteria.



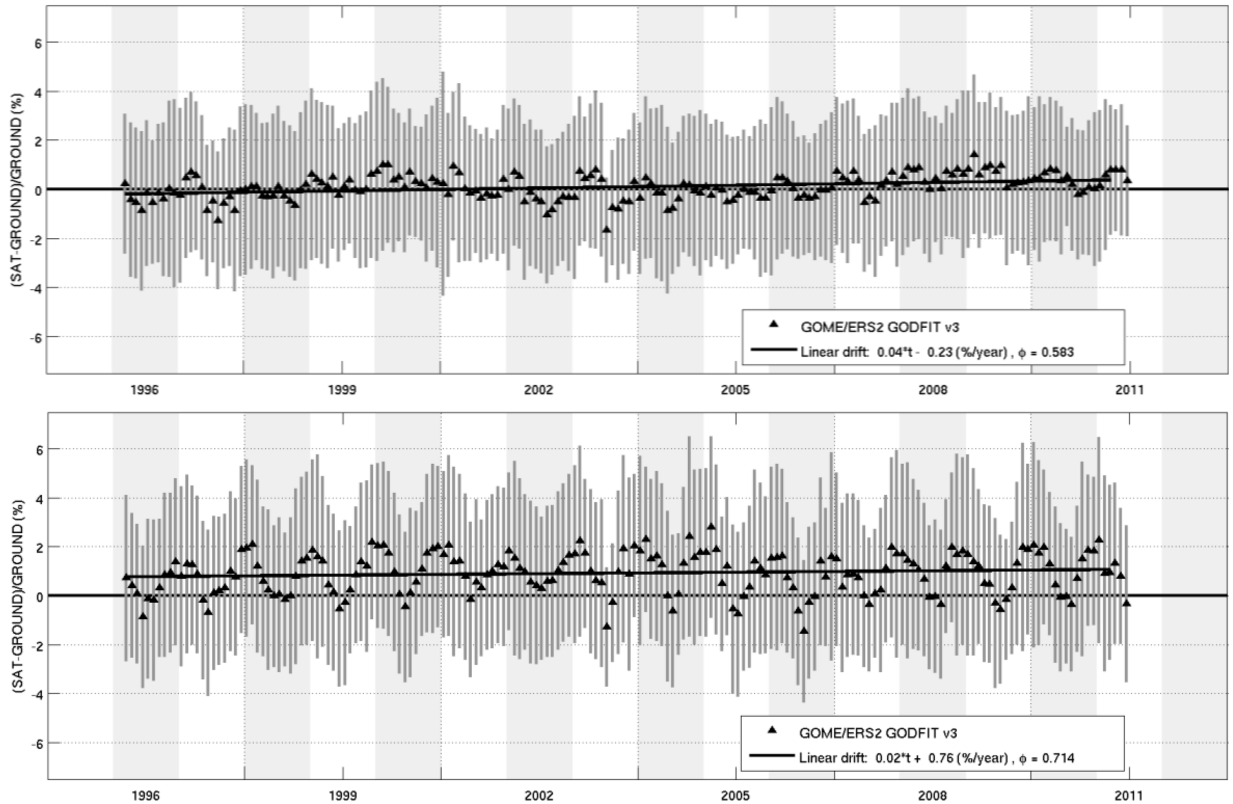


GODFITV3 – stability wrt. GB network



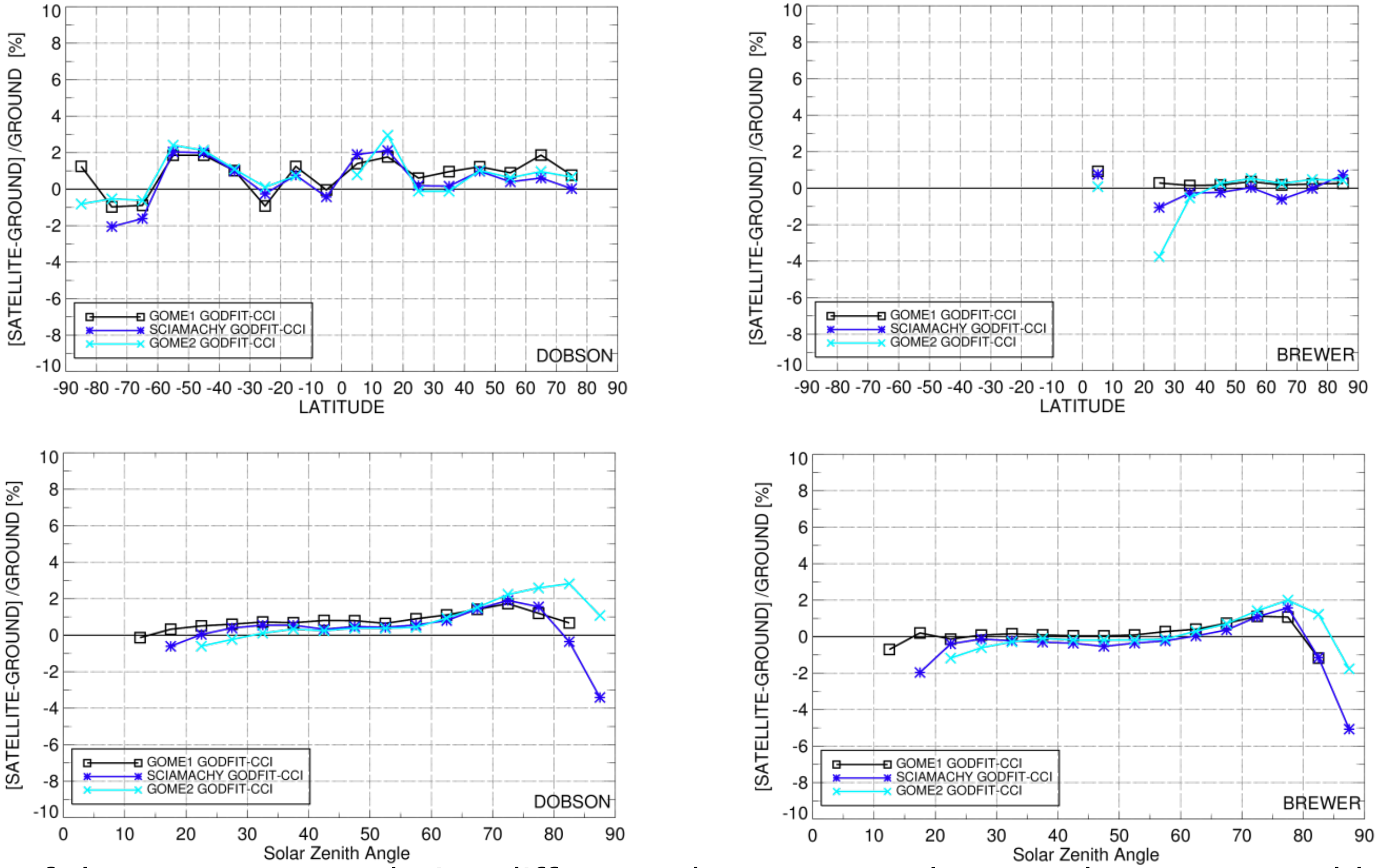
Latitude-time evolution of the percent relative difference between GOME [upper left], SCIAMACHY [upper right] and GOME-2 [lower] satellite total ozone data and Dobson network measurements. The mean difference falls around the 0-1% levels, with some peaks around ±2% for the high latitudes.

GODFITV3 – GOME stability wrt. GB network (used as 'anker' for merging)



Long-term drift of the percentage relative difference between total ozone data measured by ERS-2 GOME (GODFIT v3) and by the Northern Hemisphere Brewer network (top) and the Northern Hemisphere Dobson network (bottom)

TOC Validation: Latitudinal and SZA dependencies



Variation of the percentage relative difference between total ozone data measured by the three satellites and by ground-based networks [Dobson on the left, Brewer on the right], as a function of latitude [upper row] and the solar zenith angle of the satellite measurement [lower row].

TOC – Fitness for Purpose?

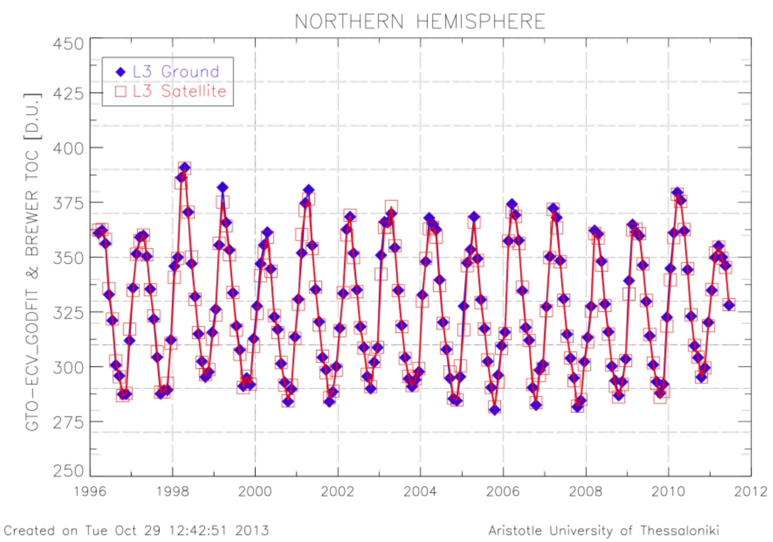
Compliance of MetOp-A GOME-2 GODFIT v3 total ozone data with user requirements (URD v2.1).

Topic	Requirement	Compliance / evaluation
Horizontal resolution	< 20-100 km	40 km along track x 80 km across track
Observation frequency	< 3 days	1.5 days at equator, 1 day at polar latitudes
Time period	(1980-2010) – (2003-2010)	01/2007 – 12/2012
Total uncertainty	2% (radiative forcing studies)	-0.5% to +2% up to 75° SZA
	3% (variability studies)	
Dependences	–	SZA: ±2% beyond 75° SZA
		Latitude: negligible vs. Brewers
		Clouds: -1% over cloudy skies
		Effective temperature: ±1%
Stability	1 – 3 % / decade	+0.4 to -0.8% / decade

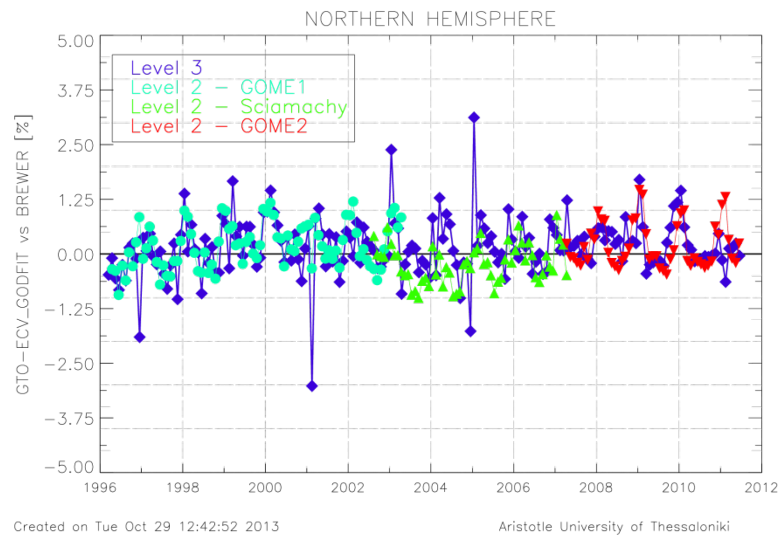
Compliance of MetOp-A GOME-2 GODFIT v3 total ozone data with user requirements

Comparisons with the Brewer network
NH time series

Time series of the level 2 & level 3 TOCs



Time series of the level 2 & level 3 differences



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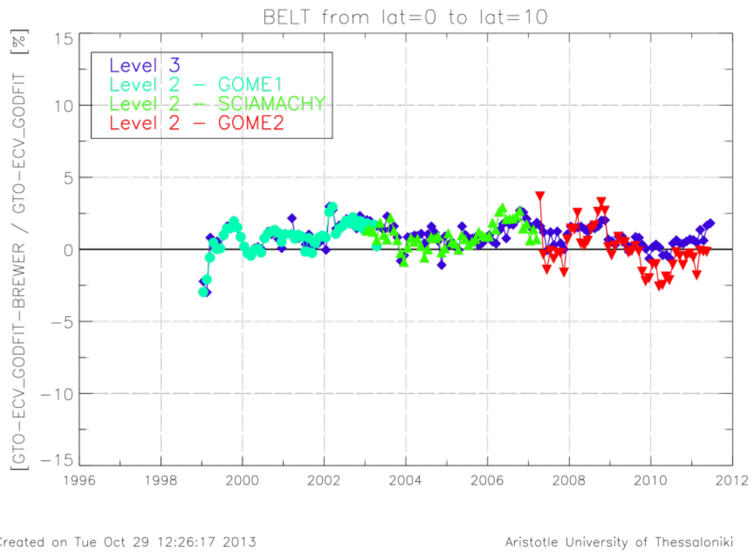
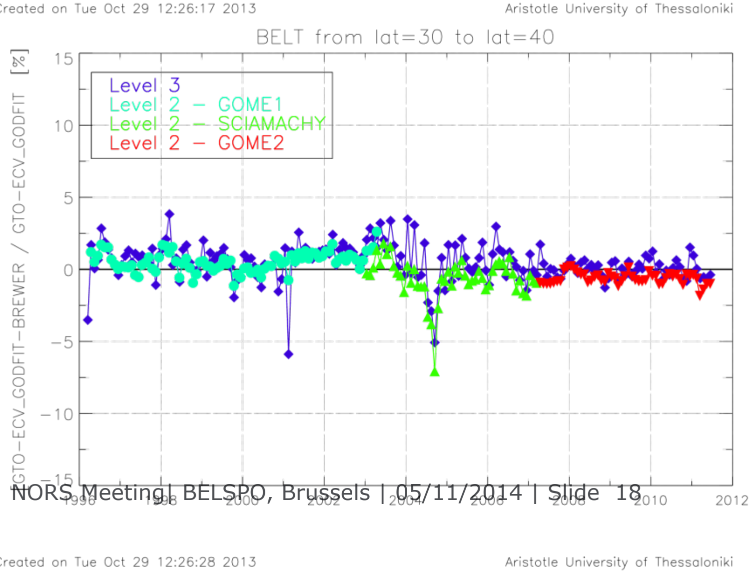
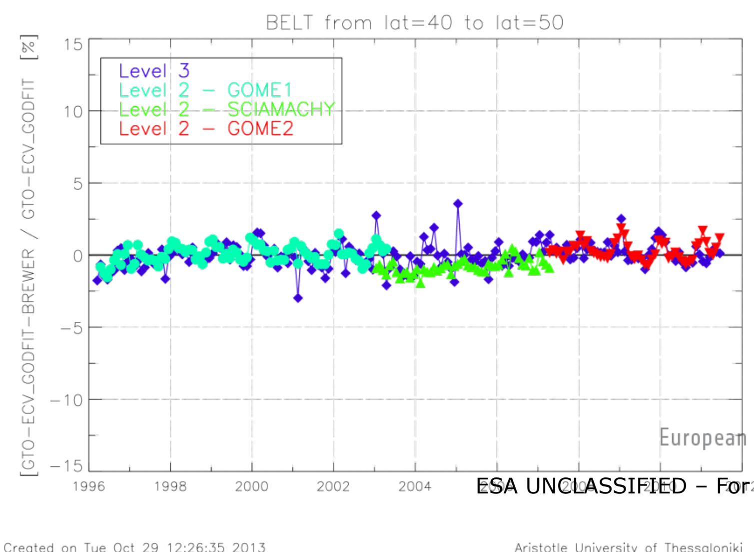
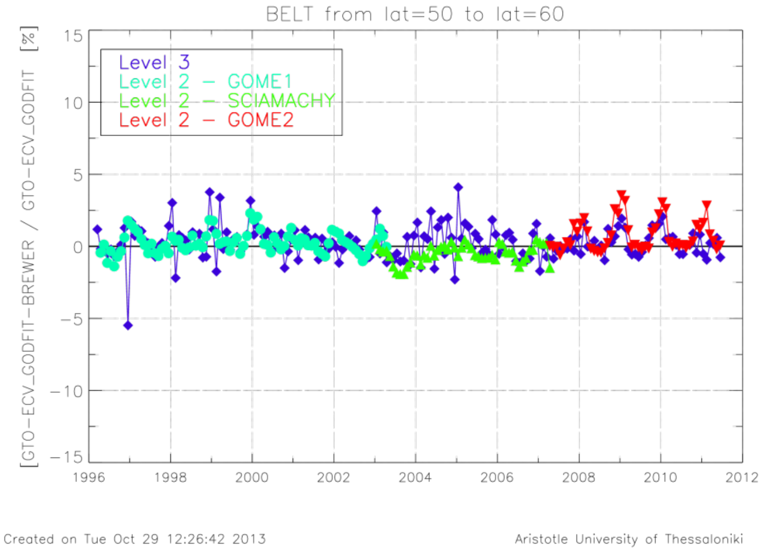
NH Belt Statistics
Tropics & Middle Latitudes

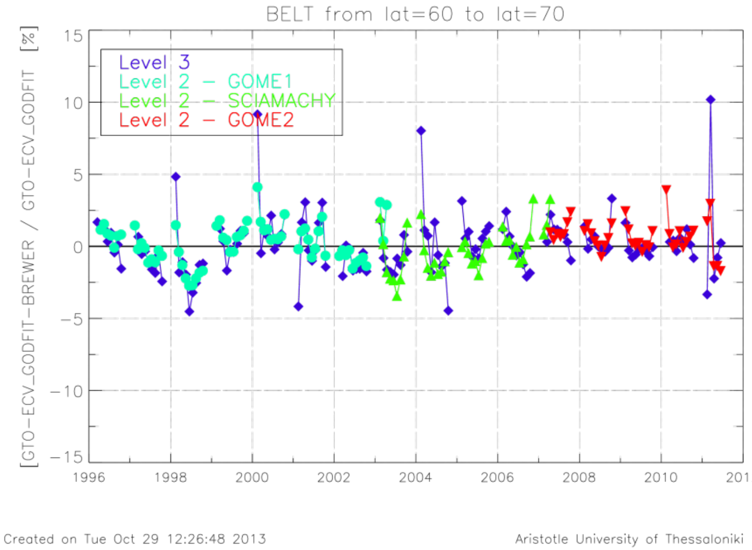


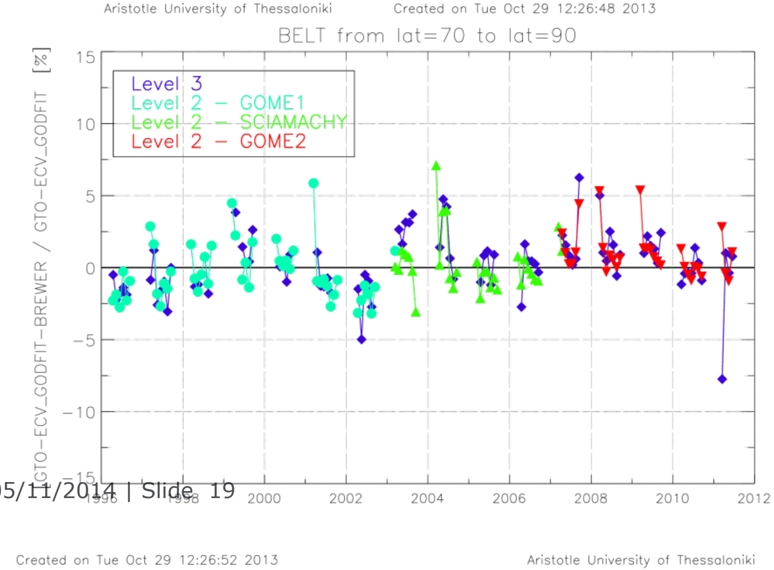




NH Belt Statistics
Middle and High Latitudes







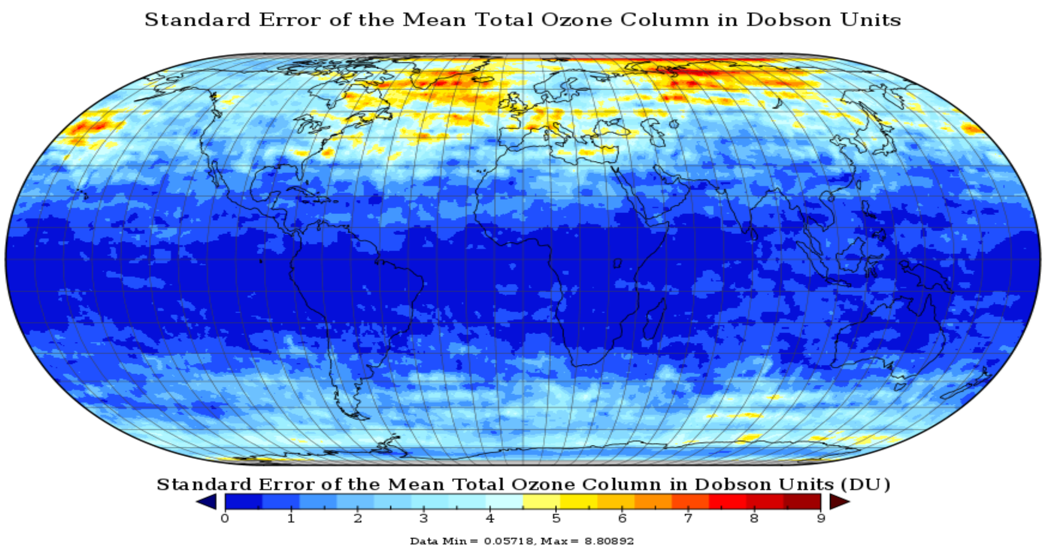
TOC - Validation Results

	GOME GODFIT v3	SCIA GODFIT v3	GOME-2A GODFIT v3	TC_L3_MRG
NH drift [/ decade]	B: 0.4% D: 0.2%	B: 0.3% D: -0.8%	B: -0.8% D: 0.4%	B: 0.0% (ML) D: 0.0% (ML)
Mean bias	+0.1%	-0.2%	-1%	B: 0 %
Seasonality	<1.5%	<1%	<1%	<1.5% (D)
Scatter	±2/2.5%	±2/2.5%	±2/2.5%	±3-4%
Latitude	Reflects rather station-to-station inhomogeneities			
SZA	-1% SZA>80°	-1% SZA>80°	-1% SZA>84°	NA
Clouds	-1% if cloudy	-1% if cloudy	-1% if cloudy	NA
Teff	Flat	Flat	Flat	NA

TOC - Validation Results

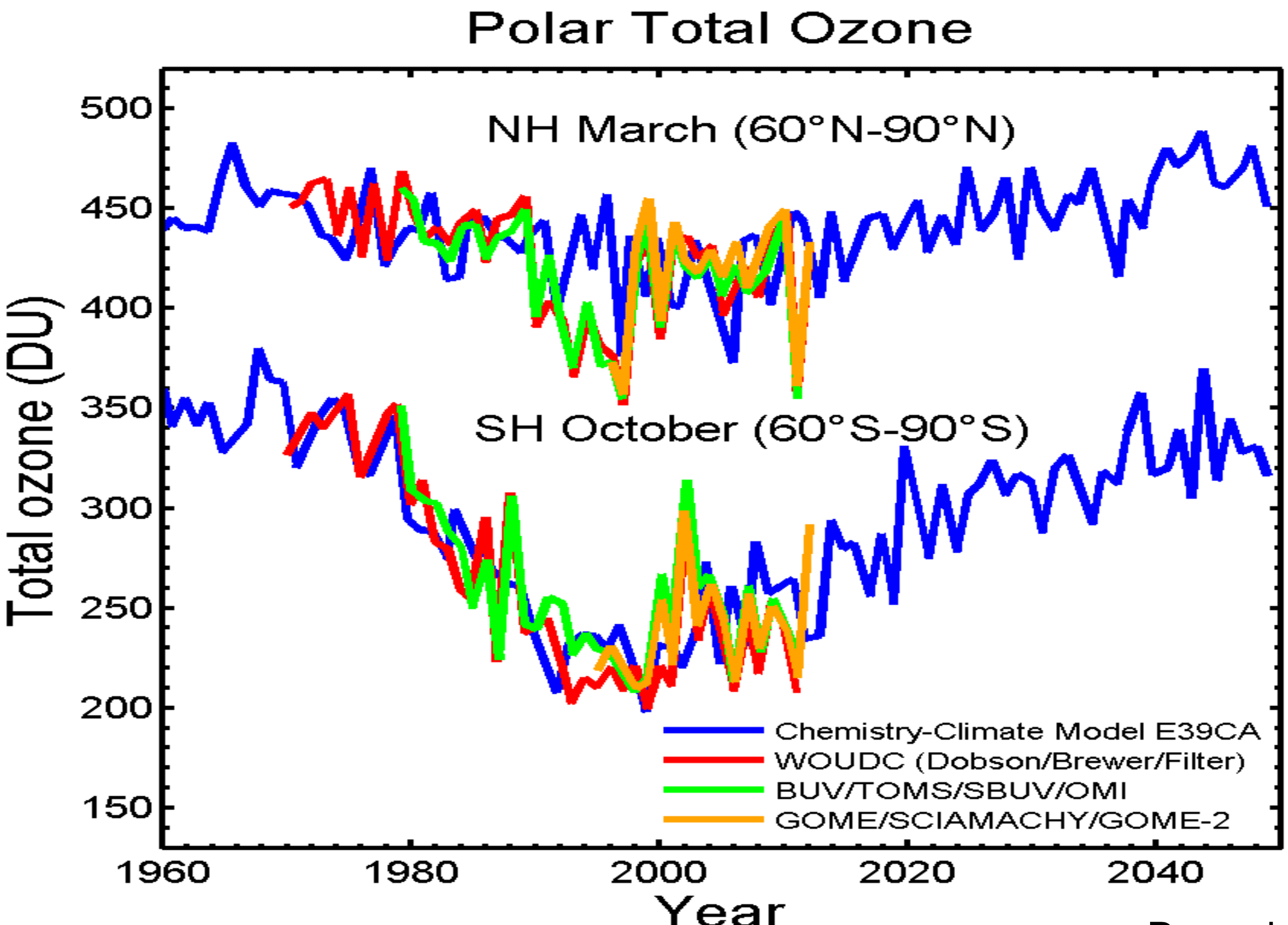
Sampling errors are the dominating error source for the total ozone L3 ECV (>5% at high latitudes)

To be resolved during next CCI-phase by Spatio-temporal statistical tools to reduce sampling errors (Kriging, RBF,...)



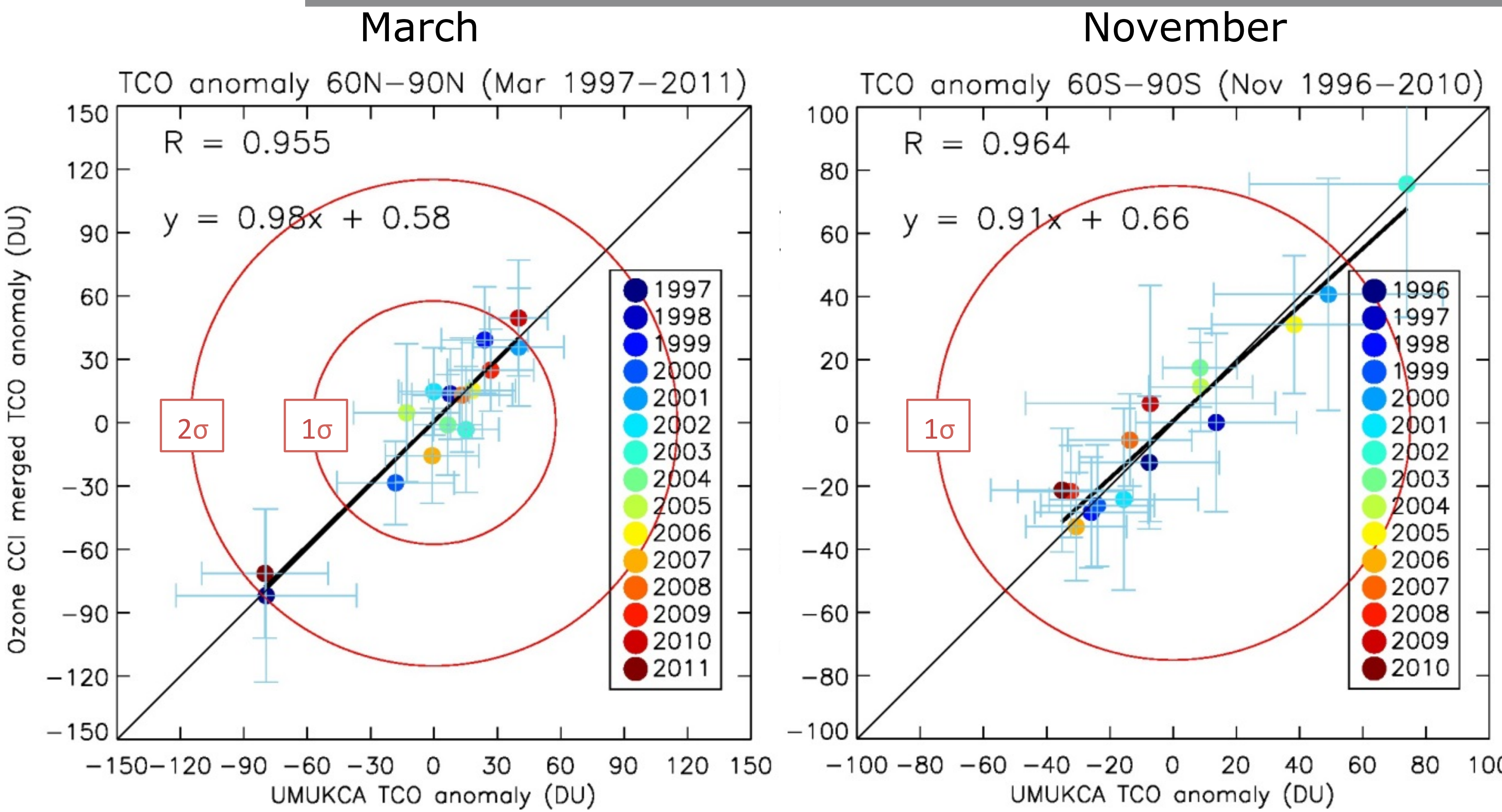
ECV Assessment/ Evaluation

"free running" atmospheric models (CCMs)



Dameris and Loyola, 2011

Ozone Anomalies Scatter Plots



ECV Evaluation/Assessment

The biases (model/observations) do not necessarily “kill“:

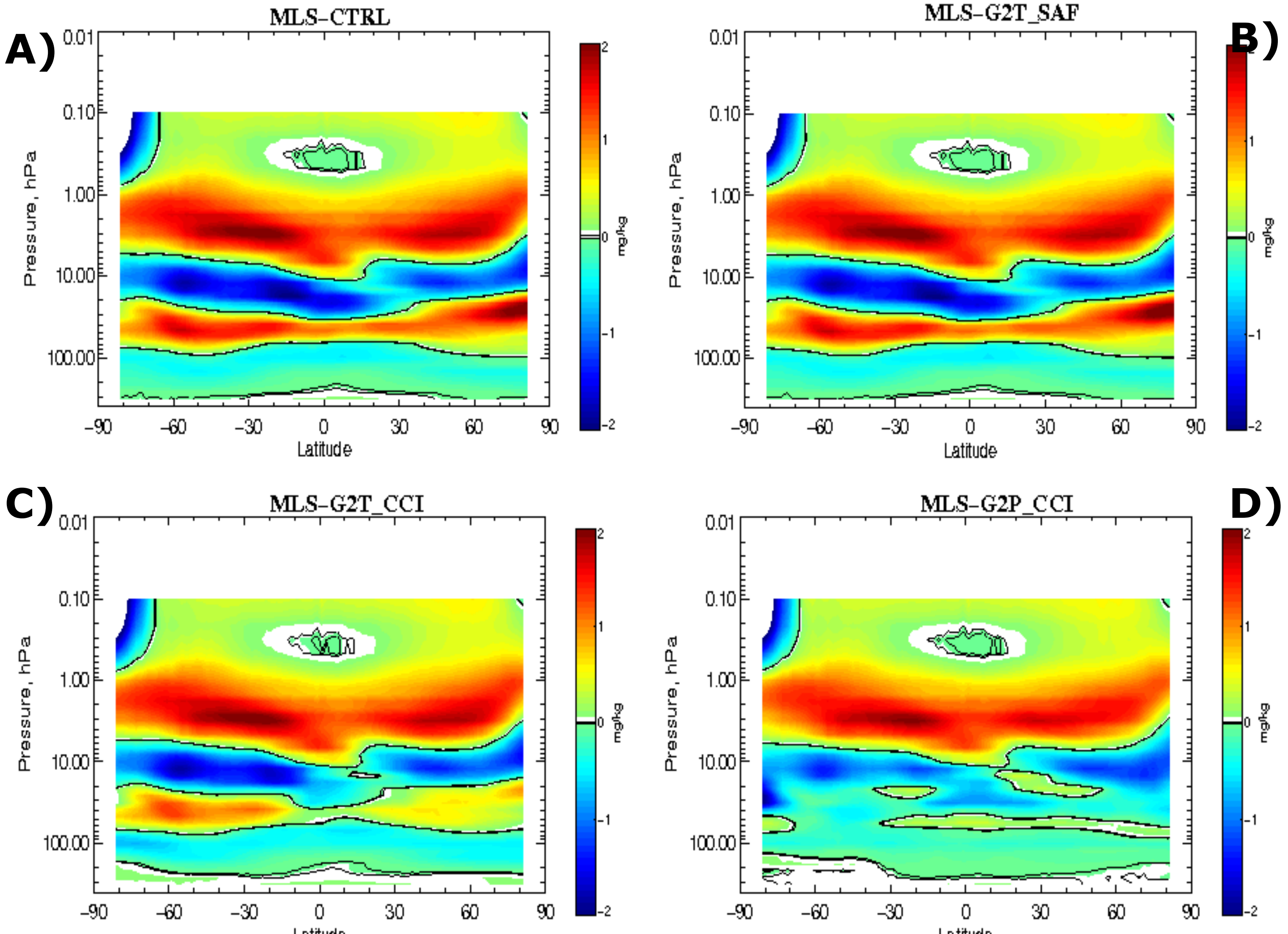
- Spring ozone anomalies for cold years in the NH can be modelled.
- Spring ozone anomalies for the SH vortex split in 2002 are captured.

Interannual ozone variability:

- The chemistry is doing well, when the meteorological biases are small.
- Variability in the free running model is realistic with a small overestimate in the SH (underlying dynamical model).

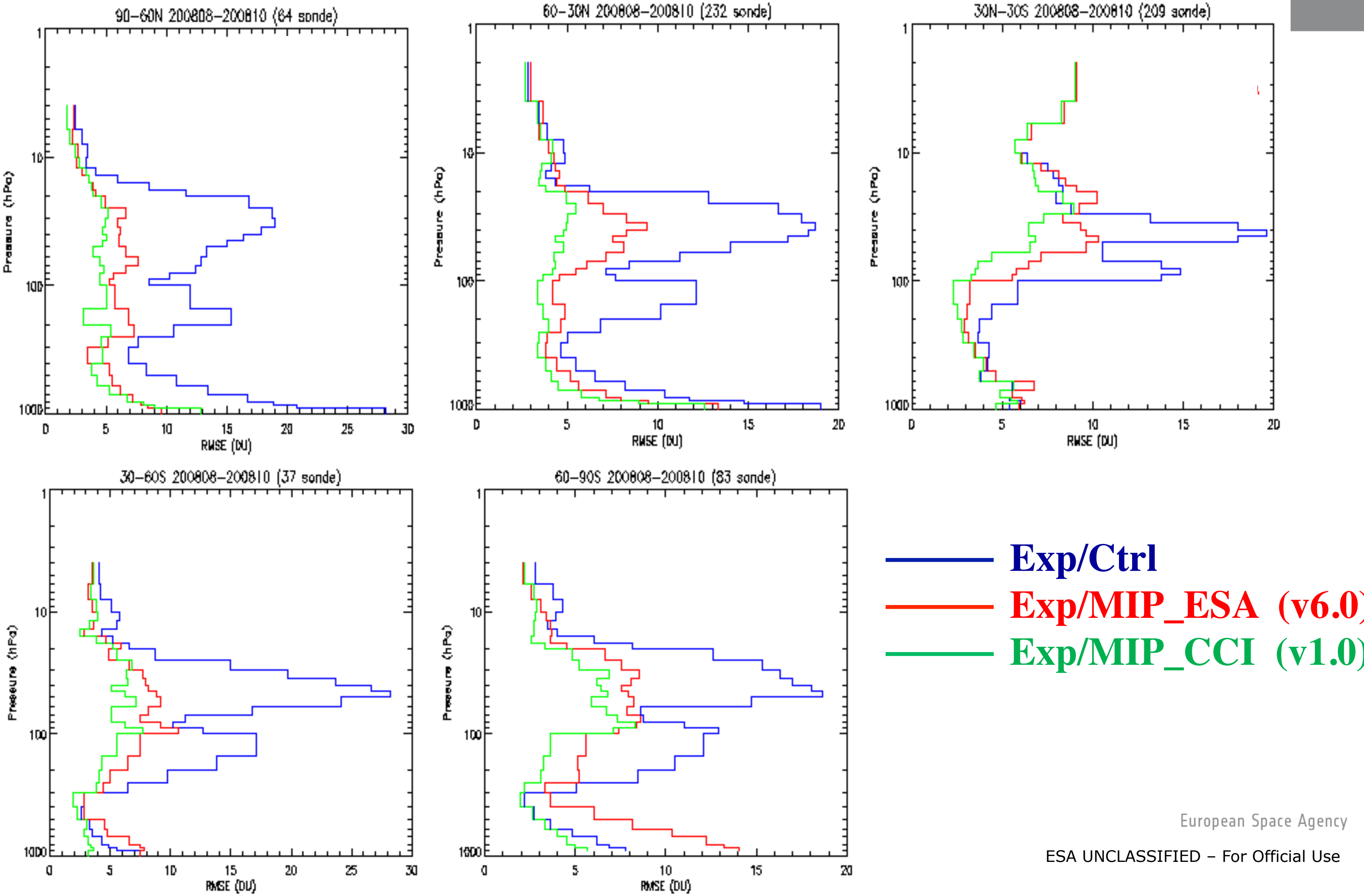
New data provides excellent benchmark for model performance (including standard deviations)!

GOME-2 O_3 to be used for Reanalysis at ECMWF



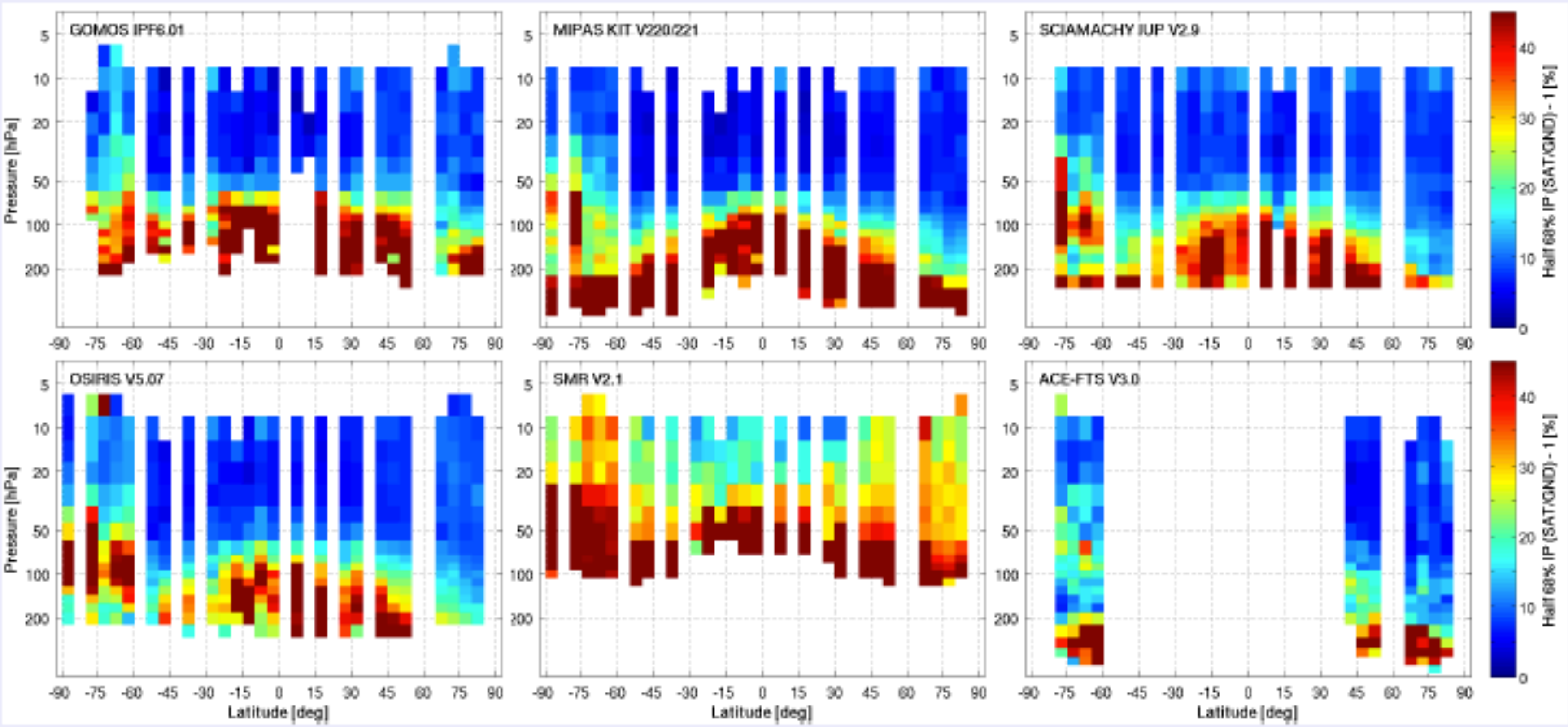
Zonal Mean Temporal Mean (MLS-Analyses): Aug – Oct

MIPAS Algorithm Selection for Reanalysis at ECMWF

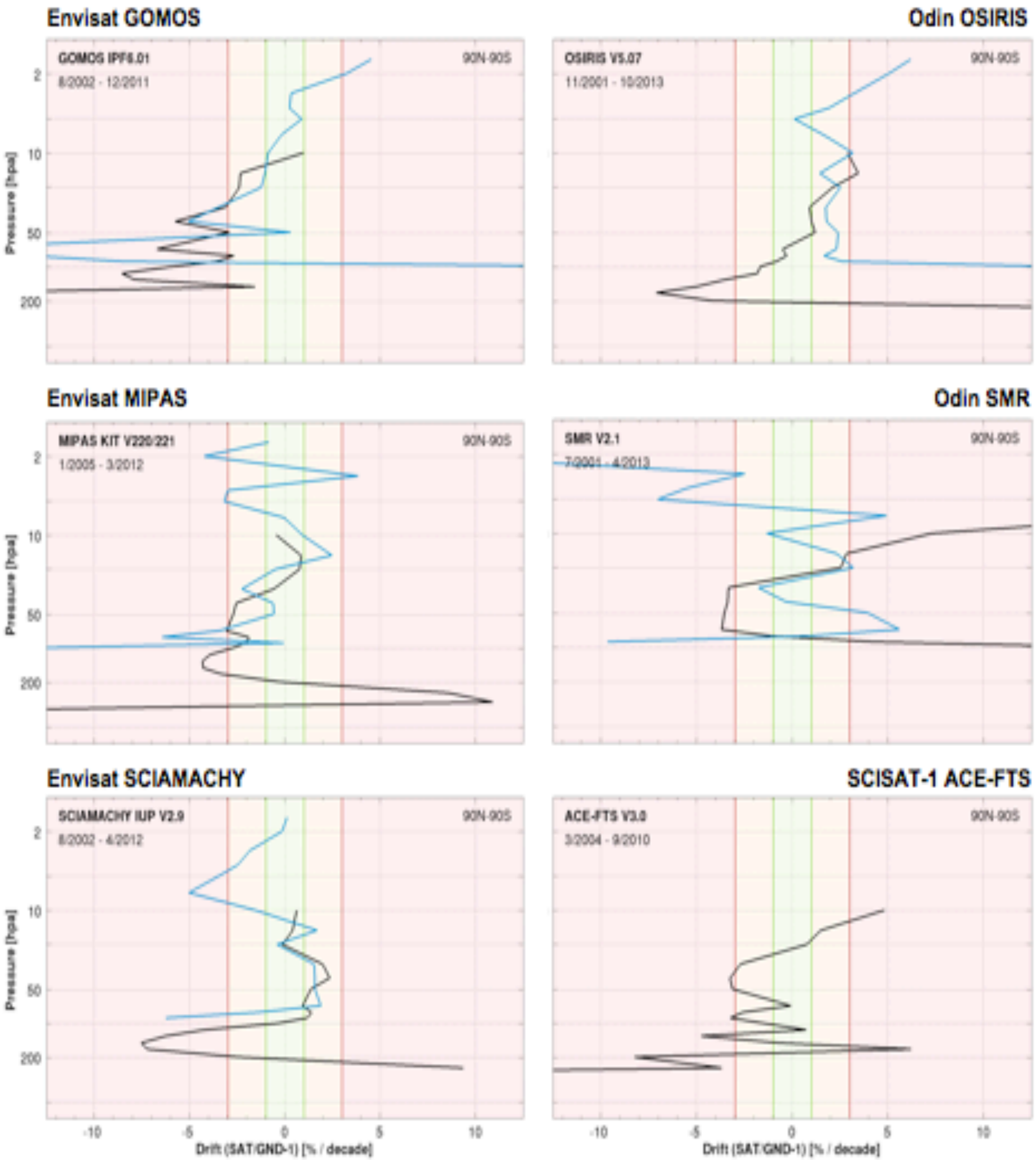


Comparison spread: meridian structure

- Typical distinction UTLS and middle atmosphere, increase in variability during Antarctic O3 hole conditions
- Comparison spread above 50hPa similar for most instruments: 5-10%
- Except SMR: 20-30%, due to (much) lower single profile precision



Drifts



Decadal stability (in %/decade) of CCI limb ozone profile data as a function of altitude (pressure), and its compliance with stringent (green) and looser (yellow) user requirements.

Decadal stability is estimated as the drift between satellite data and reference measurements (GAW/NDACC/SHADOZ ozonesonde (black) and NDACC lidar (blue) network data)

SCIAMACHY Limb Profiles: Fitness for Purpose?

Compliance of SCIAMACHY IUP v2.9 with user requirements

	Requirement	Compliance / evaluation
Horizontal resolution	< 100–300 km	300–400 km
Vertical resolution	< 1–3 km	4–5 km
Observation frequency	< 3 days	6 days
Time period	(1980-2010) – (2003-2010)	08/2002 – 04/2012
Total uncertainty in height attribution	< ± 500 m	± 200 m
Dependences	–	latitude, altitude

		UT / LS*	Lower stratosphere			Middle atmosphere		
Layer	**[hPa]** **[km]**	>200 <11	100-200 11-16	50-100 16-21	20-50 21-27	10-20 27-32	5-10 32-37	2-5 37-44
Uncertainty including systematic and random component								
Requirement				< 8-15%			< 8-15%	
• Arctic								
• Mid N								
• Tropics								
• Mid S								
• Antarctic				O3 hole				
Uncertainty including random component								
Requirement				< 8-15%			< 8-15%	
• Arctic								
• Mid N								
• Tropics								
• Mid S								
• Antarctic				O3 hole				
Stability								
Requirement				< 1-3% / decade			< 1-3% / decade	
• Ground network								

* The URD does not give requirements specific for the UT / LS region.

CCI Ozone Phase-I Data Overview

freely available at: http://www.esa-ozone-cci.org/?q=node/160

Product identifier	Source/ Processing center	Time periods																
		96	97	98	99	00	01	02	03	04	05	06	07	08	09	10	11	12
Level-2 Data Sets																		
TC_L2_GOME	BIRA	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	
TC_L2_SCIA	BIRA							■	■	■	■	■	■	■	■	■	■	■
TC_L2_GOME2	BIRA												■	■	■	■	■	■
NP_L2_GOME	RAL		■															
NP_L2_GOME2	RAL												■	■				
LP_L2_SCIA	IUP-Bremen							■	■	■	■	■	■	■	■	■	■	■
LP_L2_MIPAS	KIT										■	■	■	■	■	■	■	■
LP_L2_GOMOS	ESA							■	■	■	■	■	■	■	■	■	■	■
LP_L2_OSIRIS	SASK						■	■	■	■	■	■	■	■	■	■	■	■
LP_L2_SMR	CHALMERS						■	■	■	■	■	■	■	■	■	■	■	■
LP_L2_ACE	UOFT									■	■	■	■	■	■	■	■	■
Level-3 Data Sets																		
TC_L3_MRG	DLR/BIRA	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	
NP_L3_MRG	RAL/KNMI		■										■	■				
LP_L3_SCIA	IUP-Bremen							■	■	■	■	■	■	■	■	■	■	■
LP_L3_MIPAS	KIT										■	■	■	■	■	■	■	■
LP_L3_GOMOS	FMI							■	■	■	■	■	■	■	■	■	■	■
LP_L3_OSIRIS	SASK						■	■	■	■	■	■	■	■	■	■	■	■
LP_L3_SMR	CHALMERS						■	■	■	■	■	■	■	■	■	■	■	■
LP_L3_ACE	UOFT									■	■	■	■	■	■	■	■	■
LP_L3_MRG-MZM	FMI												■	■				
LP_L3_MRG-MBW	FMI												■	■				
Level-4 Data Sets																		
NP_L4_MRG	KNMI		■										■	■				

Qualitative assessment of compliance w.r.t. requirements

1. General: GCOS requirements for ozone can only be *partially met* using current and near-future satellite instruments.

2. Reprocessed GOME, SCIAMACHY and GOME-2 total ozone data sets match GCOS requirements on *spatial resolution, accuracy and stability*. Requirements on time resolution cannot be met with current sensors, but likely for Europe with Sentinel-4. Additional requirements on length of data series are not fulfilled with European data sets, but will after merging with US data series.

3. Demonstration nadir profile data products (GOME, GOME-2) match requirements on *horizontal resolution, temporal resolution and accuracy in the stratosphere* (and they are close to match the same requirements in the troposphere). Vertical resolution requirements cannot be met with nadir sensors. Accuracy and temporal resolution requirements are not met in the UTLS region with UV sensors, however the addition of the IASI instrument in Phase-II will improve on this situation.

4. Limb and occultation instruments match all requirements in the *stratosphere*. In the UTLS, the requirements on vertical resolution, temporal resolution and accuracy are not met.

Lessons Learned on Validation

General:

Round-Robin (algorithm selection): Validation activities provide QA material but cannot decide, external decision is required for algorithm selection.

Validation tasks are definitely part of the development cycle…

Before public release, validation of a CRDP product is required, even if "representative" data already verified.

Good user requirements make good validation requirements.

Without an realistic uncertainty characterisation the products are useless (wrong trends, no impact in data assimilation etc.)

Provide Traceability (e.g. data content study, data selection criteria, documentation etc.)

Lessons Learned on Validation

Reference data:

Stringent user requirements ⇒ Need for dedicated selection of ground-based (and satellite) "reference" data

Need for improved handling of borderline data points with poor occurrence: largest and lowest sun elevation…

Data manipulations: Error propagation not straightforward

Nadir ozone column:

Climate data validation at 1%(/decade) level ⇒ Improved selection of ground-based network data required

Unequal/unstable quality of GB data in the Tropics

Complementarity of detailed/global studies, of reference measurements, of validation methods

Level-3 validation:

Representativeness of ozone monitoring networks not suitable for validation of L3 zonal means

Basic principle: show that L3 generation does not degrade L2 quality ⇒ L2-type validation of L3 & L3 data inspection

L3/L4: How to proceed further? Adopt evaluation techniques used for DA systems?

Additional Ozone_cci Phase-II Data Sets – light green

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esa

Data product	Processing entity	Time period																				
		96	97	98	99	00	01	02	03	04	05	06	07	08	09	10	11	12	13	14	15	16
Level-2 data sets																						
GOME TC	BIRA																					
SCIAMACHY TC	BIRA																					
GOME-2A TC	BIRA																					
GOME-2B TC	BIRA																					
OMI TC	BIRA																					
GOME NP	RAL																					
SCIAMACHY NP	RAL																					
GOME-2A NP	RAL																					
IASI NP	ULB																					
SCIAMACHY LP	UBR																					
MIPAS LP	KIT																					
GOMOS LP	ESA																					
OSIRIS LP	UoS																					
SMR LP	CHALMERS																					
ACE LP	UofT																					
Level-3 data sets																						
Merged TC	DLR																					
MRG NP	KNMI																					
GOME TTOC	DLR																					
Limb-nadir TC	UBR																					
Merged MZM LP	FMI																					
Merged MBW LP	FMI																					
Merged FRM LP	FMI																					
Level-4 data sets																						
Assimilated NP	KNMI																					