SCIAMACHY
QWG-3
Final Meeting

SGP 7.00 Validation Results Summary

A. Keppens, D. Hubert, J. Granville, F. Hendrick, and J.-C. Lambert

esa UNIVERSITÄT BREMEN iup SCIAMACHY

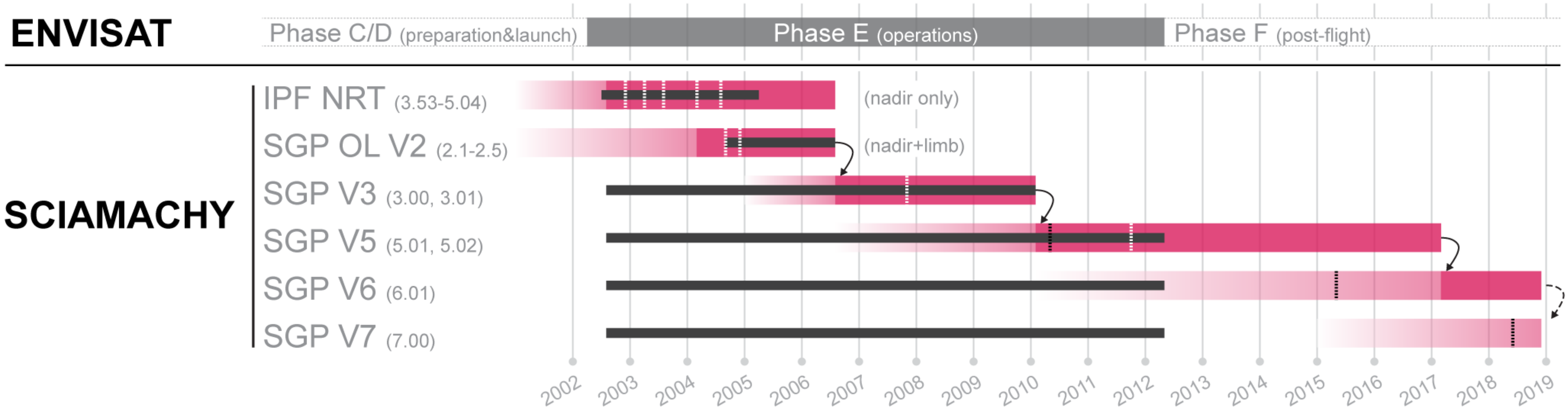
Royal Belgian Institute for Space Aeronomy
BIRA-IASB

Reference

Keppens, A., *et al.* “Multi-TASTE Phase F Validation report – Ground-based assessment of SCIAMACHY SGP 7.00 Level-2 Data Products O3, NO2, CO, CH4, BrO and H2O”, TN-BIRA-IASB-MultiTASTE-Phase-F-SCIA-SGP7-Iss1-RevA, Issue 1 / Rev. A, 6 December 2019.

Acknowledgements: This work was funded through ESA Contract 4000112017/14/I-AM/CCN#1. It relies on the versatile multi-platform validation system Multi-TASTE, its correlative measurements database CORR-2, and its observing systems metrology simulator OSSSMOSE, all developed and operated at BIRA-IASB. Multi-TASTE was developed within several heritage ESA and ProDEx projects projects and refined recently within EU Project QA4ECV, grant no. 60740. The ground-based reference data were obtained as part of WMO’s Global Atmosphere Watch and three of its main contributors, namely, GO3OS, NDACC and SHADOZ. The authors acknowledge the meticulous and sustained work of the PIs and staff at the stations to acquire and maintain long-term data records of high quality.

SCIAMACHY L2 processors overview



Final round of validation activities

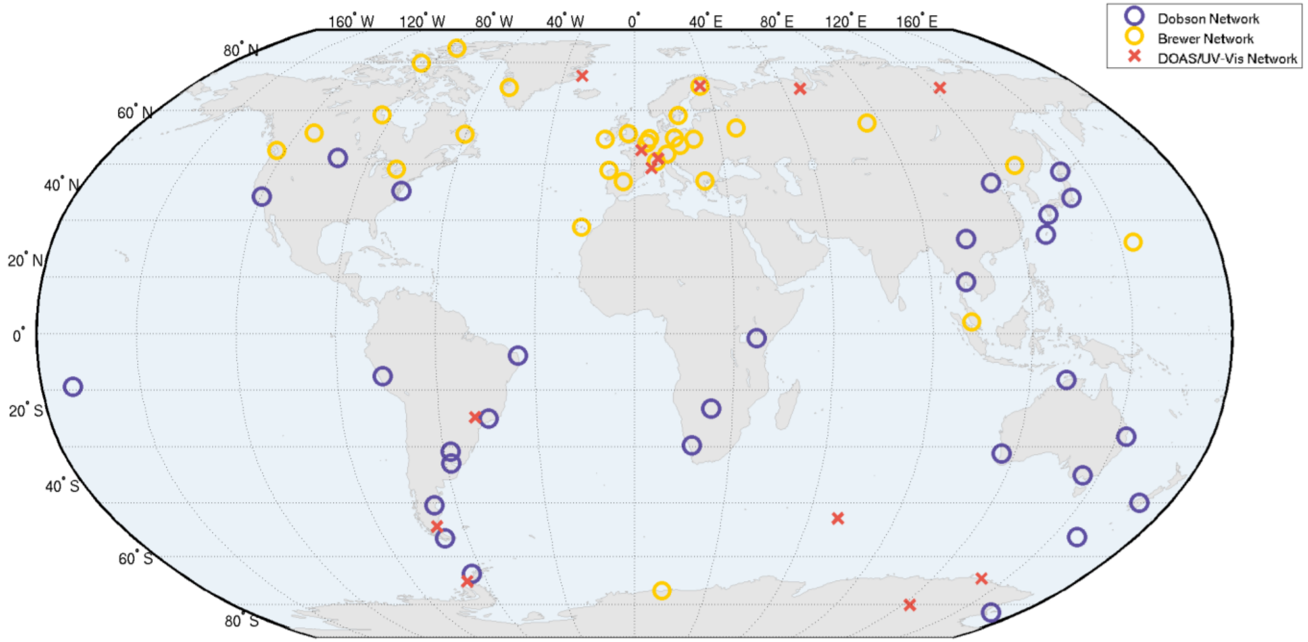
- SCIAMACHY L1 V9.0, L2 V7.00 processors
- Nadir column data products (C): O3, NO2, CO, CH4, BrO, H2O
- Limb profile data products (P): O3, BrO
- Ground-based instruments: GAW GO3OS Brewers and Dobsons, NDACC DOAS UV-visible and FTIR spectrometers, GAW/NDACC/SHADOZ ozonesondes, and NDACC lidars and millimetre wave radiometers (MWR)

	O3	H2O	NO2	BrO	CO	CH4
SCIAMACHY	C, P	C	C	C, P	C	C
Dobson	C					
Brewer	C					
UV-VIS	C		C	C, P		
FTIR					C	P
Ozonesonde	P	C, P				
Lidar	P					
MWR	P					

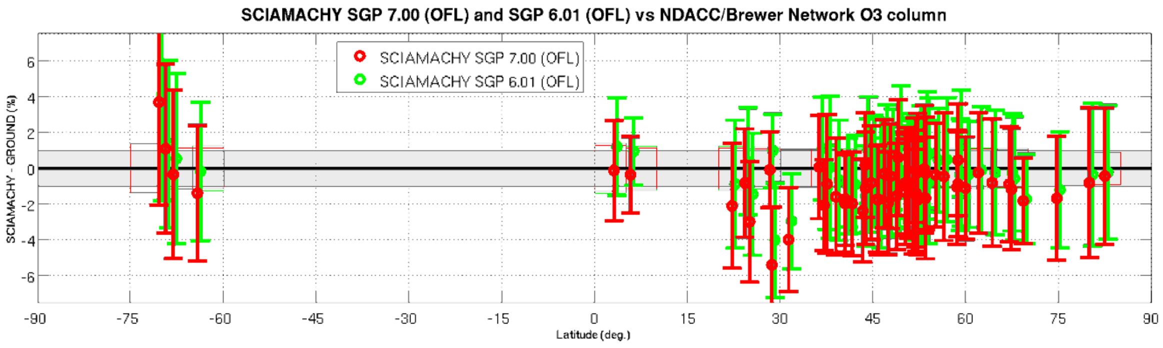
Total O3 column

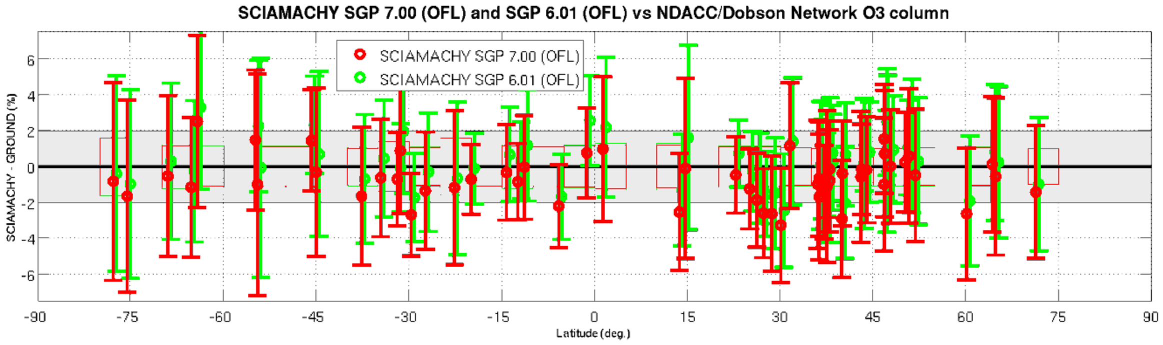
Total O3 reference data

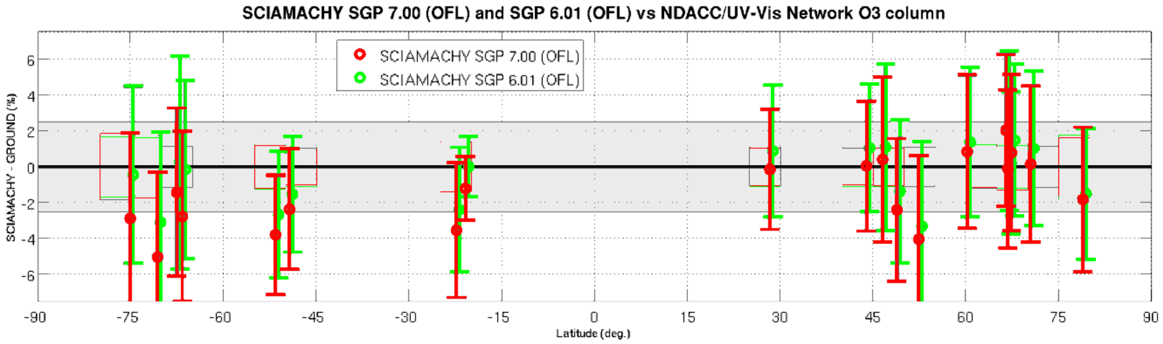
- GO3OS and NDACC Brewer and Dobson UV spectrophotometers: direct sun only, solar elevation > 15°
  - 150 km radius, 3 h co-location
- NDACC ZSL-DOAS UV-visible spectrometers: year-round, all weather
  - footprint of SCIAMACHY FOV of the same day must intercept ground-based air mass estimated with OSSSMOSE (ray tracing, weighting functions based) for dawn and dusk



Total O3 data comparison

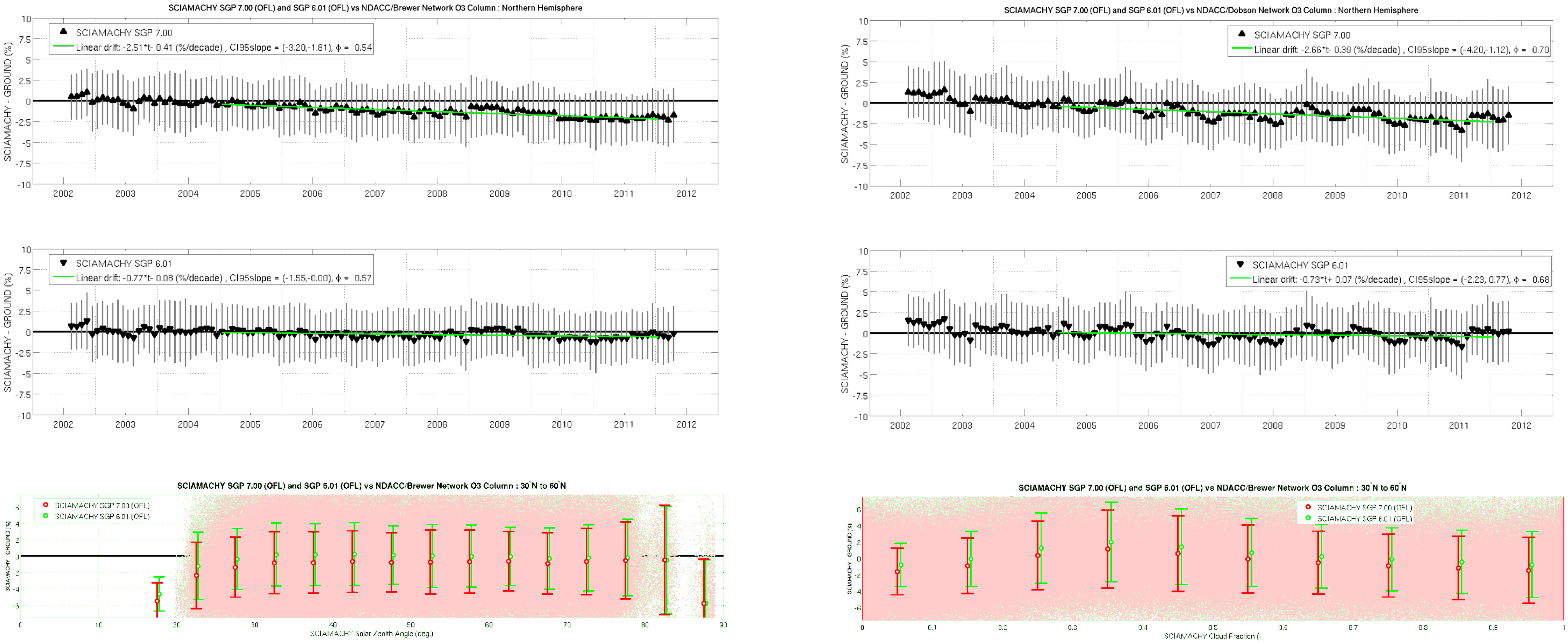






SGP 7.00	
Bias	Significant underestimation of 1.5% on average, 5% maximum.
Spread	No changes w.r.t. to previous SGP versions (dominated by a combination of measurement uncertainties and atmospheric noise).
Drift	Significant negative drift of about 2.5% from early 2005 till the end of the mission.
Other	Dependence of bias on SZA beyond 80° (total ozone underestimation of up to 4%). Slight dependence on cloud cover.

Total O3 drift, and dependences on SZA and clouds

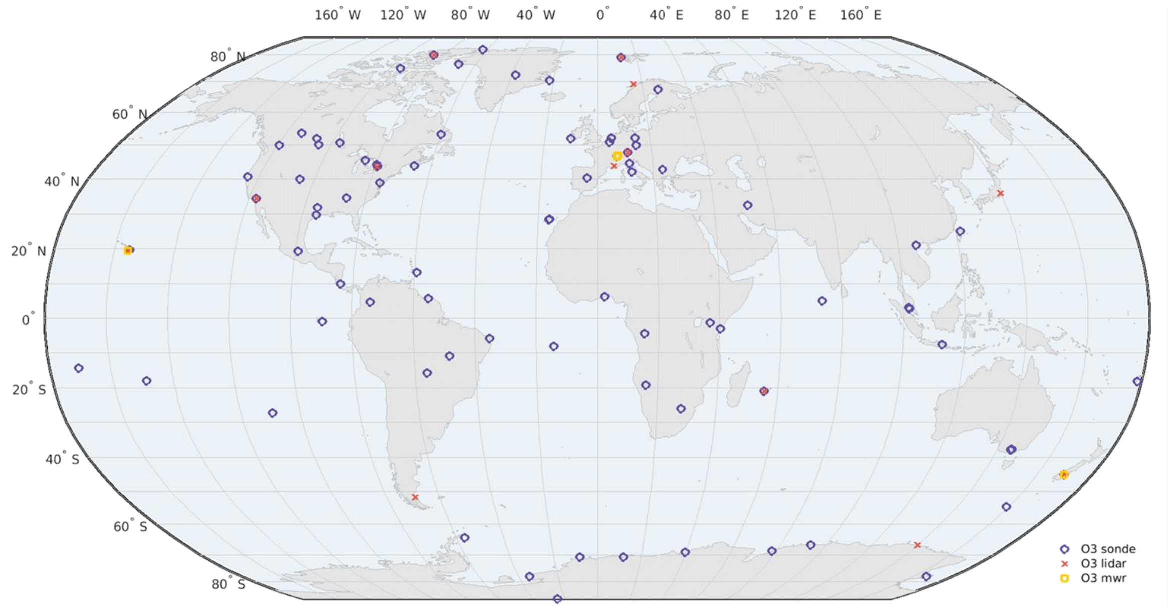


O3 profile

SGP 7.00 limb O3 profile

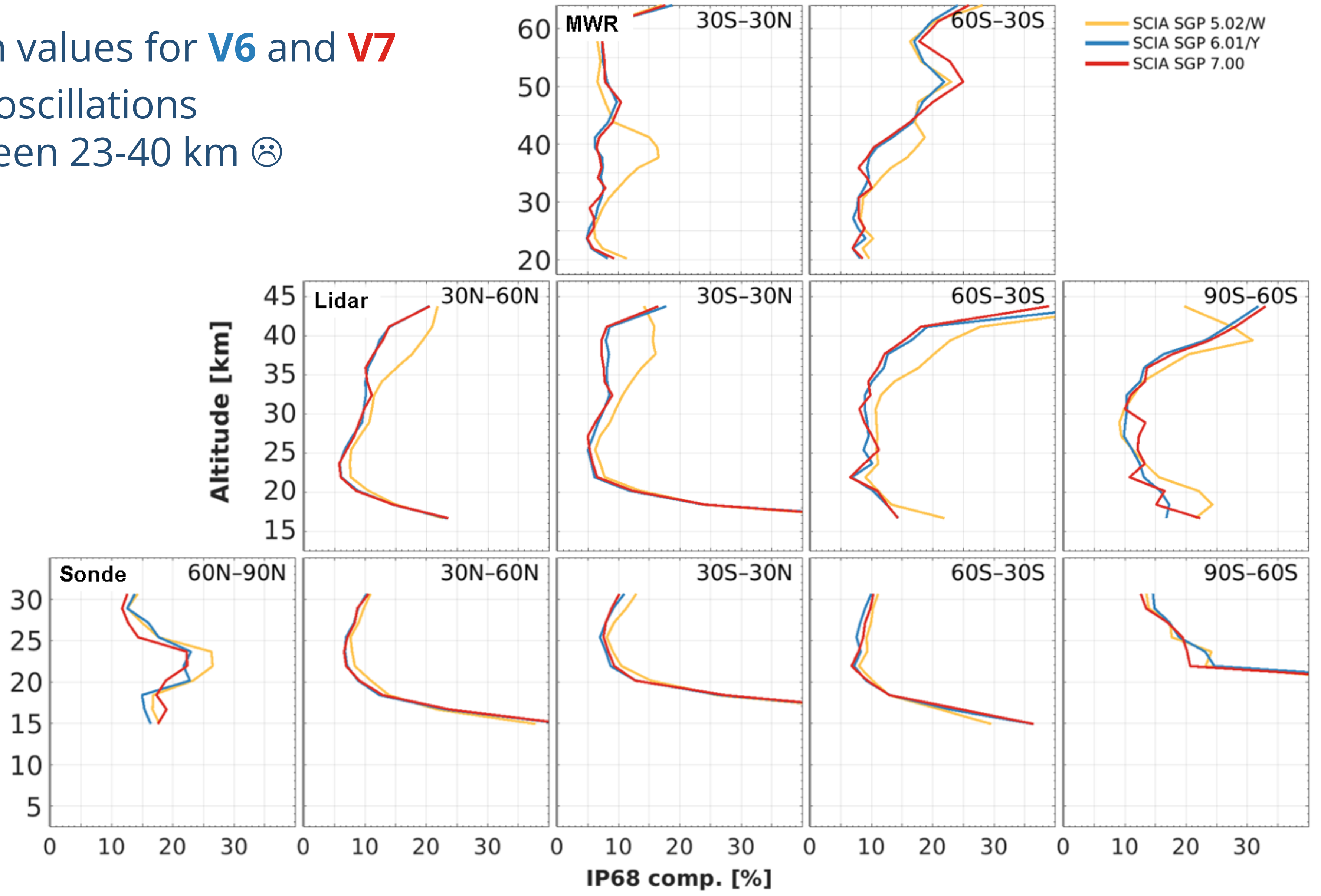
Methodology

- SCIAMACHY versus co-located ozonesonde (GO3OS, NDACC, SHADOZ), NDACC lidars and MWRs (<500km, <12/6h)
- Screening as in Hubert *et al.* (2016)
- Consider O3 number density versus altitude
- Sonde & lidar data smoothed using triangular kernel (not SCIA AKs since they lead to oscillations)



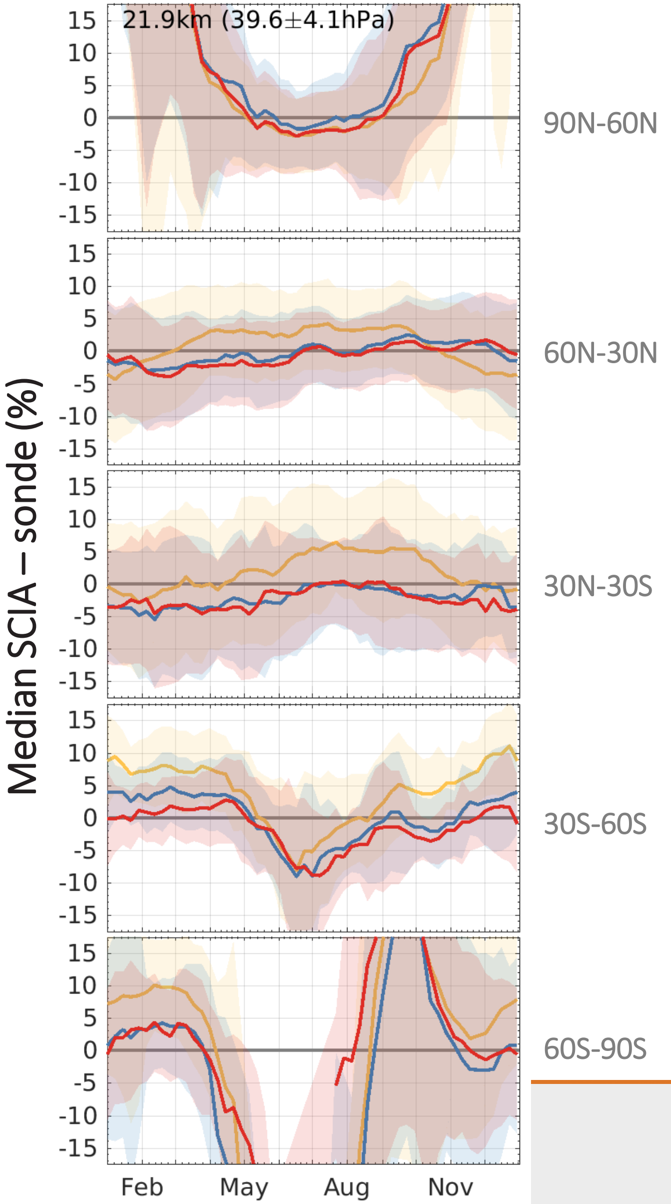
Bias & dispersion

- Similar bias & dispersion values for **V6** and **V7**
- **V7** bias exhibits vertical oscillations of 1-2% amplitude between 23-40 km ☹



All major issues inherited from V6

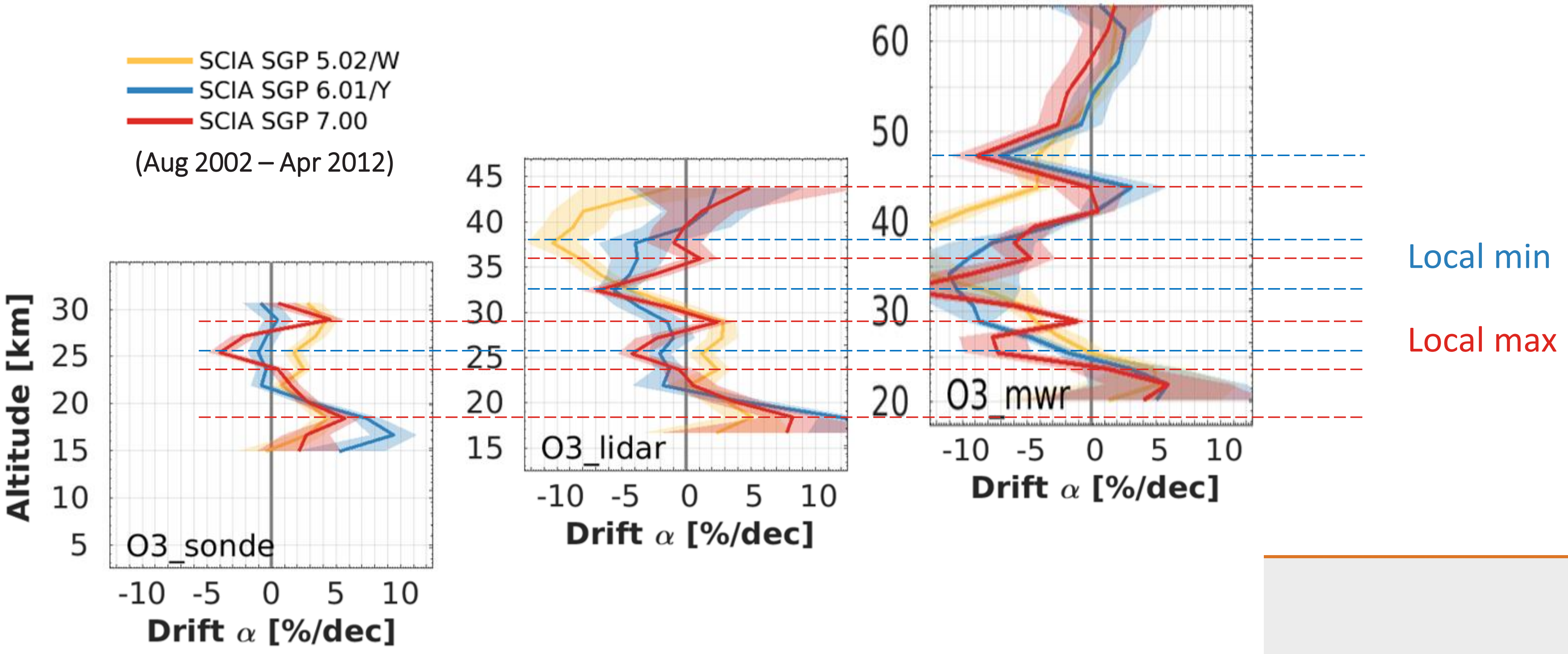
- SCIAMACHY vertical AKs cause oscillations in bias and dispersion profiles → unsuitable for smoothing in an independent validation study
- Large positive bias in US and LM, dependent on hemisphere
- Global dependence of bias and dispersion on season/SZA, especially in Arctic (and Antarctic)
- Auxiliary data clearly add uncertainty in converted profiles (O3 VMR, pressure)



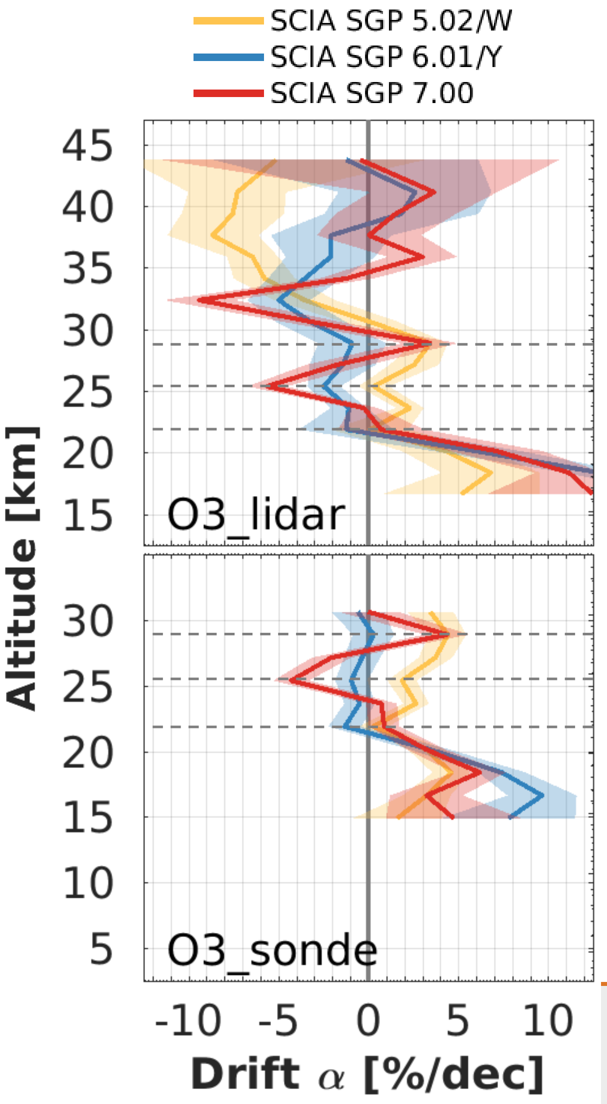
(Very) bad news : long-term stability

- Overall fairly similar vertical dependence as for **V6**
- But **V7** imprints vertical oscillations of 3-4%/decade amplitude (!) between 18-45 km
- Difference min/max altitudes correspond to differences between SCIA scan altitudes

→ SGP V7 data are unsuitable for trend studies, IUP's scientific product should be affected too!

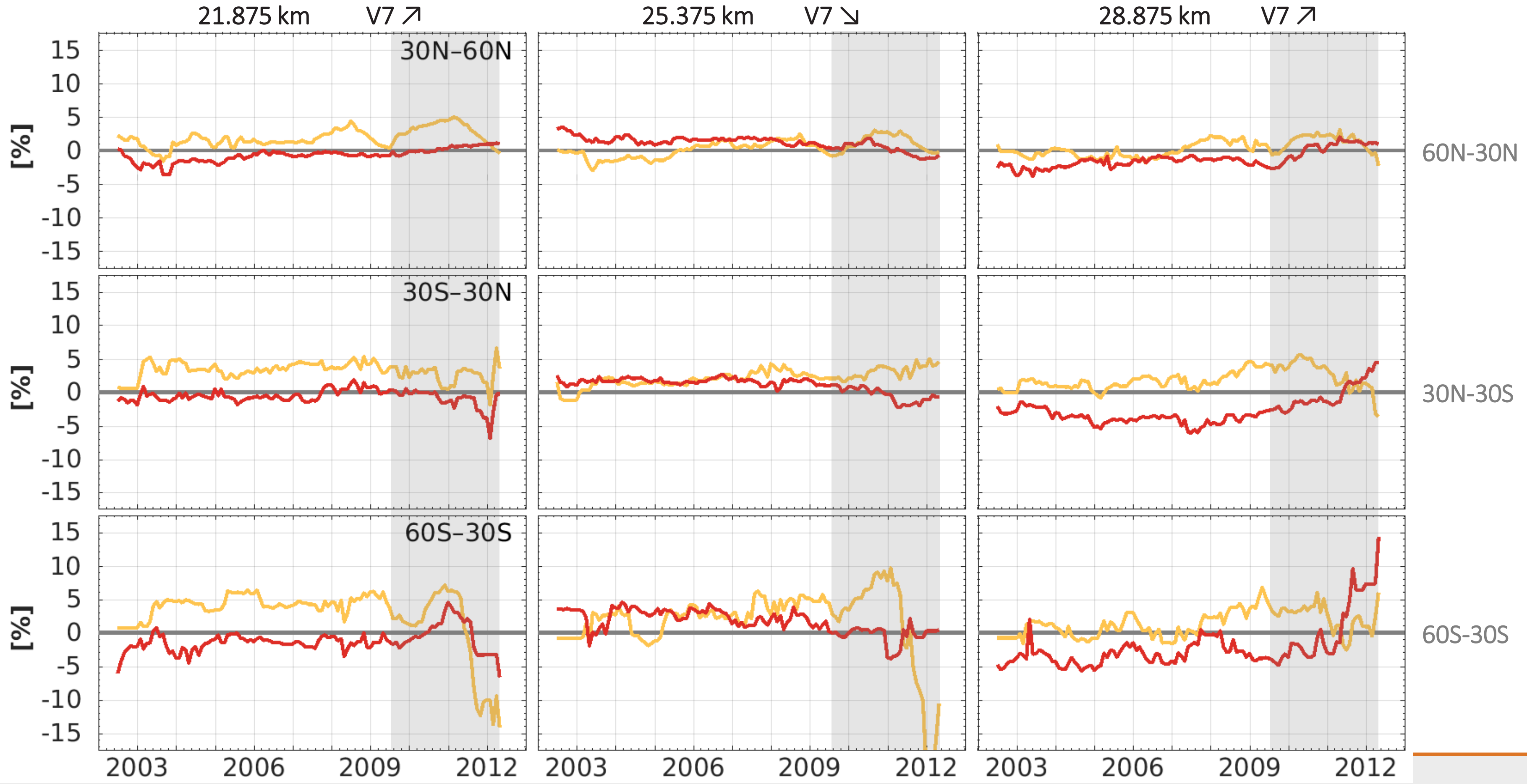


Clear changes from ~2009 onwards



(SGP 5.02/GND -1) – (SGP 6.01/GND -1)
(SGP 7.00/GND -1) – (SGP 6.01/GND -1)

(versus O3 lidar sonde)

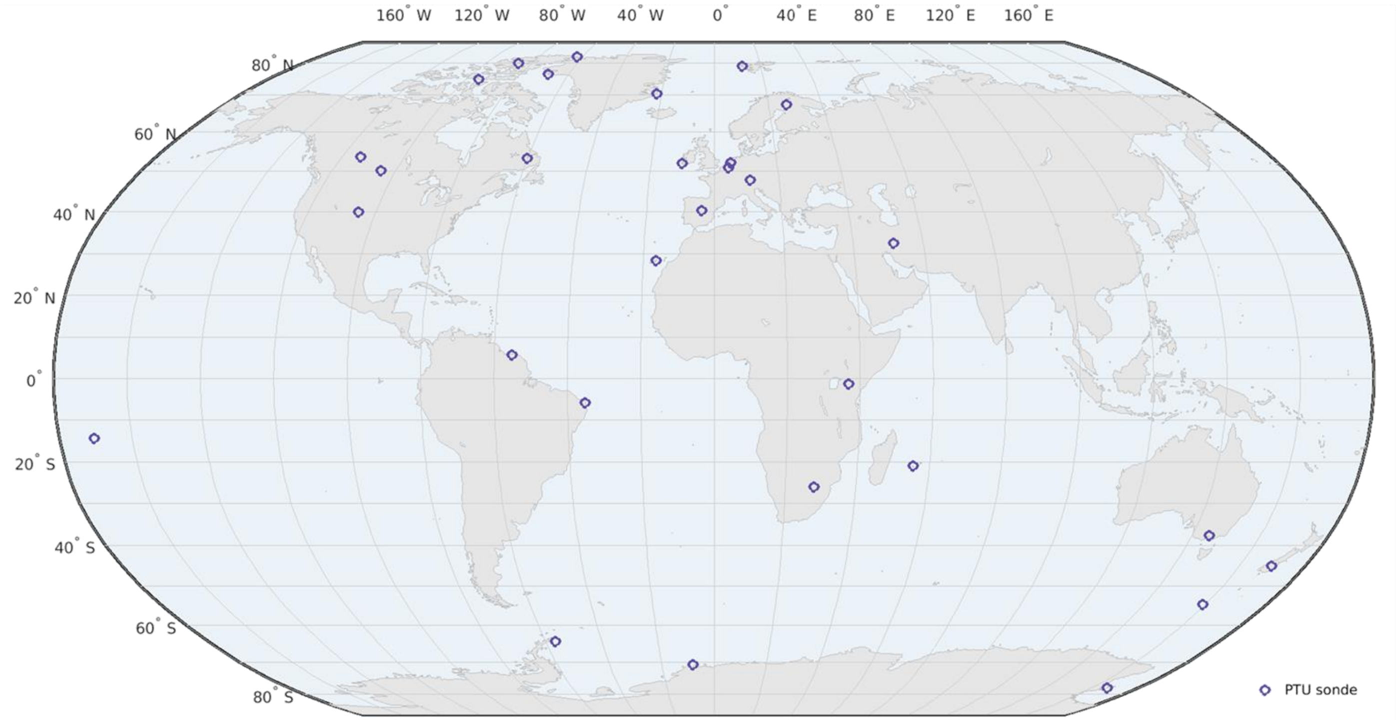


Total H2O column

SGP 7.00 nadir H2O versus sonde

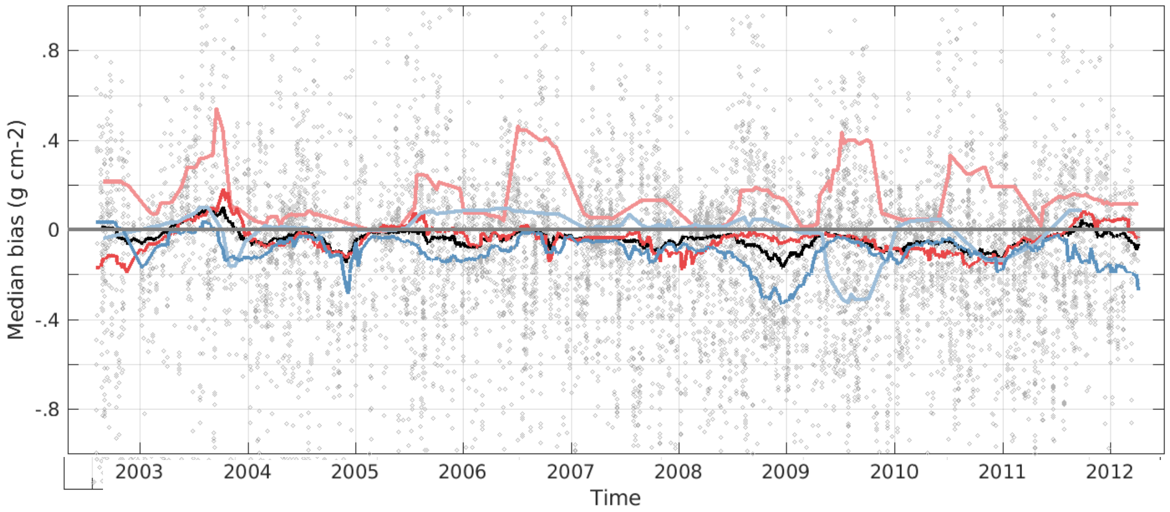
Methodology

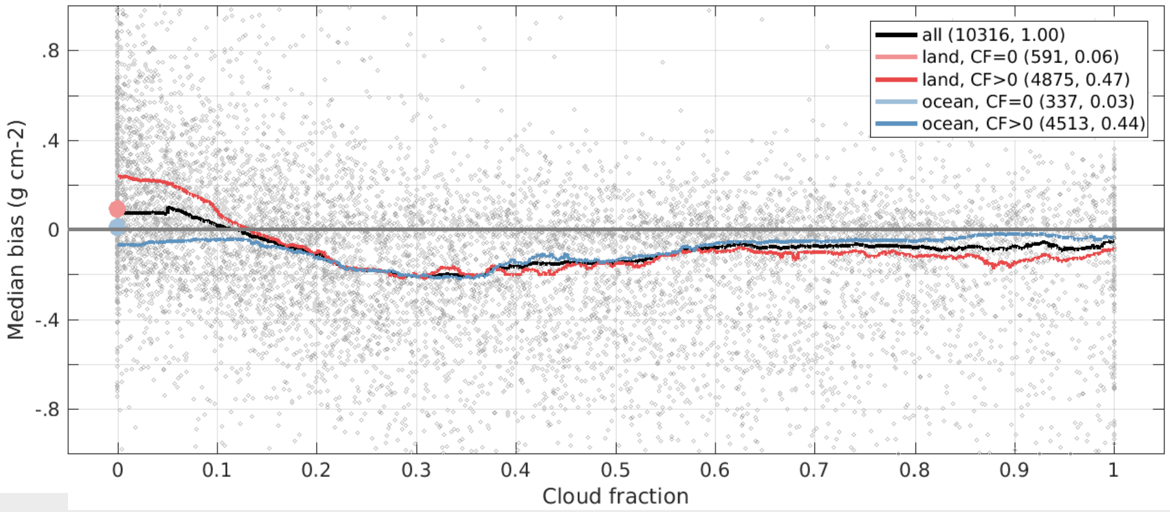
- SCIAMACHY versus co-located PTU radiosondes (<50km, <1h)
- Convert sonde measured RH to VMR, then integrate profile from surface to 10km
- Separate analysis for SCIAMACHY pixels according to land/ocean, cloud-free/cloudy



SGP V7 and V6 identical

- In general too dry (0.06 g cm^{-2}, 9%), but too wet over land and CF<0.1 (0.1-0.2 g cm^{-2}, 14-25%)
- No clear long-term change.
- Data quality degrades with increasing cloud top height under very cloudy conditions.
- At low AMF correction factor the bias becomes increasingly negative.
- Bias and spread vary over the course of a year. They are smallest in local spring and largest in local summer
- At small solar zenith angle the bias becomes positive and variability in the comparisons increases, for all pixel classes.

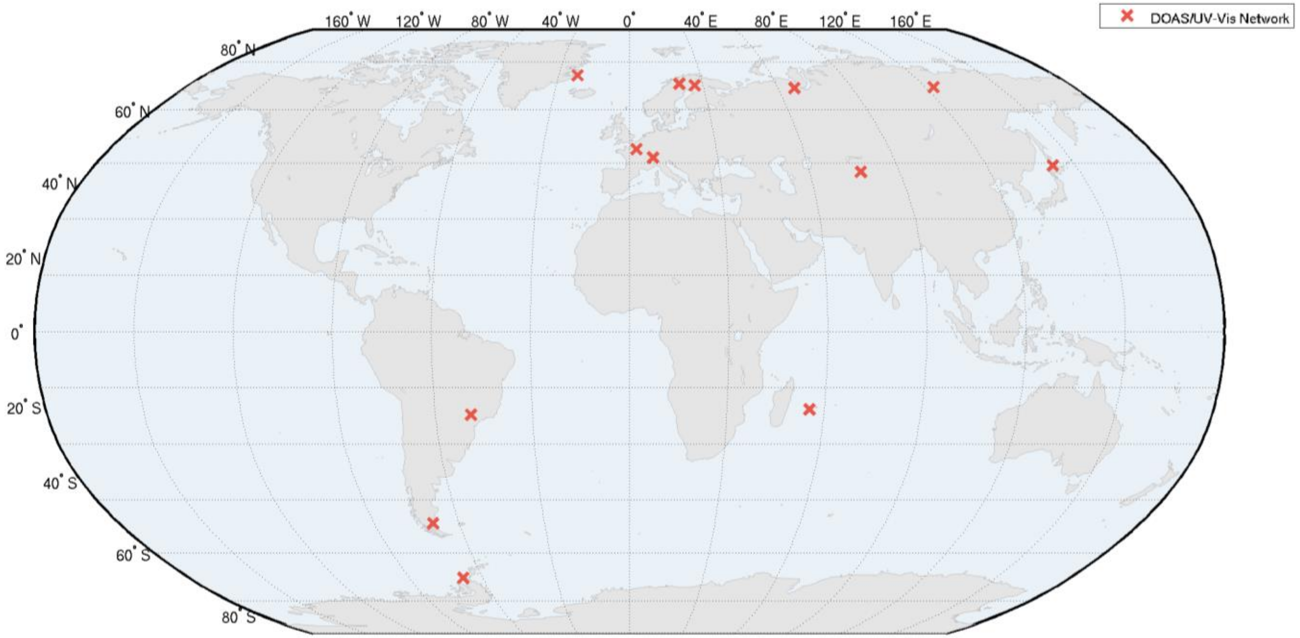




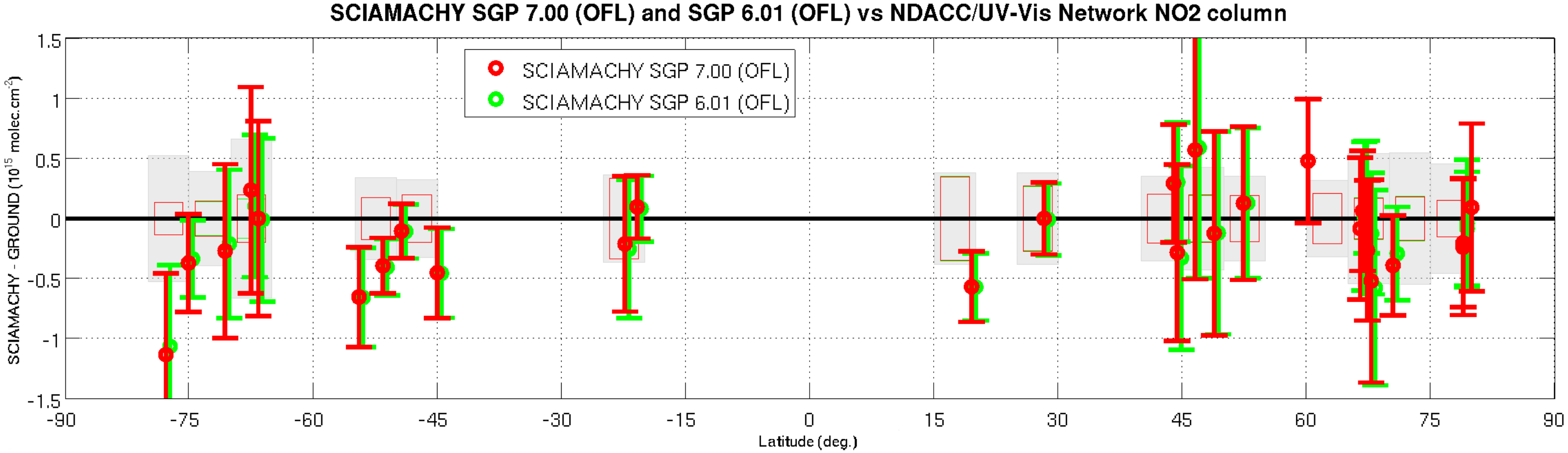
Total NO2 column

Total NO2 reference data

- NDACC ZSL-DOAS UV-visible spectrometers (mainly SAOZ network) at pristine sites
- Footprint of SCIAMACHY FOV must intercept ground-based air mass at dawn estimated with OSSSMOSE (ray tracing based)
- Photochemical correction is applied to account for diurnal cycle between SCIAMACHY and twilight NDACC data.



Total NO2 comparisons



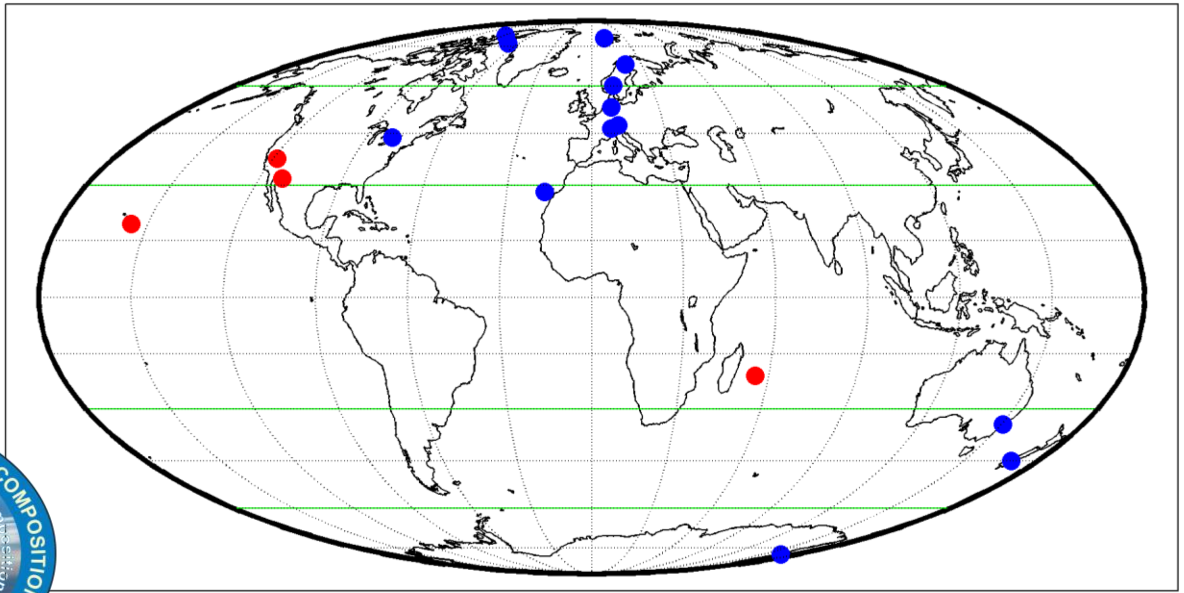
SGP 7.00	Arctic	30N-60N	30N-30S	30S-60S	Antarctic
Bias (x10^{14} molec.cm^{-2})	±3	+4	±3	-5	±3
Spread (x10^{14} molec.cm^{-2})	5	5-8	3	4	5
Other	Apparent bias between NH and SH data, maybe due to difference in sensitivity to tropospheric pollution and/or to residual diurnal cycle effects between SCIAMACHY and NDACC/UV-visible twilight data.				

CO & CH_4 column

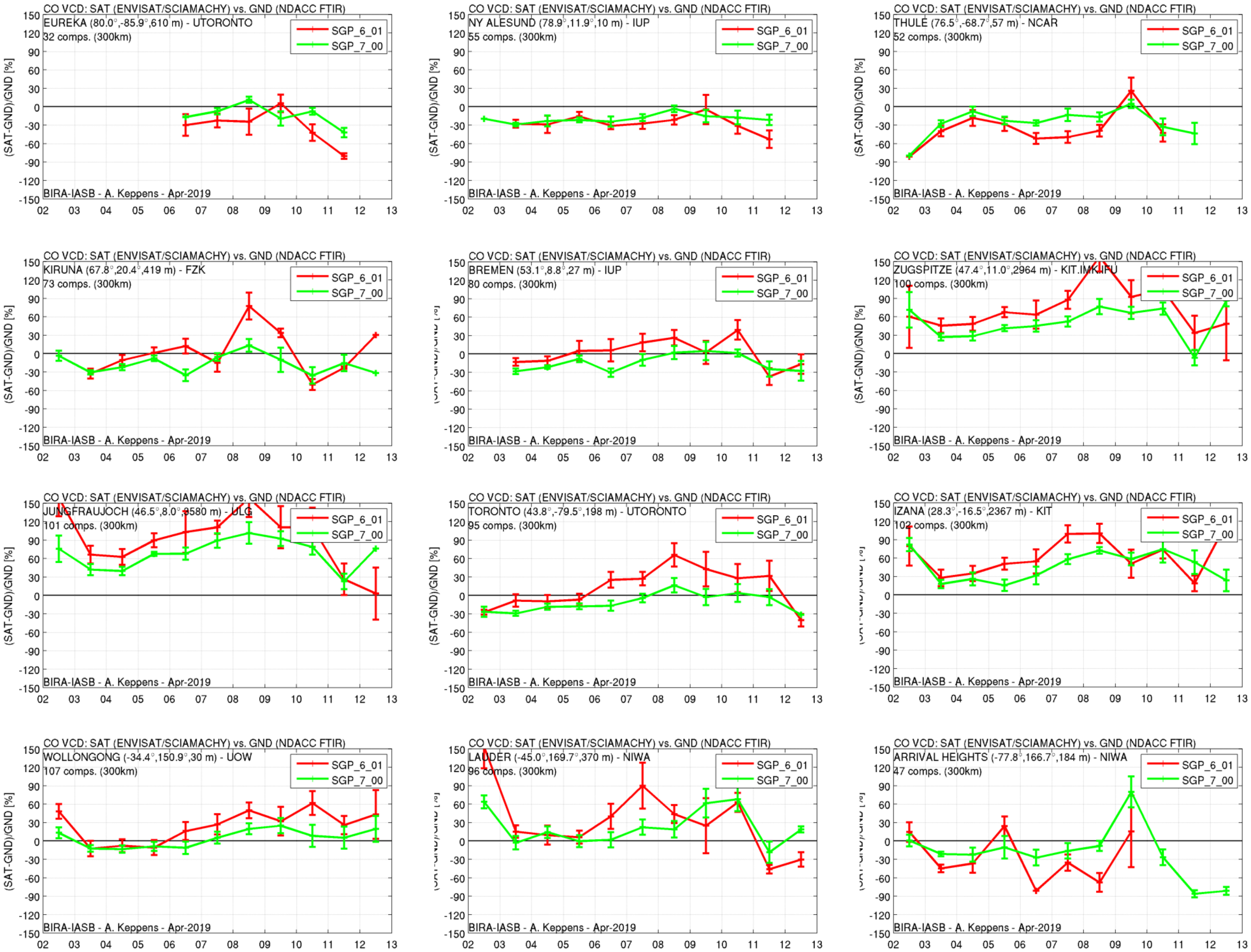
SGP 7.00 CO & CH4 versus FTIR: method

SGP V7.00 and V6.01 validation analysis on the relative difference & SEM (as error bars)

- of monthly and yearly means (neg. MM are omitted)
- of co-location pairs within 300 km and within ±3 h at 15 NDACC FTIR stations (solar IR)
- with filtering as suggested by NDACC data providers



FTIR station	Lat.	Lon.	Period
Eureka	79.99	-85.93	2006-2012
Ny-Ålesund	78.93	11.93	2002-2012
Thule	76.53	-68.74	2002-2011
Kiruna	67.84	20.41	2002-2012
Harestua	60.20	10.80	2002-2012
Bremen	53.10	8.80	2002-2012
Zugspitze	47.42	10.98	2002-2011
Jungfraujoch	46.55	7.98	2002-2012
Toronto	43.78	-79.47	2004
~~Mt. Barcroft~~	~~37.58~~	~~-118.24~~	~~2002~~
~~Kitt Peak~~	~~31.90~~	~~-111.60~~	~~2002-2005~~
Izaña	28.30	-16.50	2002-2012
Mauna Loa	19.53	-155.58	2003-2010
St. Denis	-20.90	55.50	2004-2011
Wollongong	-34.41	150.88	2002-2008
Lauder	-45.04	169.68	2002-2012
Arrival Heights	-77.83	166.67	2002-2012


CO VCD: SAT (ENVISAT/SCIAMACHY) vs. GND (NDACC FTIR)
EUREKA (80.0°,-85.9°,610 m) - UTORONTO
32 comps. (300km)
CO VCD: SAT (ENVISAT/SCIAMACHY) vs. GND (NDACC FTIR)
NY ALESUND (78.9°,11.9°,10 m) - IUP
55 comps. (300km)
CO VCD: SAT (ENVISAT/SCIAMACHY) vs. GND (NDACC FTIR)
THULE (76.5°,-68.7°,57 m) - NCAR
52 comps. (300km)
CO VCD: SAT (ENVISAT/SCIAMACHY) vs. GND (NDACC FTIR)
KIRUNA (67.8°,20.4°,419 m) - FZK
73 comps. (300km)
CO VCD: SAT (ENVISAT/SCIAMACHY) vs. GND (NDACC FTIR)
BREMEN (53.1°,8.8°,27 m) - IUP
80 comps. (300km)
CO VCD: SAT (ENVISAT/SCIAMACHY) vs. GND (NDACC FTIR)
ZUGSPITZE (47.4°,11.0°,2964 m) - KIT.IMK.IFU
100 comps. (300km)
CO VCD: SAT (ENVISAT/SCIAMACHY) vs. GND (NDACC FTIR)
JUNGFRAUJOCH (46.5°,8.0°,3580 m) - ULG
101 comps. (300km)
CO VCD: SAT (ENVISAT/SCIAMACHY) vs. GND (NDACC FTIR)
TORONTO (43.8°,-79.5°,198 m) - UTORONTO
95 comps. (300km)
CO VCD: SAT (ENVISAT/SCIAMACHY) vs. GND (NDACC FTIR)
IZANA (28.3°,-16.5°,2367 m) - KIT
102 comps. (300km)
CO VCD: SAT (ENVISAT/SCIAMACHY) vs. GND (NDACC FTIR)
WOLLONGONG (-34.4°,150.9°,30 m) - UOW
107 comps. (300km)
CO VCD: SAT (ENVISAT/SCIAMACHY) vs. GND (NDACC FTIR)
LAUDER (-45.0°,169.7°,370 m) - NIWA
96 comps. (300km)
CO VCD: SAT (ENVISAT/SCIAMACHY) vs. GND (NDACC FTIR)
ARRIVAL HEIGHTS (-77.8°,166.7°,184 m) - NIWA
47 comps. (300km)
SGP_6_01
SGP_7_00
(SAT-GND)/GND [%]
BIRA-IASB - A. Keppens - Apr-2019

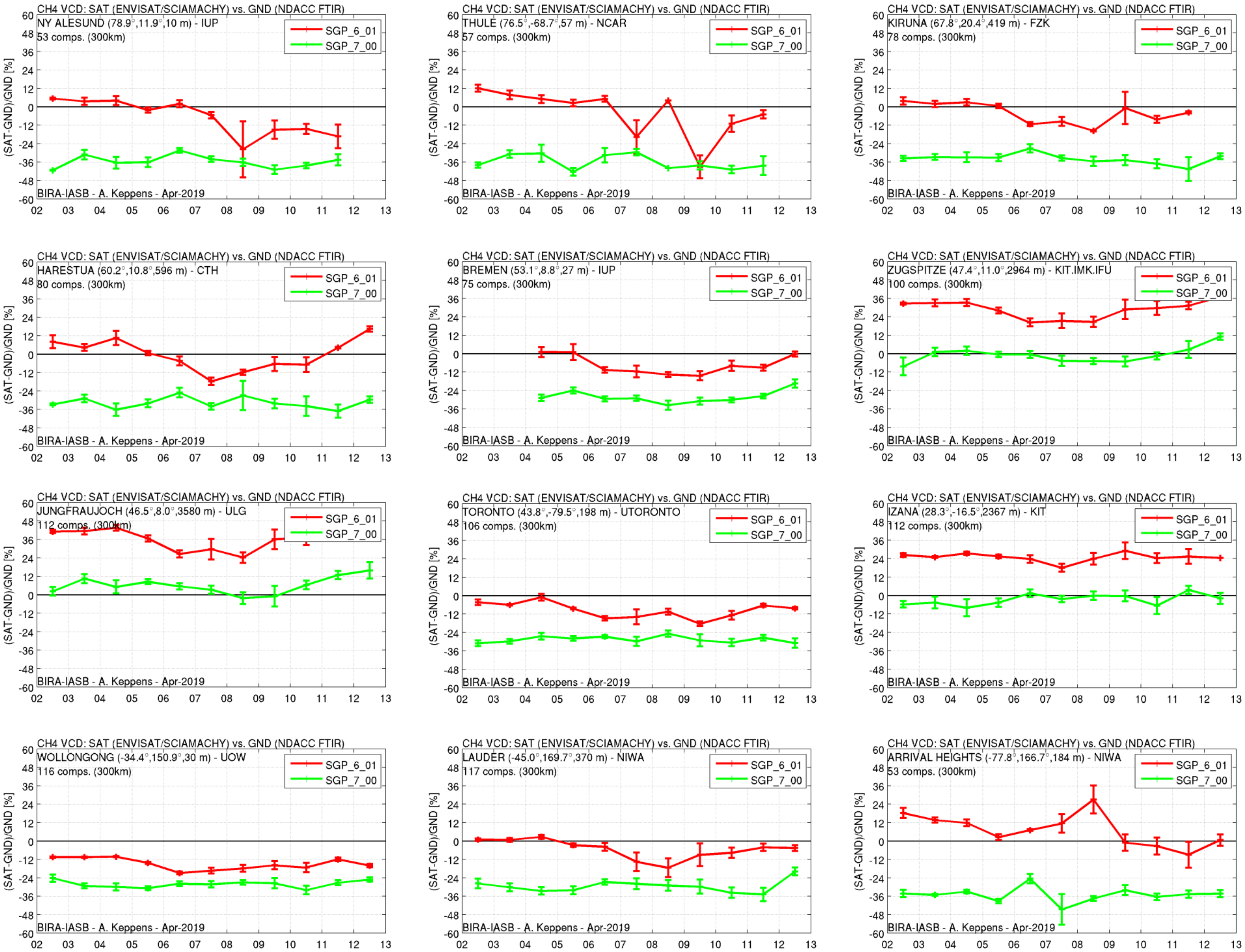
SGP 7.00 CO versus NDACC FTIR

- Overall V7 values are smaller than V6, which generally reduces the SCIA bias
- Large amount of positive and negative outliers remains (even for monthly means)
- No seasonal cycle, decadal trend or meridian dependence can be observed
- Product remains inadequate in both precision and bias

Conclusion:

- Continue V7 processing

Latitude band	# stations	# MM	Bias SGP V6 - FTIR	Bias SGP V7 - FTIR	Spread SGP V6 & V7
Arctic (60N-90N)	4	212	-23 %	-19 %	10-30 %
Mid-north (30N-60N)	4	376	46 %	21 %	10-30 %
Tropics (30N-30S)	2	125	66 %	45 %	10-30 %
Mid-south (30S-60S)	2	203	25 %	14 %	10-30 %
Antarctic (60S-90S)	1	47	-27 %	-20 %	10-30 %


CH4 VCD: SAT (ENVISAT/SCIAMACHY) vs. GND (NDACC FTIR)
NY ALESUND (78.9°,11.9°,10 m) - IUP
53 comps. (300km)
SGP_6_01
SGP_7_00
(SAT-GND)/GND [%]
BIRA-IASB - A. Keppens - Apr-2019
CH4 VCD: SAT (ENVISAT/SCIAMACHY) vs. GND (NDACC FTIR)
THULE (76.5°,-68.7°,57 m) - NCAR
57 comps. (300km)
SGP_6_01
SGP_7_00
(SAT-GND)/GND [%]
BIRA-IASB - A. Keppens - Apr-2019
CH4 VCD: SAT (ENVISAT/SCIAMACHY) vs. GND (NDACC FTIR)
KIRUNA (67.8°,20.4°,419 m) - FZK
78 comps. (300km)
SGP_6_01
SGP_7_00
(SAT-GND)/GND [%]
BIRA-IASB - A. Keppens - Apr-2019
CH4 VCD: SAT (ENVISAT/SCIAMACHY) vs. GND (NDACC FTIR)
HARESTUA (60.2°,10.8°,596 m) - CTH
80 comps. (300km)
SGP_6_01
SGP_7_00
(SAT-GND)/GND [%]
BIRA-IASB - A. Keppens - Apr-2019
CH4 VCD: SAT (ENVISAT/SCIAMACHY) vs. GND (NDACC FTIR)
BREMEN (53.1°,8.8°,27 m) - IUP
75 comps. (300km)
SGP_6_01
SGP_7_00
(SAT-GND)/GND [%]
BIRA-IASB - A. Keppens - Apr-2019
CH4 VCD: SAT (ENVISAT/SCIAMACHY) vs. GND (NDACC FTIR)
ZUGSPITZE (47.4°,11.0°,2964 m) - KIT.IMK.IFU
100 comps. (300km)
SGP_6_01
SGP_7_00
(SAT-GND)/GND [%]
BIRA-IASB - A. Keppens - Apr-2019
CH4 VCD: SAT (ENVISAT/SCIAMACHY) vs. GND (NDACC FTIR)
JUNGFRAUJOCH (46.5°,8.0°,3580 m) - ULG
112 comps. (300km)
SGP_6_01
SGP_7_00
(SAT-GND)/GND [%]
BIRA-IASB - A. Keppens - Apr-2019
CH4 VCD: SAT (ENVISAT/SCIAMACHY) vs. GND (NDACC FTIR)
TORONTO (43.8°,-79.5°,198 m) - UTORONTO
106 comps. (300km)
SGP_6_01
SGP_7_00
(SAT-GND)/GND [%]
BIRA-IASB - A. Keppens - Apr-2019
CH4 VCD: SAT (ENVISAT/SCIAMACHY) vs. GND (NDACC FTIR)
IZANA (28.3°,-16.5°,2367 m) - KIT
112 comps. (300km)
SGP_6_01
SGP_7_00
(SAT-GND)/GND [%]
BIRA-IASB - A. Keppens - Apr-2019
CH4 VCD: SAT (ENVISAT/SCIAMACHY) vs. GND (NDACC FTIR)
WOLLONGONG (-34.4°,150.9°,30 m) - UOW
116 comps. (300km)
SGP_6_01
SGP_7_00
(SAT-GND)/GND [%]
BIRA-IASB - A. Keppens - Apr-2019
CH4 VCD: SAT (ENVISAT/SCIAMACHY) vs. GND (NDACC FTIR)
LAUDER (-45.0°,169.7°,370 m) - NIWA
117 comps. (300km)
SGP_6_01
SGP_7_00
(SAT-GND)/GND [%]
BIRA-IASB - A. Keppens - Apr-2019
CH4 VCD: SAT (ENVISAT/SCIAMACHY) vs. GND (NDACC FTIR)
ARRIVAL HEIGHTS (-77.8°,166.7°,184 m) - NIWA
53 comps. (300km)
SGP_6_01
SGP_7_00
(SAT-GND)/GND [%]
BIRA-IASB - A. Keppens - Apr-2019

SGP 7.00 CH4 versus NDACC FTIR

- V6 yearly biases often insignificant (towards poles) and within random uncertainty
- V7 few 10 % below V6, introducing negative bias at most stations
- But V6 positive bias in Tropics reduced in V7 as a result
- Strong and significant seasonal cycle (up to 30 %) for both versions

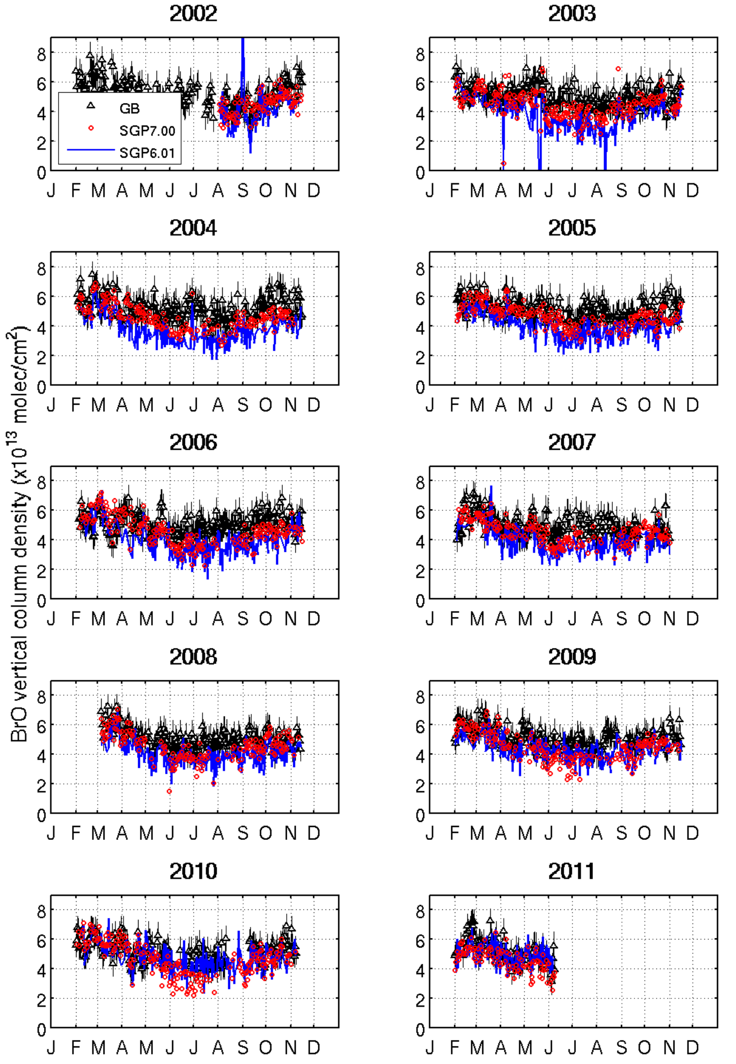
Conclusions:

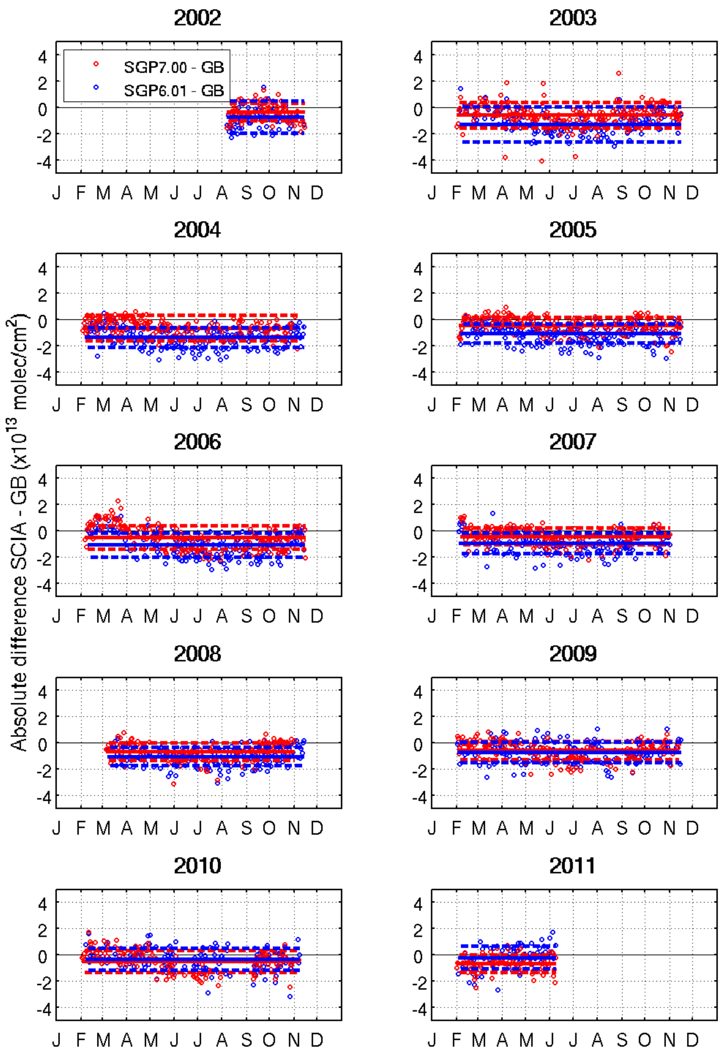
- V7 has 20-40 % lower values than V6
- V7 better towards equator, V6 better towards poles
- Decide on V7 data release?

Latitude band	# stations	# MM	Bias SGP V6 - FTIR	Bias SGP V7 - FTIR	Spread SGP V6 & V7
Arctic (60N-90N)	5	299	-7 %	-34 %	5-15 %
Mid-north (30N-60N)	4	393	14 %	-12 %	5-15 %
Tropics (30N-30S)	3	193	19 %	-7 %	5-15 %
Mid-south (30S-60S)	2	233	-9 %	-28 %	5-15 %
Antarctic (60S-90S)	1	53	8 %	-35 %	5-15 %

BrO column & profile

BrO total column over Harestua (Norway)





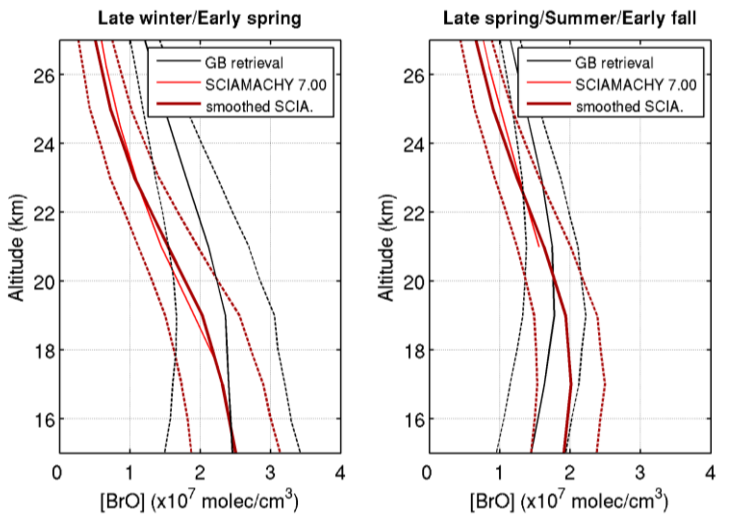
		SGP 6.01 - GB	SGP 7.00 - GB
Absolute difference ($x10^{12}$ molec/cm^2)	Bias	-7.3	-5.5
	Standard deviation	9.8	8.0
Relative difference (%)	Bias	-14.8	-10.5
	Standard deviation	19.9	15.8
Remark	V6 standard deviation affected by outliers in 2002 and 2003.		

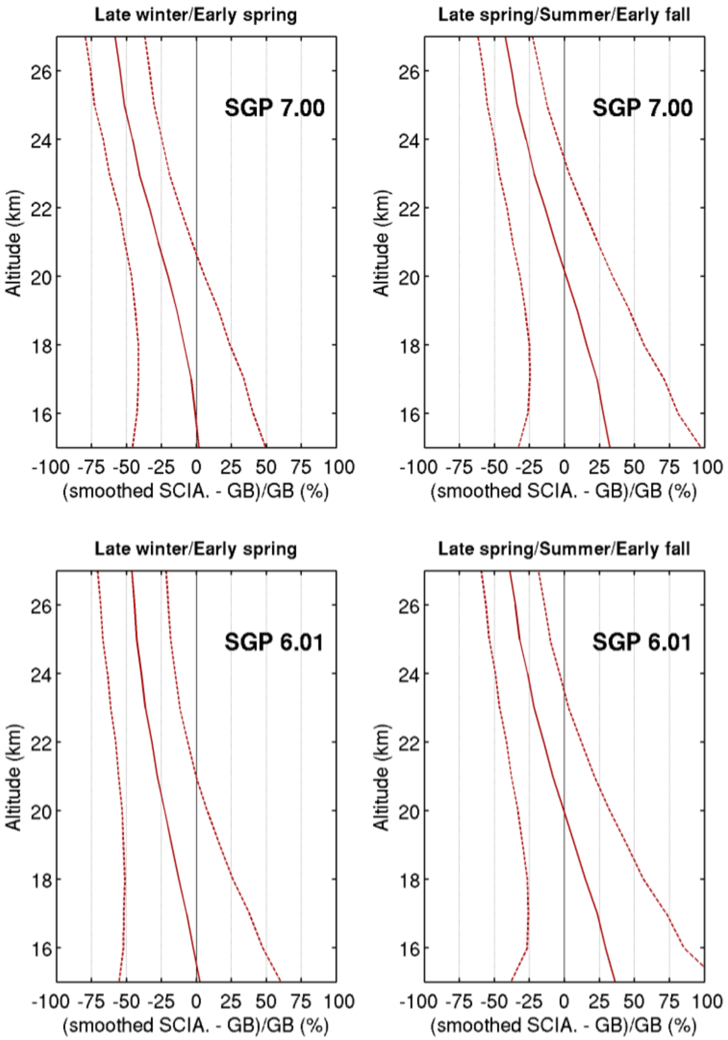
- Co-location criteria:
  - Spatial: <300km from the station
  - Temporal: Ground-based sunrise columns converted to satellite overpass SZA (Hendrick et al., ACP, 2007 & 2009)

➢ On overall, smaller negative biases with ground-based UV-vis data for SGP 7.00

➢ Smaller spread for SGP 7.00

BrO stratospheric profile over Harestua (Norway)





- Co-location criteria:
  - Spatial: <500km from the station
  - Temporal: Ground sunrise profiles converted to satellite overpass SZA (Hendrick et al., ACP, 2007 & 2009)
- ➢ Positive bias for the lower altitude levels and negative bias up to -30% (late spring/early fall) and -50% (late spring/summer/early fall) for higher altitude levels
- ➢ Larger bias than those obtained for the IUP-Bremen scientific product at the same station (+10/-20%; see Hendrick et al., ACP, 2009

Summary / Conclusions

SCIAMACHY SGP 7.00 vs. ground-based	Nadir (total column)						Limb (vertical profile)	
	O3	NO2	BrO	H2O	CO	CH4	O3	BrO
Domain of validation results	Representative global sample	Representative global sample for stratospheric NO_2	1 sub-Arctic site	Representative for land and coastal areas, not above ocean	15 stations, mostly NH	15 stations, mostly NH	Representative global sample 15-45 km, only 2 sites 45-65 km	1 Arctic site 15-27 km
Bias ± spread	-1.5 ± 5 %	-10 ± 15 %	-11 ± 16 %	-7 ± 29 %	For monthly / yearly averages	20 ± 20 %	+10 ± 7 %, a lot of substructure	+25 to -50 %
Long-term stability	3%/dec. neg. drift in NH	No significant drift	No significant drift	No significant drift	No significant drift	No detectable drift (large σ)	**Large drifts, strong height-dependence**	No significant drift
Evolution w.r.t. SGP 6.01	Few % lower	~	Negative bias reduced	V7 = V6	V7 < V6	- (20-40) %	Vertical oscillations in V7 drift & bias	~
Recommendation	**Not suitable for trend studies**	/	/	/	/	Need for bias correction	**Not suitable for trend studies**	/