climate change initiative

LONG-LIVED GREENHOUSE GAS PRODUCTS PERFORMANCES

Dataset harmonization and validation/intercomparison: Limb products

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Overview of WP2200 - limb

Task

Collect data products and auxiliary data and harmonize content formats

Output

Consistent dataset of all limb satellite products under consideration, filtered according to the recommendations provided by each instrument team

Satellite limb datasets to harmonize

ACE-FTS (SCISAT): 2004-present

HIRDLS (Aura): 2005-2008

MIPAS (ENVISAT) 2002-2012 (ESA and IMK-IAA retrieval processors)
Note two different periods: full-resolution (2002-2004) and reduced/optimized resolution (2005-2012).

MLS (Aura): 2004-present (N_2O only)

SMR (Odin): 2002-present (N_2O only)

To be compared with each other and with balloon and aircraft limb data.

Gases of interest

Step 1: N_2O

-All satellite datasets under consideration include N_2O retrievals.

-Starting here allows easier testing across all instruments.

Step 2: CFC-11, CFC-12, and SF_6

-CFCs available from HIRDLS, MIPAS, and ACE-FTS.

-SF_6 available from MIPAS IMK-IAA and ACE-FTS.

Step 3: Other halogenated compounds (to support further work)

-CFC-113, CCl_4, CF_4, and HCFC-22 from MIPAS and ACE-FTS. ← We are here

-HCFC-141b, HCFC-142b, HFC-23, HFC-134a from ACE-FTS.

Harmonization (limb): Format

Mandatory variables

The format was adapted from the HARMOZ (harmonized ozone) files.

Table 2. Mandatory parameters in the HARMOZ netCDF files. N_{alt} and N_{prof} denote the number of pressure levels and the number of profiles, respectively.

Parameter and unit	Dimensions	Description
time (days since 1900-01-01 00:00:00)	$N_{prof} \times 1$	The parameter to index the profiles
air_pressure (hPa)	$N_{alt} \times 1$	The vertical coordinate
altitude (km)	$N_{alt} \times N_{prof}$	The geometric altitude above the mean sea-level
latitude (deg north)	$N_{prof} \times 1$	Latitude of each profile (given at altitude ~ 35 km)
longitude (deg east)	$N_{prof} \times 1$	Longitude of each profile (given at altitude ~ 35 km) [-180,180]
mole_concentration_of_ozone_in_air (moles cm^{-3})	$N_{alt} \times N_{prof}$ In VMR (ppv)	Vertical profiles of ozone. Number density (cm^{-3}) is acquired by multiplying the variable with Avogadro constant $N_A = 6.02214 \times 10^{23}$ moles^{-1}
mole_concentration_of_ozone_in_air standard_error (moles cm^{-3})	$N_{alt} \times N_{prof}$ In VMR (ppv)	Uncertainty (random error) associated with the ozone profiles
vertical_resolution (km)	$N_{alt} \times N_{prof}$ ~~or $N_{alt} \times 1$~~	FWHM of the averaging kernel Instrument-dependent, explanation provided in files
air_temperature (K)	$N_{alt} \times N_{prof}$	Temperature profiles at the locations of measurements, for conversion from concentration to mixing ratio

Sofieva et al., *ESSD*, 2013.

The variables listed as N_alt x N_prof are actually N_prof x N_alt.

Added
-local_solar_time
-solar_zenith_angle
-LOLIPOP-specific quality flags to allow for future removal of measurements (currently all set to zero)

Some instrument-specific variables are also included.

Harmonization (limb): Dataset size

Approximate size of the harmonized datasets

Instrument	Dataset size [GB]
ACE-FTS	~1
HIRDLS	~57
MIPAS (ESA)	~30
MIPAS (IMK-IAA)	~30
MLS	~65
SMR	~4

This includes the datasets for N_2O, CFC-11, CFC-12, and SF_6.

Overview of WP2400 - limb

Task

Perform an intercomparison analysis and validation of all relevant satellite limb products using independent reference data (balloon and aircraft).

Output

Product Validation and Intercomparison Report [D2.3], contribution to publication.

Intercomparisons: Finding coincidences

Coincidence criteria considered

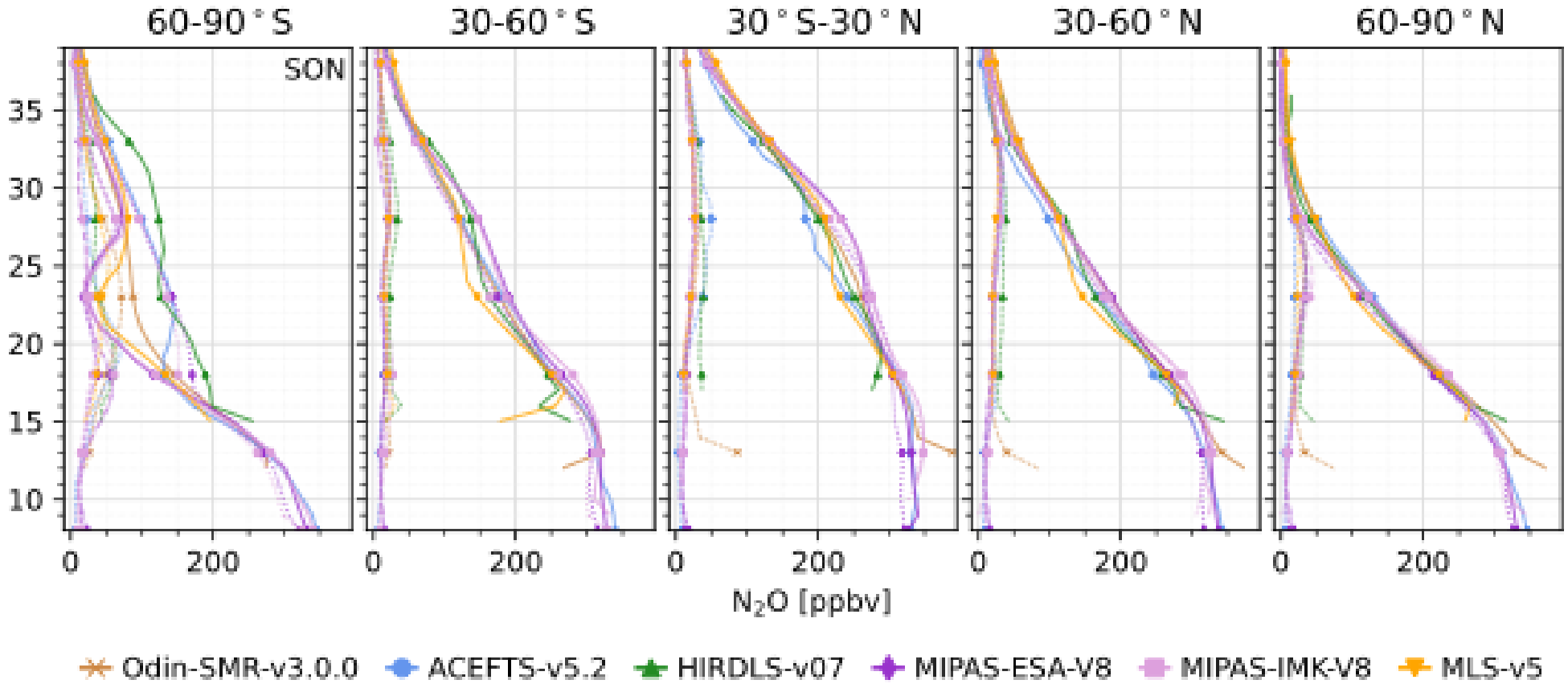
- Different time criteria (within 3 hr, 6 hr, 12 hr).
- Using distance (within 100 km, 300 km, 1000 km).
- Using latitude (within 5°).

Final coincidence criteria

- Within 6 hr.
- Within 300 km.
- The closest profile in distance that met these criteria that had not already been matched with another profile was used.

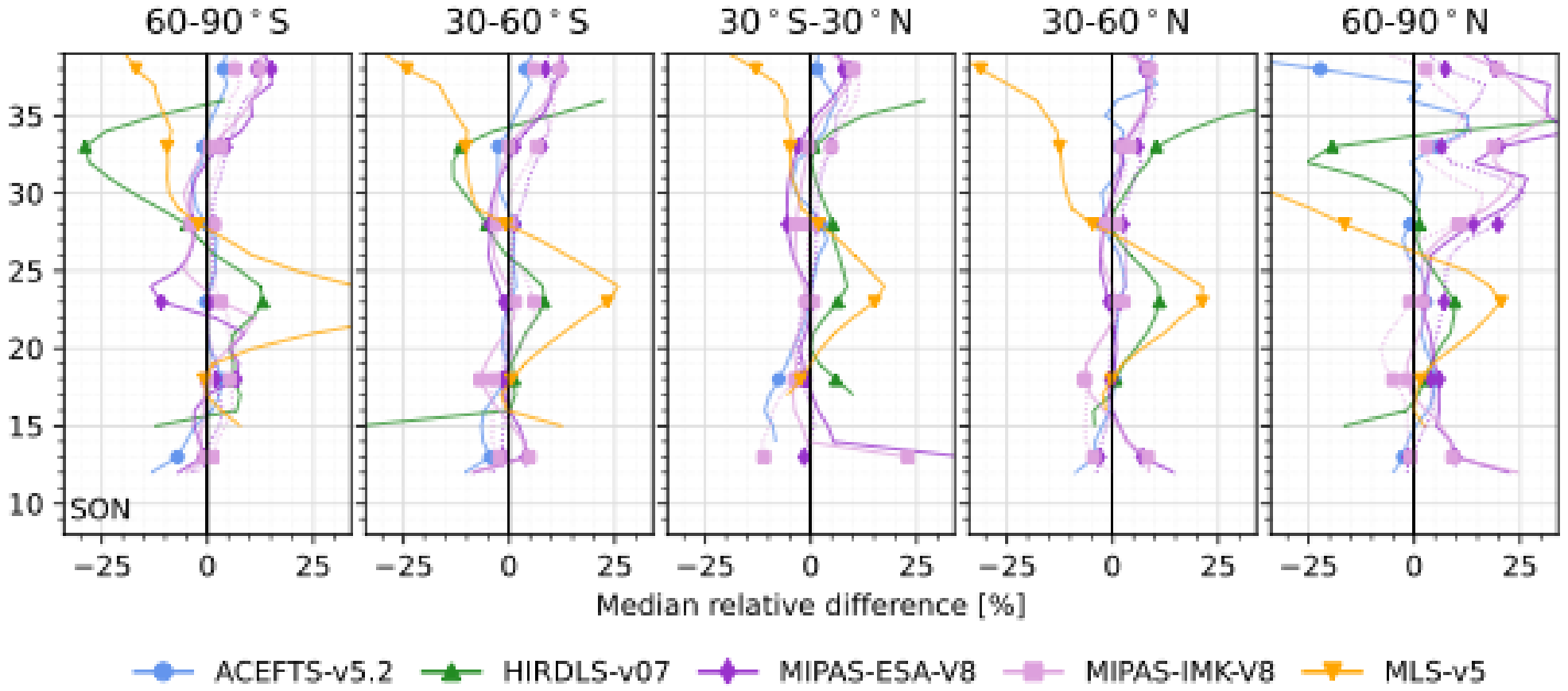
Coincidences were identified between each pair of datasets (6 datasets = 15 unique pairs).

Intercomparisons: Profiles (N_2O)



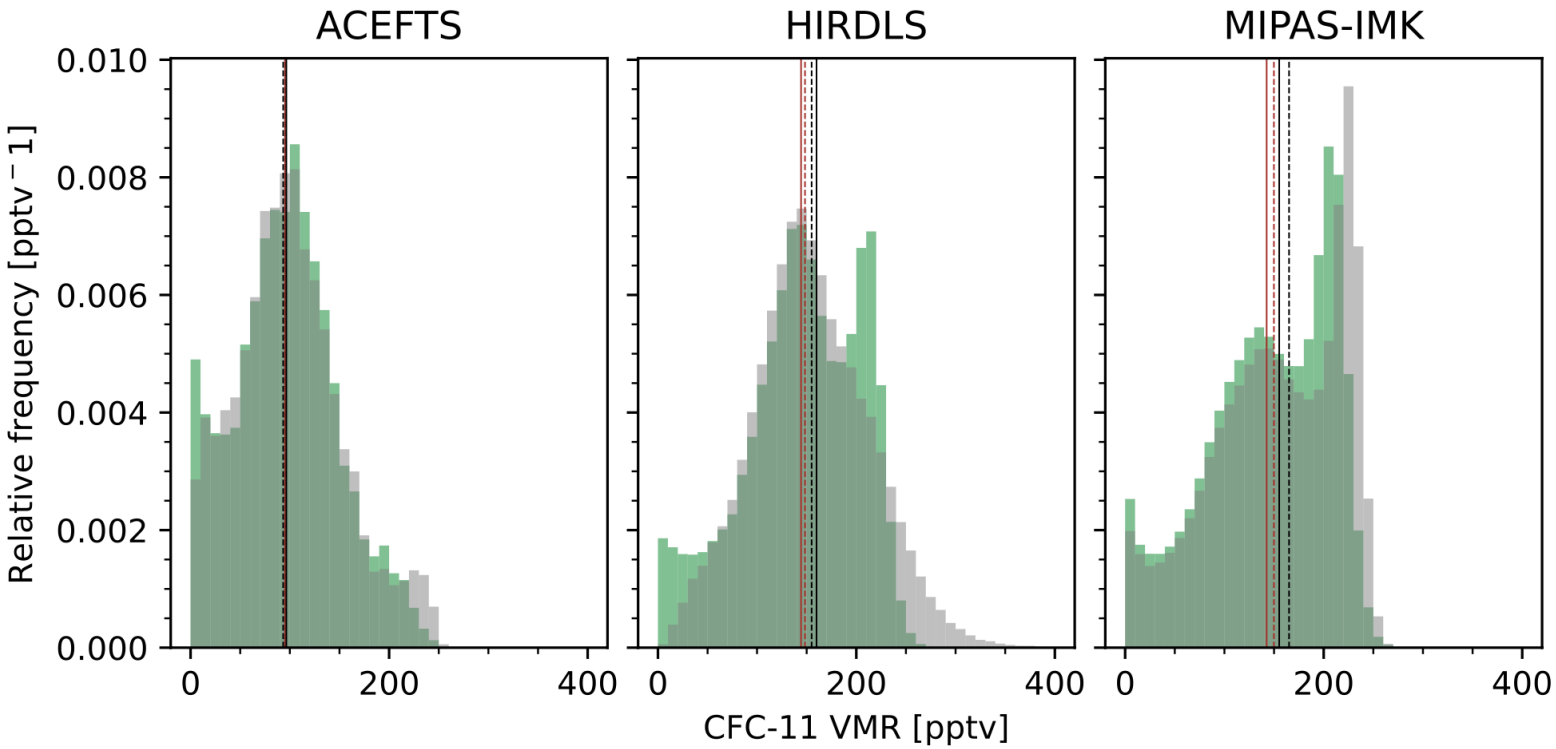
Median VMR (solid, except MIPAS full-resolution period is dotted) and median absolute deviation of the VMR (dashed) for each instrument. Only profiles coincident with an **SMR** profile were included.

Intercomparisons: Difference profiles (N_2O)



Median absolute difference between **SMR** and coincident measurements from each other instrument. The MIPAS full-resolution period is shown with dotted lines.

Intercomparisons: Probability density functions (CFC-11)



The differences between the panels show the importance of sampling.

The basic shapes agree with ACE-FTS and MIPAS-IMK.

Biased slightly low compared to MIPAS-IMK.

HIRDLS is missing the peak just above 200 pptv.

Probability density functions of **MIPAS-ESA** (reduced resolution period, green) CFC-11 measurements at 18 km that are coincident with each other dataset (grey). The mean is shown as a solid line (MIPAS-ESA RR brown, other black) and the median is shown as a dashed line.

Intercomparisons: Summary plots (N_2O)

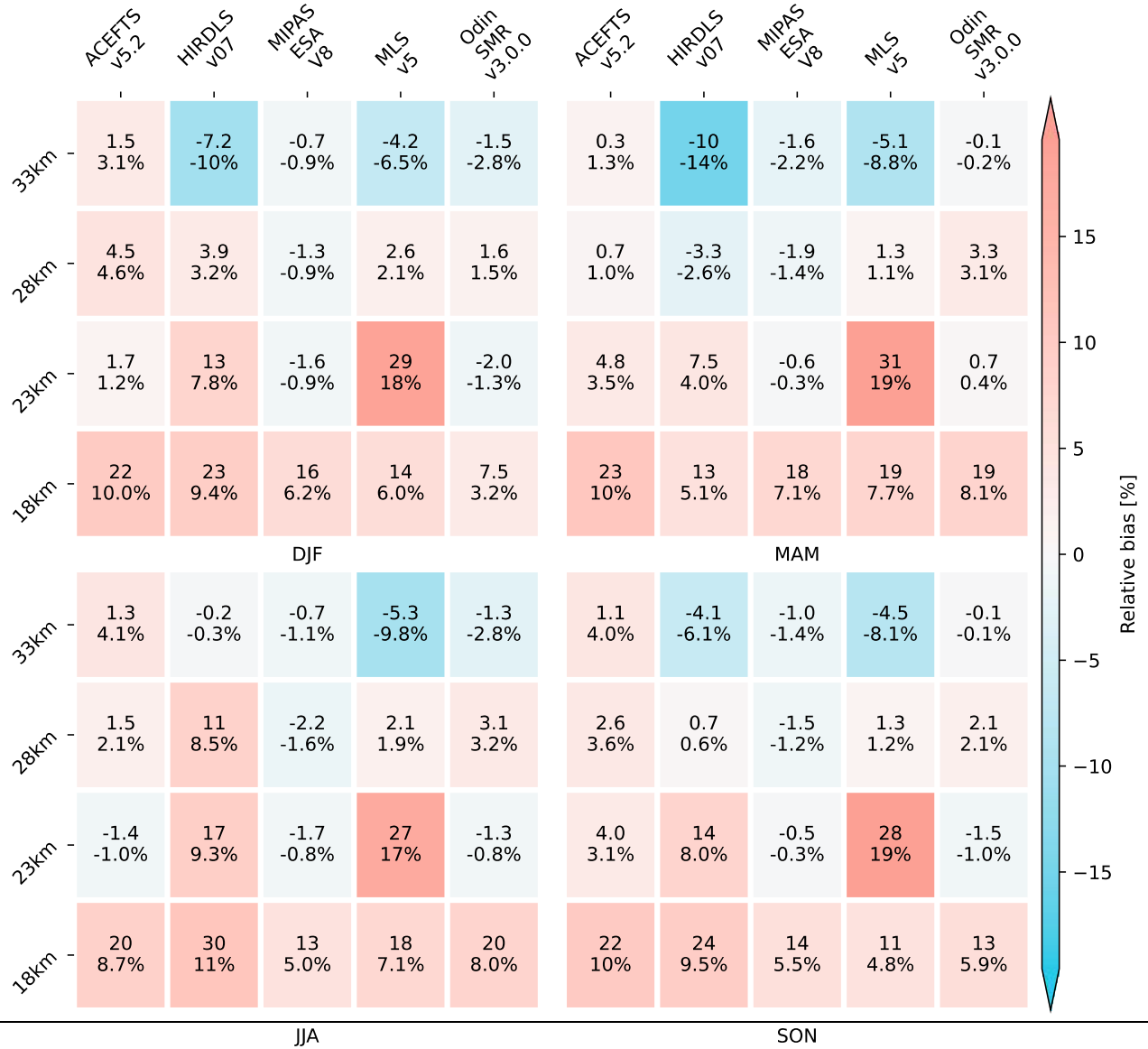
Absolute N_2O bias (ppbv) and relative bias between **MIPAS-IMK RR** and each other instrument.

MIPAS-IMK RR consistently has a high bias of up to 11% at 18 km.

There is a tendency toward a low bias at 33 km.

The worse agreement with MLS at 23 km is due to the kink in the MLS profile (i.e. MLS has a low bias here).

Otherwise, the agreement is very good (within 10%).



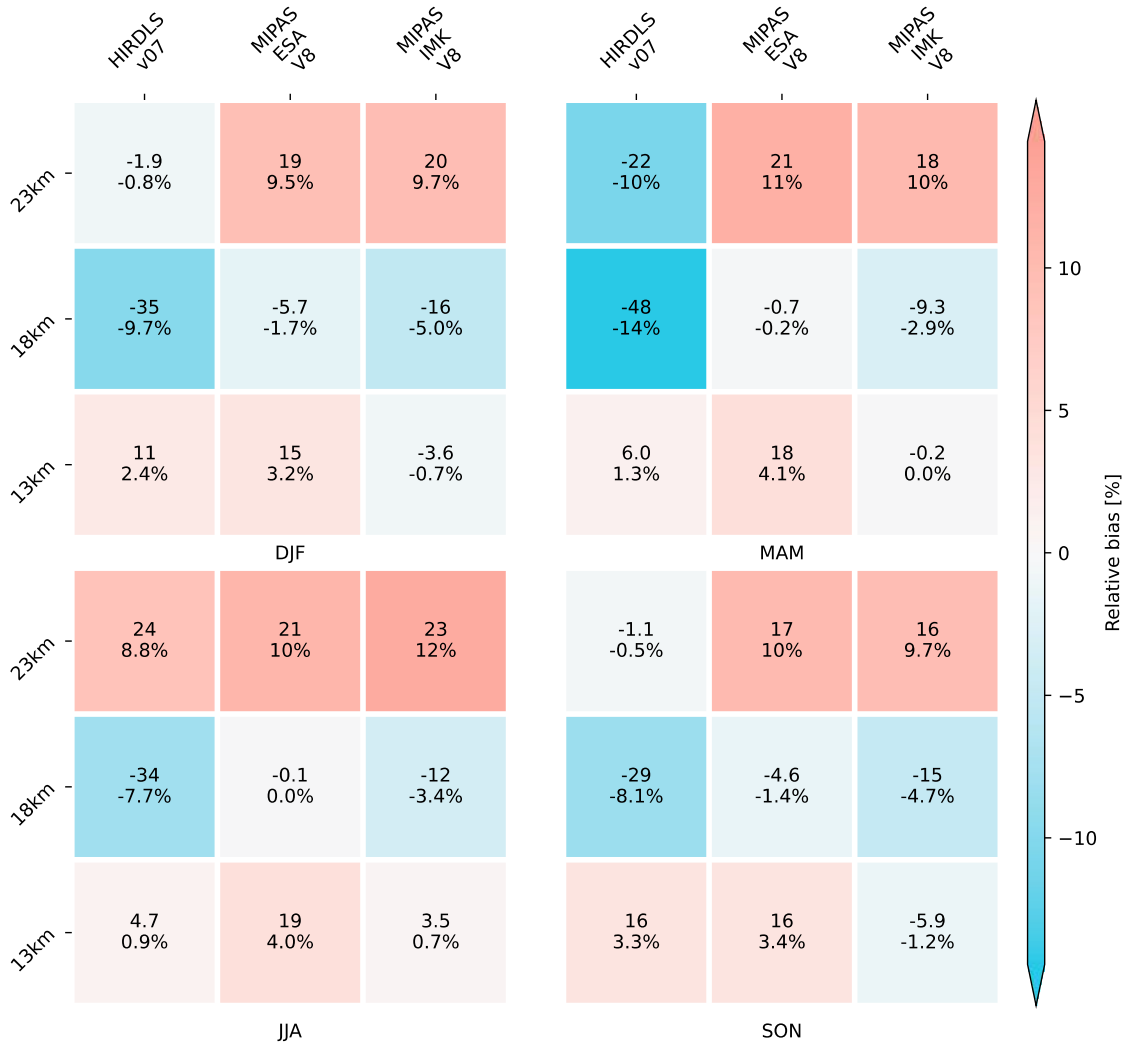
Intercomparisons: Summary plots (CFC-12)

Absolute CFC-12 bias (pptv) and relative bias between **ACE-FTS** and each other instrument.

ACE-FTS has a mostly positive bias (up to 5%) at 13 km, except compared to MIPAS-IMK during DJF, MAM, and SON.

ACE-FTS has a consistent negative bias at 18 km, mostly within 10%.

ACE-FTS has a mostly positive bias (up to 12%) at 23 km, except compared to HIRDLS.



Validation: Datasets and finding coincidences

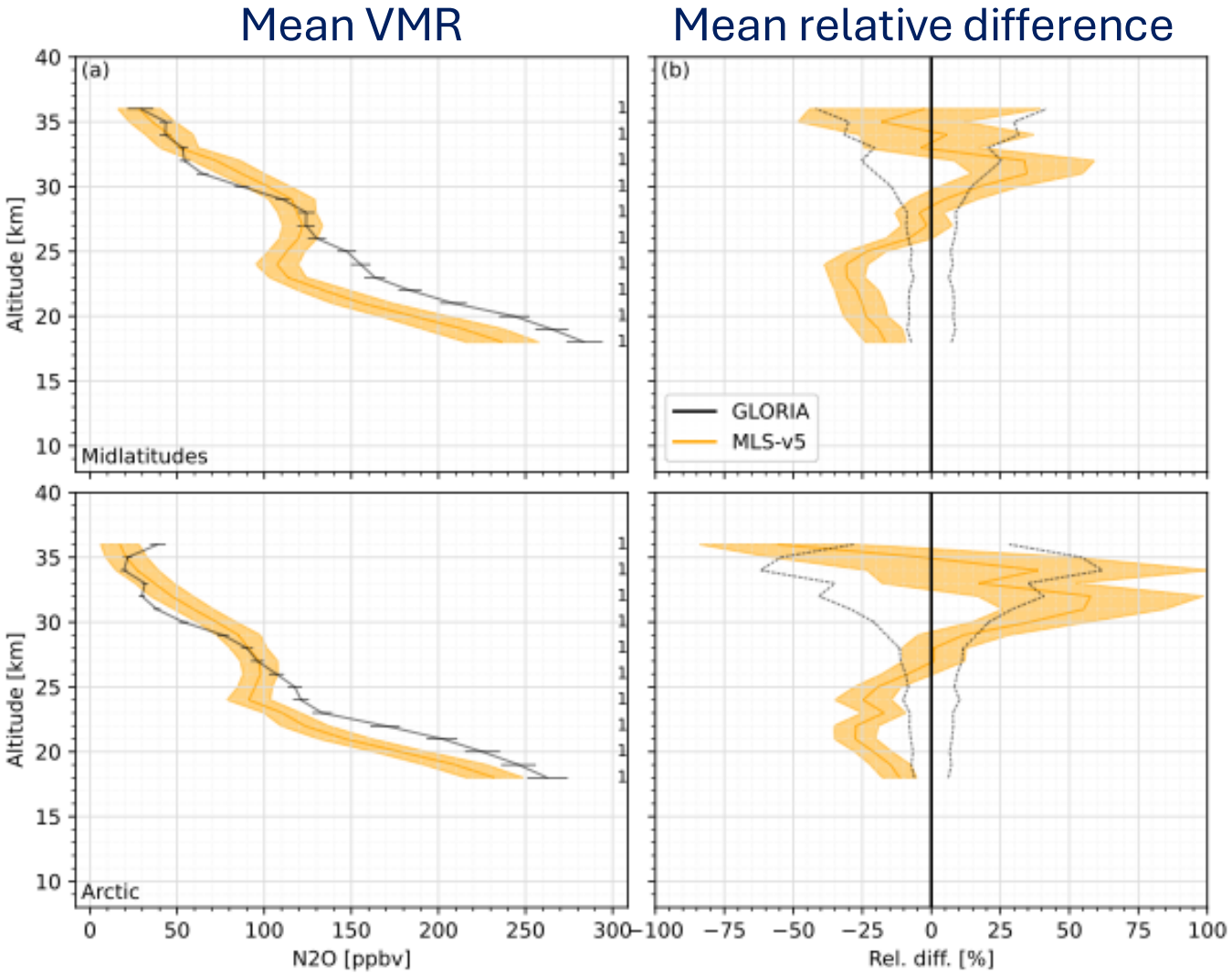
Independent reference datasets

GLORIA: two mean profiles (one for each flight), in August 2021 and August 2022
MIPAS-B: 10 flights, from February 2002-September 2014
MarkIV (MkIV): 17 flights, from December 2002-September 2023

Coincidence criteria selected

- Within 72 hr (all except ACE-FTS, which is within 720 hr/30 days).
- Within 5° latitude.
- On the same side of the polar vortex edge (determined using scaled potential vorticity from the Jet Propulsion Laboratory Derived Meteorological Products, based on MERRA-2 reanalysis data).
- All satellite profiles that met these criteria were averaged.

Validation: Profiles (N_2O)



Shading represents one standard deviation, error bars show reported uncertainty of the **GLORIA** mean profiles. The number indicates how many GLORIA profiles were averaged.

These comparisons were done for each balloon profile, for each satellite instrument.

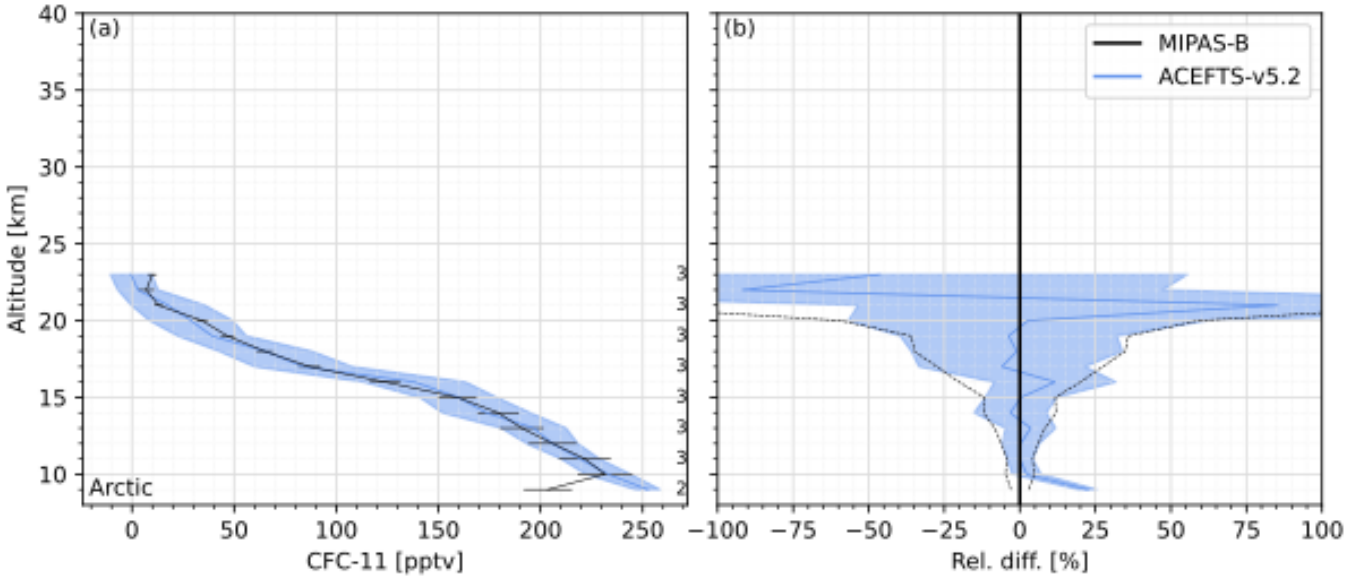
The kink in the **MLS** profile at 25 km is present in the midlatitudes and the Arctic.

The profiles are mostly consistent above 25 km except from 30-32 km.

Validation: Profiles (CFC-11)

Mean VMR

Mean relative difference

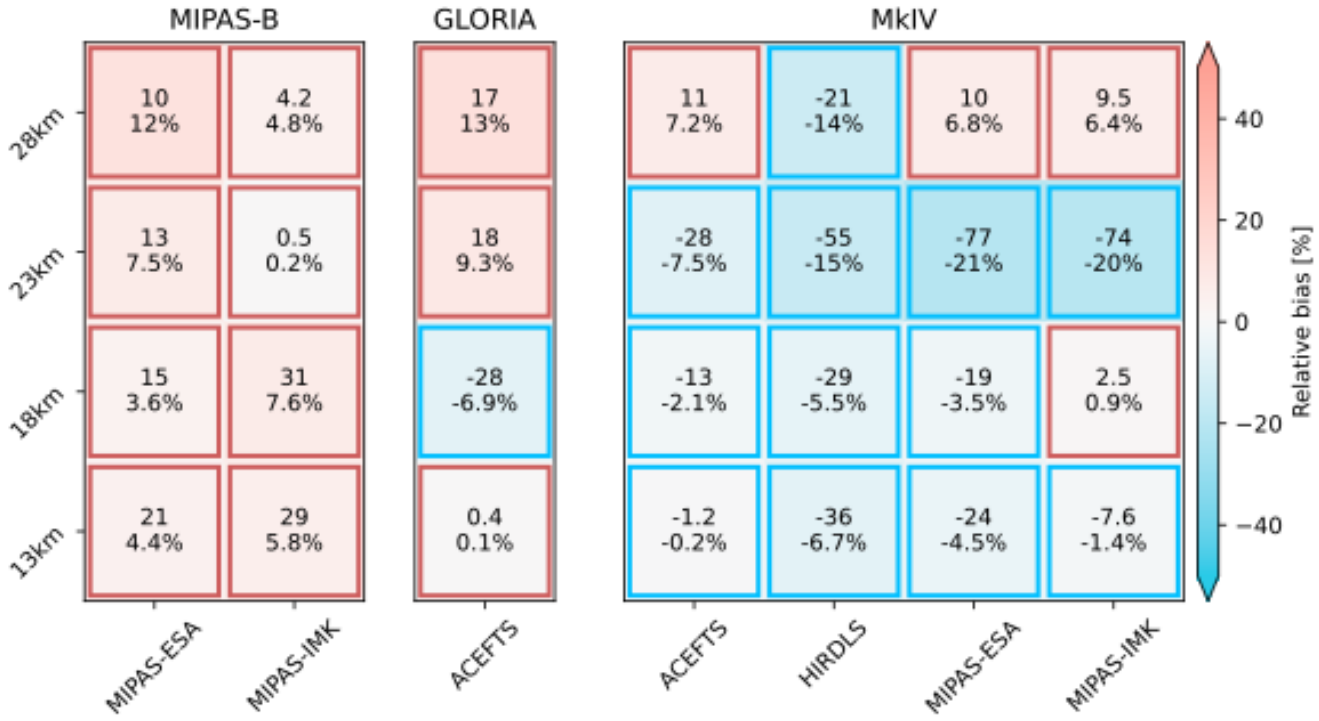


Shading represents one standard deviation, error bars show reported uncertainty of the **MIPAS-B** mean profiles. The number indicates how many MIPAS-B profiles were averaged.

Filtering for vortex vs. extravortex air greatly improved comparisons in the Arctic: the mean profiles are consistent except at 9 km, where the MIPAS-B profile has an unrealistic decrease.

The **ACE-FTS** relative differences are large at higher altitudes due to the low VMRs.

Validation: Summary plots



Summary of CFC-12 comparisons in the **midlatitudes**. Absolute differences are shown in pptv above the relative differences. Borders are coloured when the relative difference magnitude is below 50%.

Agreement is very good: 22/28 boxes have relative differences within 10%.

All comparisons with MIPAS-B show a high bias. Does this indicate a low bias in the MIPAS-B measurements?

Most comparisons relative to MkIV show a negative bias.

Summary

WP 2200: Limb dataset harmonization

- Files are available for N_2O, CFC-11, CFC-12, and SF_6.

WP 2400: Limb dataset intercomparison and validation

- Coincident profiles were intercompared using profile plots, PDFs, and summary grid plots.

- ACE-FTS v5.2, MIPAS V8, and SMR v3.0.0 perform well across all comparisons, with only minor biases found in some regions.

-HIRDLS v07 has variable performance; check the intercomparisons in different regions and seasons for your application.

-The MLS N_2O profiles have a kink centred near 32 hPa (24 km).

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