



Product Quality Assessment Report (PQAR) – ANNEX E for IASI CO₂ and CH₄ (v9.1) and AIRS CO₂ mid-tropospheric products

C3S2_312a_Lot2_DLR – Atmosphere

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History of modifications

Version	Date	Description of modification	Chapters / Sections
1.1	20-October-2017	New document for data set CDR1 (until 2016)	All
2.0	4-October-2018	Update for CDR2 (until 2017)	All
3.0	12-August-2019	Update for CDR3 (until 2018) and additional information of Metop-C	All, esp. Sects. 1.1 and 2.1
3.1	03-November-2019	Update after review by Assimila: Correction of typos and broken links. Some references added.	All
4.0 beta	18-August-2020	Update for CDR4 (until 2019) with new version of each IASI product	All
4.0	17-September-2020	Correction of issues with numbering of tables and figures based on review by Assimila	All
5.0	18-February-2021	Update for CDR5 (until 2020)	All
6.0	4-August-2022	Update for CDR6 (until 2021)	All
6.1	14-December-2022	Update after review (use of new template, several improvements at various places)	All
6.2	14-February-2023	Update after 2 nd review (several improvements at various places)	All
6.3	02-March-2023	Minor updates after 2 nd review to generate clean version.	All



List of datasets covered by this document

Deliverable ID	Product title	Product type (CDR, ICDR)	Version number	Delivery date
WP2-FDDP-GHG-v1	CO2_IASA_NLIS, CH4_IASA_NLIS, CO2_IASB_NLIS, CH4_IASB_NLIS CO2_AIRS_NLIS (v3.0)	CDR 6	9.1	31-Aug-2022

Related documents

Reference ID	Document
D1	Main PQAR: Buchwitz, M., et al., Product Quality Assessment Report (PQAR) – Main document for Greenhouse Gas (GHG: CO₂ & CH₄) data set CDR 6 (01.2003-12.2021), project C3S2_312a_Lot2_DLR – Atmosphere, v6.3, 2023. Important Note: <i>This document is an ANNEX to the Main PQAR document and contains the quality assessment results of the data provider.</i> For the final overall quality assessment results of the data products described in this document see the Main PQAR document.
D2	Crevoisier, C., et al., Algorithm Theoretical Basis Document (ATBD) – ANNEX E for IASI CO₂ and CH₄ and AIRS CO₂ mid-tropospheric products, project C3S2_312a_Lot2_DLR – Atmosphere, v6.3, 2023.



Acronyms

Acronym	Definition
AIRS	Atmospheric Infrared Sounder
AMSU	Advanced Microwave Sounding Unit
ATBD	Algorithm Theoretical Basis Document
BESD	Bremen optimal ESTimation DOAS
CAR	Climate Assessment Report
C3S	Copernicus Climate Change Service
CCDAS	Carbon Cycle Data Assimilation System
CCI	Climate Change Initiative
CDR	Climate Data Record
CDS	(Copernicus) Climate Data Store
CMUG	Climate Modelling User Group (of ESA's CCI)
CoMet	Carbon Dioxide and Methane Mission
CONTRAIL	Comprehensive Observation Network for Trace gases by Airlines
CRG	Climate Research Group
D/B	Data base
DOAS	Differential Optical Absorption Spectroscopy
EC	European Commission
ECMWF	European Centre for Medium Range Weather Forecasting
ECV	Essential Climate Variable
EMMA	Ensemble Median Algorithm
ENVISAT	Environmental Satellite (of ESA)
EO	Earth Observation
ESA	European Space Agency
EU	European Union
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FCDR	Fundamental Climate Data Record
FoM	Figure of Merit
FP	Full Physics retrieval method
FTIR	Fourier Transform InfraRed
FTS	Fourier Transform Spectrometer
GCOS	Global Climate Observing System
GEO	Group on Earth Observation
GEOSS	Global Earth Observation System of Systems
GHG	GreenHouse Gas
GOME	Global Ozone Monitoring Experiment
GMES	Global Monitoring for Environment and Security
HIPPO	HIAPER Pole-to-Pole Observations



GOSAT	Greenhouse Gases Observing Satellite
IAGOS	In-service Aircraft for a Global Observing System
IASI	Infrared Atmospheric Sounding Interferometer
ICOS	Integrated Carbon Observation System
IMAP-DOAS (or IMAP)	Iterative Maximum A posteriori DOAS
IPCC	International Panel in Climate Change
IUP	Institute of Environmental Physics (IUP) of the University of Bremen, Germany
JAXA	Japan Aerospace Exploration Agency
JCGM	Joint Committee for Guides in Metrology
L1	Level 1
L2	Level 2
L3	Level 3
L4	Level 4
LMD	Laboratoire de Météorologie Dynamique
MACC	Monitoring Atmospheric Composition and Climate, EU GMES project
NA	Not applicable
NASA	National Aeronautics and Space Administration
NetCDF	Network Common Data Format
NDACC	Network for the Detection of Atmospheric Composition Change
NIES	National Institute for Environmental Studies
NIR	Near Infra Red
NLIS	LMD/CNRS <i>neuronal</i> network mid/upper tropospheric CO ₂ and CH ₄ retrieval algorithm
NOAA	National Oceanic and Atmospheric Administration
Obs4MIPs	Observations for Climate Model Intercomparisons
OCO	Orbiting Carbon Observatory
OE	Optimal Estimation
PBL	Planetary Boundary Layer
ppb	Parts per billion
ppm	Parts per million
PR	(light path) PROxy retrieval method
PVIR	Product Validation and Intercomparison Report
QA	Quality Assurance
QC	Quality Control
REQ	Requirement
RMS	Root-Mean-Square
RTM	Radiative transfer model
SCIAMACHY	SCanning Imaging Absorption spectroMeter for Atmospheric ChartographY
SCIATRAN	SCIAMACHY radiative transfer model
SRON	SRON Netherlands Institute for Space Research
SWIR	Short Wava Infra Red



TANSO	Thermal And Near infrared Sensor for carbon Observation
TANSO-FTS	Fourier Transform Spectrometer on GOSAT
TBC	To be confirmed
TBD	To be defined / to be determined
TCCON	Total Carbon Column Observing Network
TIR	Thermal Infra Red
TR	Target Requirements
TRD	Target Requirements Document
WFM-DOAS (or WFMD)	Weighting Function Modified DOAS
UoL	University of Leicester, United Kingdom
URD	User Requirements Document
WMO	World Meteorological Organization
Y2Y	Year-to-year (bias variability)



General definitions

Essential climate variable (ECV)

An ECV is a physical, chemical, or biological variable or a group of linked variables that critically contributes to the characterization of Earth's climate.

Climate data record (CDR)

The US National Research Council (NRC) defines a CDR as a time series of measurements of sufficient length, consistency, and continuity to determine climate variability and change.

Fundamental climate data record (FCDR)

A fundamental climate data record (FCDR) is a CDR of calibrated and quality-controlled data designed to allow the generation of homogeneous products that are accurate and stable enough for climate monitoring.

Thematic climate data record (TCDR)

A thematic climate data record (TCDR) is a long time series of an essential climate variable (ECV).

Intermediate climate data record (ICDR)

An intermediate climate data record (ICDR) is a TCDR which undergoes regular and consistent updates, for example because it is being generated by a satellite sensor in operation.

Satellite data processing levels

The NASA Earth Observing System (EOS) distinguishes six processing levels of satellite data, ranging from Level 0 (L0) to Level 4 (L4) as follows.

- L0 Unprocessed instrument data
- L1A Unprocessed instrument data alongside ancillary information
- L1B Data processed to sensor units (geo-located calibrated spectral radiance and solar irradiance)
- L2 Derived geophysical variables (e.g., XCO₂) over one orbit
- L3 Geophysical variables averaged in time and mapped on a global longitude/latitude horizontal grid
- L4 Model output derived by assimilation of observations, or variables derived from multiple measurements (or both)



Additional definitions as relevant for this document:

In the following some relevant Target Requirement (TR) related definitions are given. For details please see TRD (D4), 2017, ESA-CCI-GHG-URDv2.1 and CMUG-RBD, 2010:

Systematic error: component of measurement error that in replicate measurements remains constant or varies in a predictable manner

Note: “Systematic error” = “Absolute systematic error” (in contrast to “Relative systematic error” defined below).

For satellite GHG ECV products especially the “Relative systematic error” is important. The definition as used here is as follows:

Relative systematic error: Identical with “Systematic error” but after bias correction and without considering a possible “global offset” (overall mean bias). Reflects the importance of spatially and temporally correlated errors (“spatio-temporal biases”). Computed from standard deviations of spatial and temporal biases.

Bias: estimate of a systematic measurement error (JCGM, 2008).

Precision is the measure of reproducibility or repeatability of the measurement without reference to an international standard so that precision is a measure of the random and not the systematic error. Suitable averaging of the random error can improve the precision of the measurement but does not establish the systematic error of the observation (CMUG-RBD, 2010).

Note: Precision (as explained in TRD (D4)) is quantified with the standard deviation (1-sigma) of the error distribution.

Stability is a term often invoked with respect to long-term records when no absolute standard is available to quantitatively establish the systematic error - the bias defining the time-dependent (or instrument-dependent) difference between the observed quantity and the true value (CMUG-RBD, 2010).

Note: Stability requirements cover inter-annual error changes. If the change in the average bias from one year to another is larger than the defined values, the corresponding product does not meet the stability requirement.

Representativity is important when comparing with or assimilating in models. Measurements are typically averaged over different horizontal and vertical scales compared to model fields. If the measurements are smaller scale than the model it is important. The sampling strategy can also affect this term (CMUG-RBD, 2010).

Threshold requirement: The threshold is the limit at which the observation becomes ineffectual and is not of use for climate-related applications (CMUG-RBD, 2010).



Goal requirement: The goal is an ideal requirement above which further improvements are not necessary (CMUG-RBD, 2010).

Breakthrough requirement: The breakthrough is an intermediate level between the “threshold” and “goal” requirements, which - if achieved - would result in a significant improvement for the targeted application. The breakthrough level may be considered as an optimum, from a cost-benefit point of view when planning or designing observing systems (CMUG-RBD, 2010).

Horizontal resolution is the area over which one value of the variable is representative of (CMUG-RBD, 2010).

Vertical resolution is the height over which one value of the variable is representative of. Only used for profile data (CMUG-RBD, 2010).

Observing Cycle (or Revisit Time) is the temporal frequency at which the measurements are required (CMUG-RBD, 2010).



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Scope of document

This document is a Product Quality Assessment Report (PQAR) for the Copernicus Climate Change Service (C3S, <https://climate.copernicus.eu/>) greenhouse gas (GHG) component as covered by project C3S2_312a_Lot2.

Within this project satellite-derived atmospheric carbon dioxide (CO₂) and methane (CH₄) Essential Climate Variable (ECV) data products will be generated and delivered to ECMWF for inclusion into the Copernicus Climate Data Store (CDS) from which users can access these data products and the corresponding documentation.

The satellite-derived GHG data products are:

- Column-averaged dry-air mixing ratios (mole fractions) of CO₂ and CH₄, denoted XCO₂ (in parts per million, ppm) and XCH₄ (in parts per billion, ppb), respectively.
- Mid/upper tropospheric mixing ratios of CO₂ (in ppm) and CH₄ (in ppb).

This document describes the validation / quality assessment of the C3S products CO₂_IASA_NLIS (v9.1), CH₄_IASA_NLIS (v9.1), CO₂_IASB_NLIS (v9.1), CH₄_IASB_NLIS (v9.1), CO₂_AIRS_NLIS (v3.0).

These products are mid-tropospheric CO₂ and CH₄ Level 2 products as retrieved from the IASI sensors on Metop-A and Metop-B and mid-tropospheric CO₂ from AIRS using algorithms developed at CNRS-LMD, France.



Executive summary

This document describes the performance for the Level 2 CO₂ and CH₄ data products retrieved from IASI observations at CNRS-LMD and delivered to the Copernicus Climate Change Service (C3S). These products are mid-tropospheric-averaged dry-air mixing ratios (mole fractions) of CH₄ and CO₂, retrieved at 9:30 am/pm (local time) from observations made by the IASI and AMSU instruments onboard the European Metop-A (July 2006-August 2021) and Metop-B (since February 2013) platforms, and mid-tropospheric-averaged dry-air mixing ratios (mole fractions) of CO₂, retrieved at 13:30 am/pm (local time) from observations made by the AIRS and AMSU instruments onboard NASA Aqua platform.

IASI and AIRS observations were spatially and temporally collocated with observations made from aircraft measurements from the CONTRAIL (Machida et al., 2007, 2008; Matsueda et al., 2008; Sawa et al., 2015) and HIPPO (Wofsy et al. 2012) programs, as well as with observations made from balloons using AirCores (Membrive et al., 2017). When enough in-situ data were available, a number of statistics, including accuracy and stability, have been computed from the difference between in-situ measurements and retrievals from space observation. Overall, the CNRS-LMD products are found to be highly stable and meet the Target Requirements (TR) for accuracy and stability. It should be noted that, due to too sparse a validation dataset for CH₄, the TR for stability could not be computed. This calls for continuous effort in performing and developing continuous airborne observations of greenhouse gases.



1. Product validation methodology

1.1 CH₄ and CO₂ mid-tropospheric column averaged mole fractions

The validation is performed for five Level 2 products:

- CO2_IASA_NLIS: mid-tropospheric column averaged mole fractions of CO₂ retrieved from IASI onboard Metop-A.
- CO2_IASB_NLIS: mid-tropospheric column averaged mole fractions of CO₂ retrieved from IASI onboard Metop-B.
- CH4_IASA_NLIS: mid-tropospheric column averaged mole fractions of CH₄ retrieved from IASI onboard Metop-A.
- CH4_IASB_NLIS: mid-tropospheric column averaged mole fractions of CH₄ retrieved from IASI onboard Metop-B.
- CO2_AIRS_NLIS: mid-tropospheric column averaged mole fractions of CO₂ retrieved from AIRS onboard Aqua.

As described in [D2], the four first products have been retrieved from simultaneous observations of the IASI and AMSU instruments flying together onboard the Metop satellites using a non-linear inference scheme based on neural networks. IASI hyperspectral observations in the thermal infrared at 7.7 μm for CH₄ or 15 μm for CO₂, which are sensitive to both temperature and gas concentrations of CH₄ or CO₂, respectively, are used in conjunction with microwave observations from the AMSU instruments, only sensitive to temperature, to decorrelate both signals (Crevoisier et al., 2009a, 2009b, 2013). The fifth product has been similarly obtained with AIRS and AMSU observations.

Potential radiative systematic biases existing between simulations used in the inference scheme and observations are computed for each channel by averaging, over the instruments full years of operation, the differences between simulations and collocated (in time and space) satellite observations. The simulations are performed using the 4A/OP-2009 forward model¹ (*Scott and Chédin, 1981*), which is based on the updated 2011 version of the GEISA spectroscopic database² (Jacquinet-Husson et al., 2011), and radiosonde measurements from the Analyzed Radio Soundings Archive database³ IASI calibrated radiance spectra (level1c) are received through the EUMETCast near real time data distribution service via the French AERIS center⁴.

The retrieved CO₂ and CH₄ integrated columns are weighted to the tropical mid-troposphere with peak sensitivity at about 230 hPa (~11 km), half the peak sensitivity at 100 and 500 hPa (~6 and 16 km), and no sensitivity to the surface. Retrievals are performed over land and sea, by night and day (9:30 am/pm local time) for clear-sky only (no clouds, no aerosols). The CO₂ retrievals are limited to the tropical region (30N:30S) because of the greater stability of the temperature atmospheric

¹ Available at <https://4aop.aeris-data.fr/>, last access January 2023

² Available at <https://geisa.aeris-data.fr/>, last access January 2023

³ Available at <http://ara.lmd.polytechnique.fr/>, last access January 2023

⁴ <https://www.aeris-data.fr/>, last access January 2023



profile, which helps decorrelating temperature from gas in the observed radiances, yielding a much better precision compared to the extratropics.

In order to cope with failure of various AMSU channels on each Metop satellites, version 9.1 of the retrieval has been designed to process the entire time series of Metop-A and Metop-B data with the same retrieval code that excludes all failed AMSU channels. This yields a homogeneous data set of mid-tropospheric CH₄ and CO₂ from both instruments over the entire time period since the first launch of IASI onboard Metop-A.

1.2 Validation data and method

Validation against high precision / low systematic errors reference observations is required for the mid/upper troposphere CO₂ and CH₄ data products. Unfortunately, measurements of both gases in the free troposphere and stratosphere are very sparse. Validation thus mostly relies on existing aircraft and airborne measurements.

A promising way consists in using 0-30 km concentration profiles measured by balloon-borne atmospheric samplers called AirCores (Karion et al., 2010; Membrive et al., 2017) to which averaging kernels can be applied to derive columns that can then be compared to those derived from space. So far, only a few profiles have been acquired, all in the northern hemisphere. In this validation exercise, use is made of CH₄ profiles from all stations operated by European teams for which data are available: three stations located in France where monthly measurements are made in the framework of the French AirCore program⁵ (Aire-sur-l'Adour, Trainou, Reims), two stations also managed by the French AirCore team (Timmins, Ontario, Canada and Kiruna in Sweden). Additional profiles acquired through a cooperation with the Finnish Meteorological Institute come from Sodankylä. Spanning 2014-2019, they are used to validate both Metop-A and Metop-B retrievals (CH₄_IASA_NLIS and CH₄_IASB_NLIS).

Additional validation data come from measurements performed by commercial aircrafts made as part of the CONTRAIL project (Matsueda et al. 2008, Machida et al., 2008, Sawa et al., 2015). Concentration of CO₂ and CH₄ are then provided at the altitude of the flight, typically at 10-12 km for most of the flight, and as profile during ascend or descent at airports. For previous years, use is made of in situ observations made by commercial airliners from April 1993 to March 2007 between Japan and Australia⁶. These observations, partly analyzed by Matsueda et al. (2002), are available on a monthly basis. They cover the altitude range 9–13 km. Several gaps have affected the measurements throughout the period, which prevents making robust statistics from them.

⁵ <https://aircore.aeris-data.fr>, last access January 2023

⁶ Data available at <https://gaw.kishou.go.jp/>



2. Validation Results

2.1 Products CO2_IASA_NLIS and CO2_IASB_NLIS

2.1.1 Validation

2.1.1.1 Validation with aircraft measurements

Figure 1 shows comparison of IASI CO₂ mid-tropospheric columns with CONTRAIL aircraft data as monthly means in 12 latitudinal bands of 5° each. Figure 2 shows the scatter plot of IASI CO₂ vs. CONTRAIL CO₂ for the whole period. The R correlation coefficient is 0.98 for IASI-A (v9.1) and 0.92 for IASI-B (v9.1), the bias and the standard deviation of the difference between both being 0.96 ± 1.20 ppm. The bias for v9.1 is larger than for previous versions (the difference was 0.57 ± 0.99 ppm for CRDP3). This might come from the change in the retrieval code that has led to a change in the vertical sensitivity to CO₂ variations as explained in [D2]. With a higher sensitivity to CO₂ at lower altitudes than previous versions, the difference between the partial column retrieved from IASI and the in-situ concentration measured at 11-12 km by CONTRAIL is expected to be higher.

To compute the various parameters summarized in the following tables, the time series in each latitudinal band displayed in Figure 1 have been used separately.

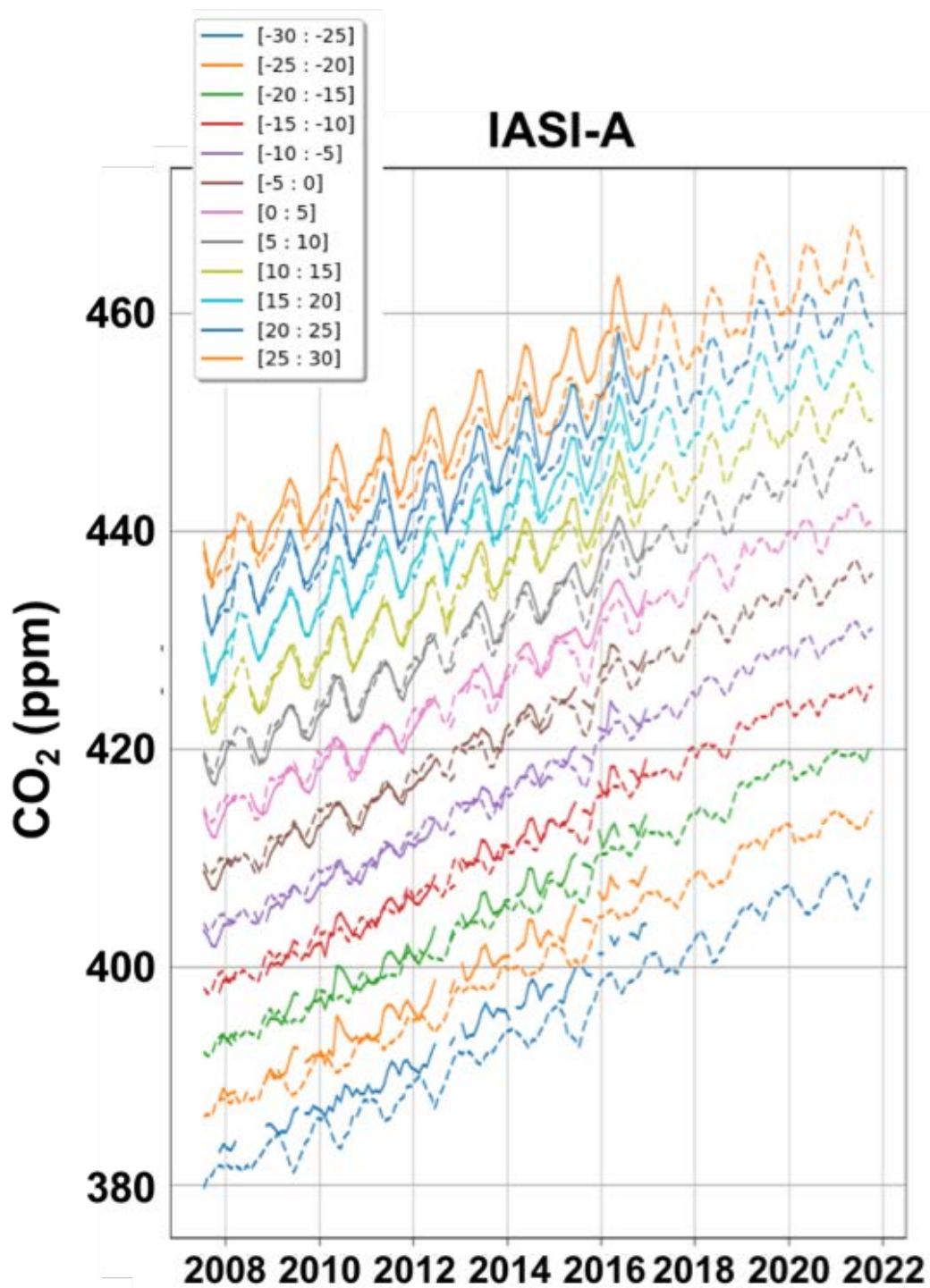
Table 2 shows the mean CONTRAIL-IASI-A CO₂ difference together with the associated standard deviation recorded in each latitudinal band. The mean CONTRAIL-IASI-A bias over all latitudinal band is 0.96 ppm.

Table 2: Mean and standard deviation (std) of CO₂ (ppm): difference between CONTRAIL and IASI (v9.1) over 12 latitudinal bands of 5° each. Statistics over July 2007-December 2019.

Latitudinal band	30S: 25S	25S: 20S	20S: 15S	15S: 10S	10S: 5S	5S :EQ	EQ: 5N	5N: 10N	10N: 15N	15N: 20N	20N: 25N	25N: 30N
IASI-CONTRAIL Mean	2.80	1.88	0.94	0.27	-0.11	0.01	0.27	0.24	0.38	0.99	1.58	2.32
IASI-CONTRAIL std	1.52	1.45	1.31	1.17	1.15	1.18	1.29	1.17	0.99	1.00	1.04	1.16



Figure 1: Monthly variation of IASI mid-tropospheric CO₂ v9.1 (dashed line) for Metop-A (left) and Metop-B (right) from July 2007 to September 2021 and of CONTRAIL CO₂ (full line) from July 2007 to December 2016 in 12 latitudinal bands of 5° each from 30S to 30N.



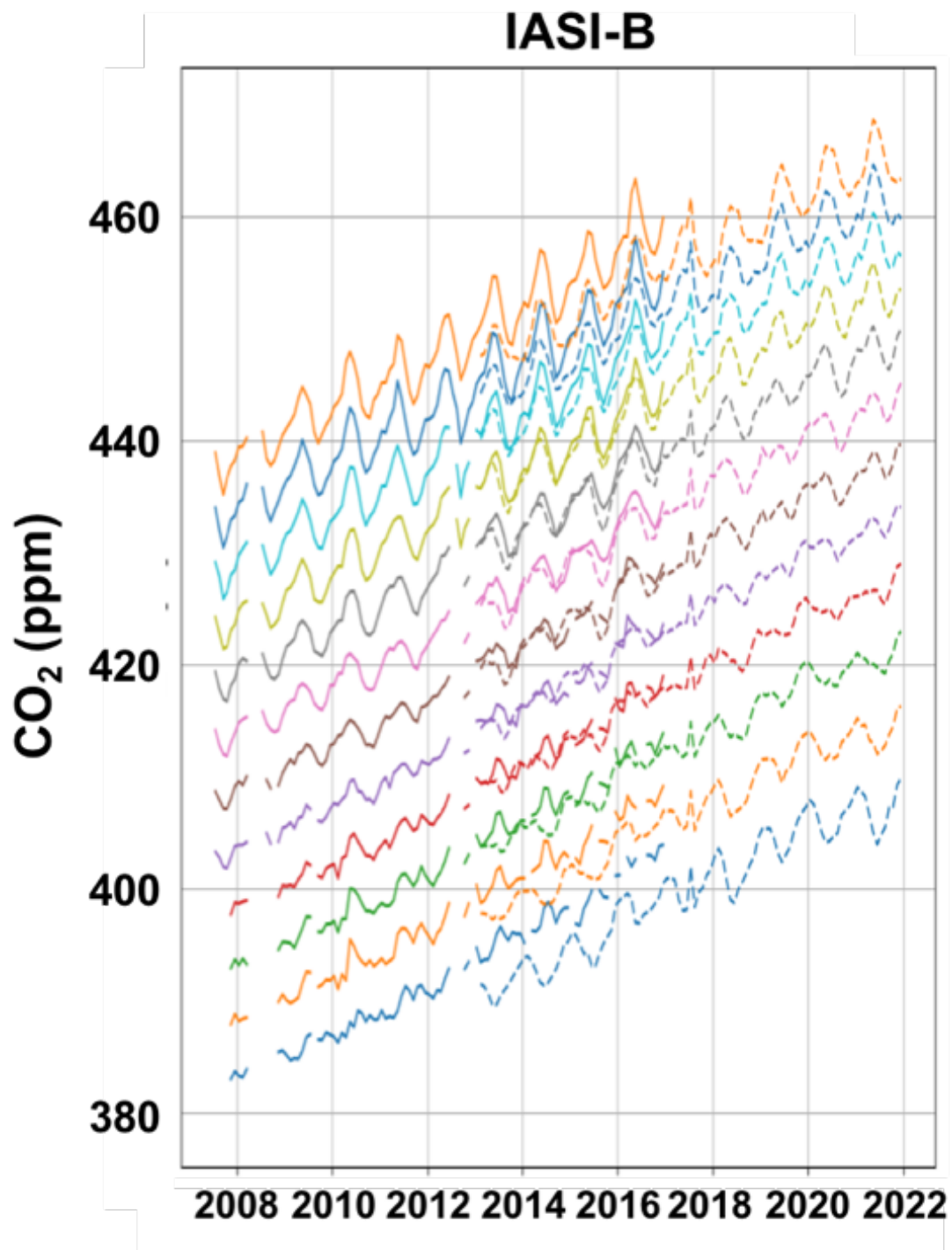
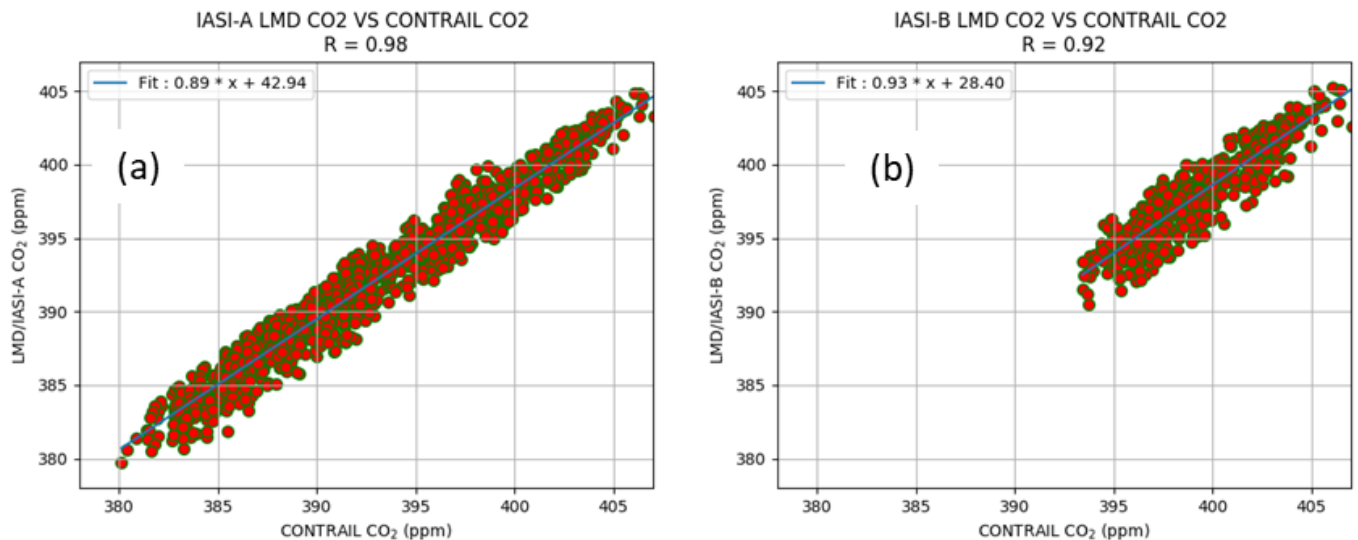




Figure 2: Scatter plot of IASI mid-tropospheric CO₂ v9.1 (IASI-A on left and IASI-B on right) vs. CONTRAIL CO₂ measured at 10 km over the whole period available for CONTRAIL depicted in Fig. 1 (July 2007 – December 2016) measured by aircraft at 10-12 km (dashed line) in 12 latitudinal bands of 5° each.



The relative systematic error is computed as the standard deviation of the CONTRAIL – IASI bias obtained in each latitudinal band. It is computed as two values:

- the “relative spatial bias”, which is the standard deviation of the mean per-latitudinal band bias computed over the entire time series. This was found to be 0.96 ppm.
- The “relative spatio-temporal bias”, which is the standard deviation of the seasonal mean bias in each latitudinal band (i.e. JFM, AMJ, JAS, OND). This was found to be 1.09 ppm.

For each latitudinal band, the linear drift was computed as the slope of the linear regression of the mean CONTRAIL –IASI bias against time. Table 3 shows the resulting drift and error. The main drift over all bands is 0.06 ± 0.10 ppm/year.

Table 3: Linear drift of CO₂ (ppm).

Latitudinal band	30S: 25S	25S: 20S	20S: 15S	15S: 10S	10S: 5S	5S :EQ	EQ: 5N	5N: 10N	10N: 15N	15N: 20N	20N: 25N	25N: 30N
Linear drift [ppm/year]	0.01	-0.06	-0.02	-0.02	-0.02	-0.06	0.06	0.12	0.20	0.24	0.14	0.11

Finally, the year-to-year stability in each latitudinal band was computed as the difference between the maximum and the minimum values of the monthly differences within each year. This stability was found to be 2.78 ± 0.81 ppm/year.



2.1.1.2 Consistency between Metop-A and Metop-B

A direct comparison between mid-tropospheric CO₂ fields retrieved from Metop-A and Metop-B (version V9.1) yields a global bias and standard deviation of -0.28 ppm +/- 0.69 ppm.

Figure 3 shows the full time series of mid-tropospheric CO₂ retrieved from Metop-A and Metop-B. For most of the common period, the two products, which are recorded at the same local time but with a 180° shift in the orbit, are coincident. However, in 2020, the CO₂ retrieved from IASI/Metop-A is lower than the one retrieved from IASI/Metop-B. This is linked to a change in the correction of the detectors non linearity on Metop-A by the end of 2019. This change at instrument level has impacted the radiances themselves in the longwave band of the IASI spectrum where the CO₂ absorption bands are located. The full characterization of this change is on-going. Once the impact has been properly characterized at Level 1, a correction of the radiances will be made and taken into account in the retrieval process.

Figure 3: Mid-tropospheric CO₂ retrieved from IASI/AMSU onboard Metop-A (blue) between July 2007 and November 2020, and from IASI/AMSU onboard Metop-B (blue) between February 2013 and September 2021.

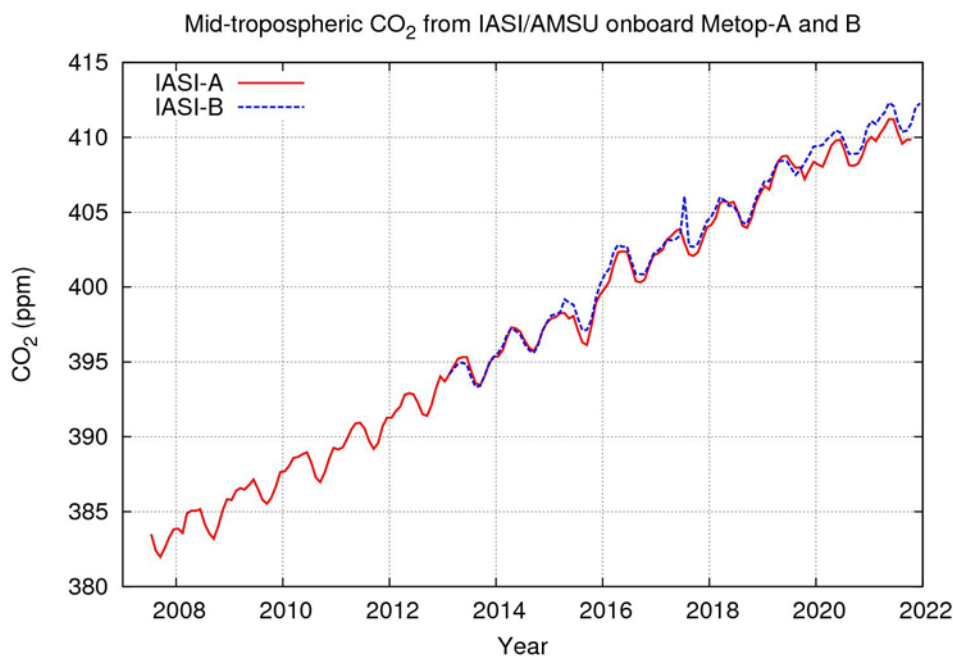




Figure 4 shows the seasonal maps (3 month average) of mid-tropospheric CO₂ retrieved from Metop-A and Metop-B. Figure 5 shows the difference between the two and the associated standard deviation, over the whole period common between the instruments (2014-2020). The Metop-A and -B derived fields are close to each other. However, a small but positive bias for latitudes higher than 30 degrees can be seen. These biases appear to be constant throughout the year. Such constant biases might be due to the change from a tropical air mass to a mid-latitude air mass that is not consistent between the two instruments; this point will be checked for future releases.



Figure 4: Seasonal maps (3 month average) of mid-tropospheric CO₂ as retrieved from Metop-A (left) and Metop-B (right), average over 2014-2021.

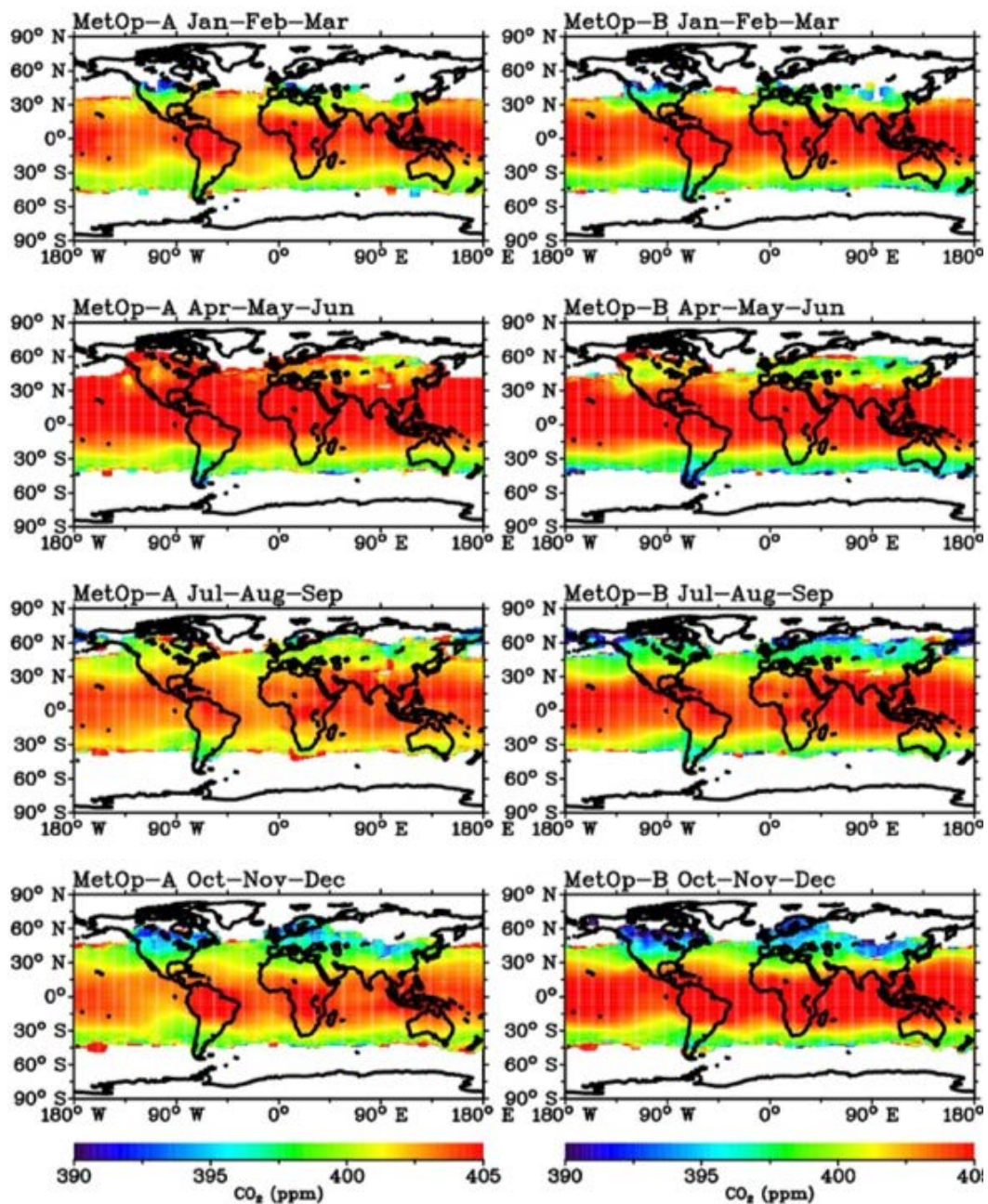
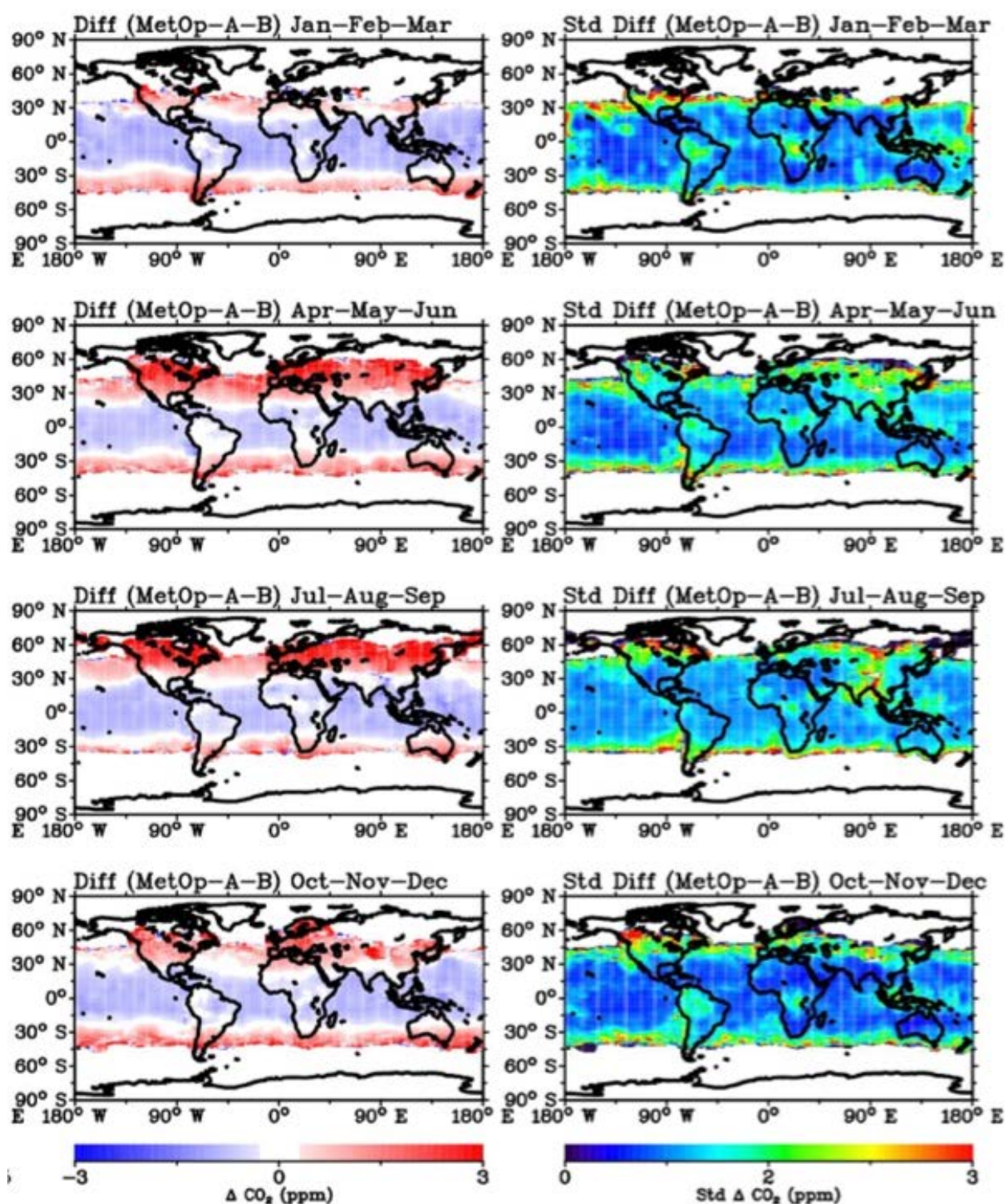




Figure 5: Seasonal maps (3 month average) of mid-tropospheric CO₂: Mean (left) and standard deviation (right) of the difference between Metop-A and Metop-B, average over 2014-2021.





2.1.2 Validation summary

The validation results are summarized in the table below.

Table 4: Product Quality Summary Table for product CO2_IASA_NLIS. T means Threshold; B means Breakthrough; G means Goal.

Product Quality Summary Table for Product: CO2_IASA_NLIS Level: 2, Version: 9.1, Time period covered: 7.2007 – 12.2021				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Single measurement precision (1-sigma) in [ppm]	0.99	< 8 (T) < 3 (B) < 1 (G)	-	-
Mean bias [ppm]	0.96	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppm]	Spatial – spatiotemporal: 0.96 / 1.09	< 0.5	Probability that accuracy TR is met: 50%	This value is based on the comparison between partial column and point measurement.
Stability: Drift [ppm/year]	0.06 ± 0.10 (1-sigma)	< 0.5	Probability that stability TR is met: 100%	-
Stability: Year-to-year bias variability [ppm/year]	2.78 ± 0.81 (1-sigma)	< 0.5	-	-



2.2 Products CH₄_IASA_NLIS and CH₄_IASB_NLIS

2.2.1 Validation

For CH₄ products, only two quantities have been evaluated so far: single measurement precision, and mean bias with both aircraft and AirCore measurements. Due to limited time series of both aircraft and balloons, it has not yet been possible to evaluate the stability criteria.

2.2.1.1 Validation with aircraft measurements

Retrievals are compared with measurements made in the framework of the CONTRAIL project (*Machida et al., 2007, 2008; Matsueda et al., 2008; Sawa et al., 2015*). All IASI retrievals falling in a 5°x5° grid cell centered on each CONTRAIL measurement are averaged. Figure 6 shows the scatter plot of each pair of CONTRAIL / IASI CH₄. Over the whole dataset, the difference between CONTRAIL and IASI CH₄ is -3.38 ± 15.59 ppb, with a correlation R factor of 0.81 for IASI-A and 0.76 for IASI-B.

Figure 6: CONTRAIL CH₄ vs. IASI CH₄ (Metop-A on left and Metop-B on right) for all CONTRAIL measurements over July 2007-December 2017. The 1x1 line is shown as black.

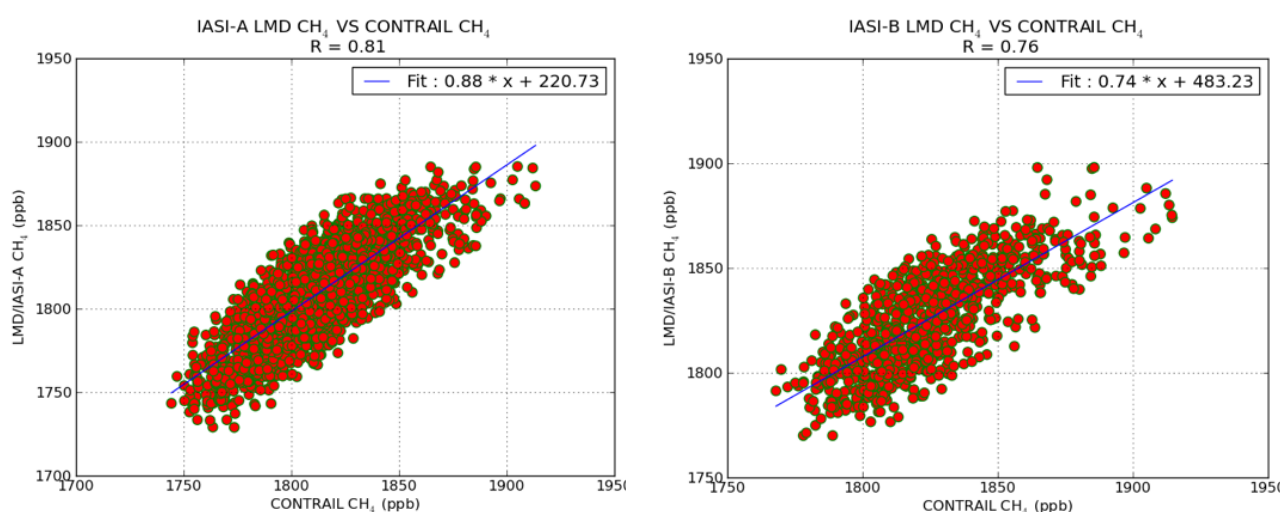


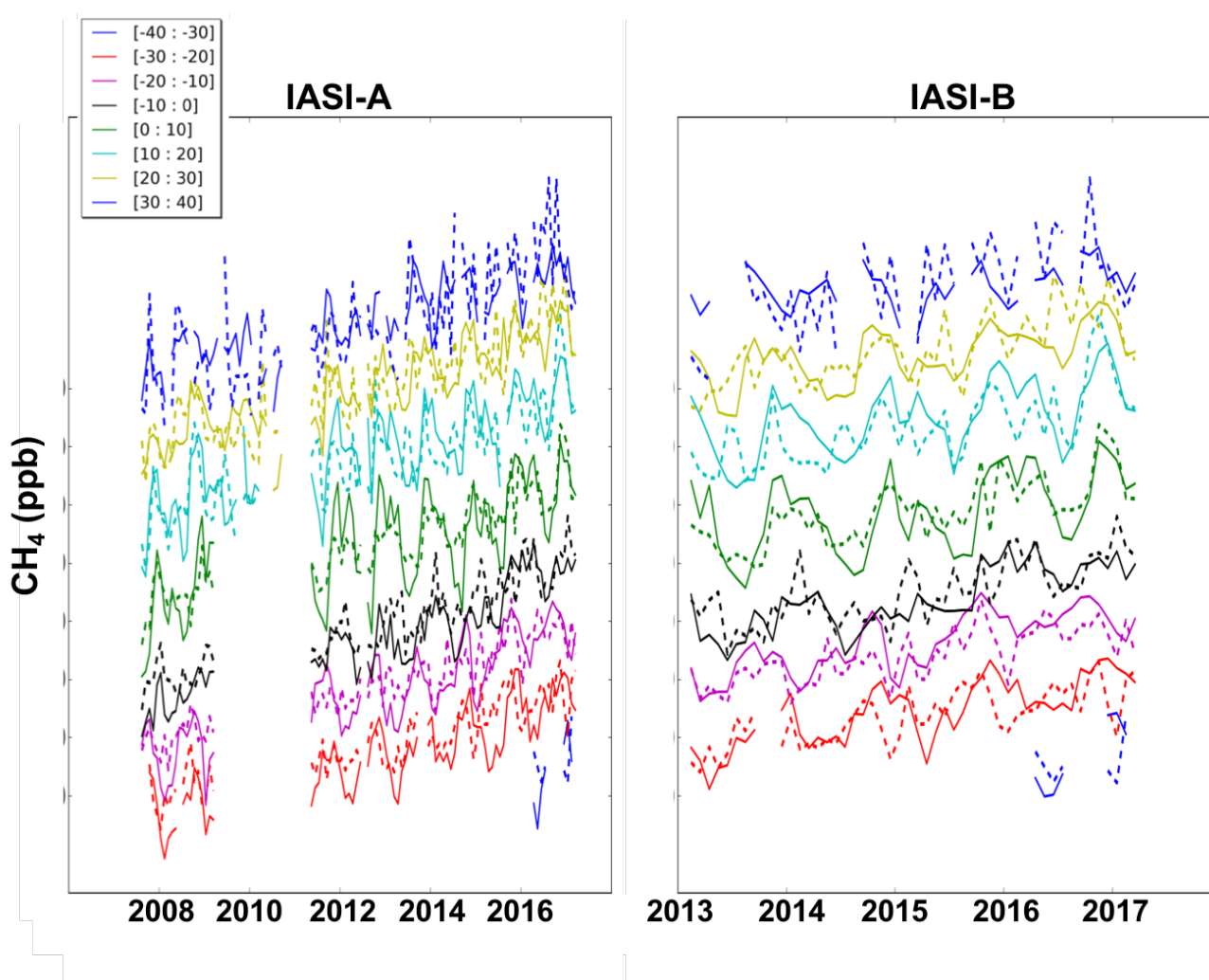
Figure 7 shows the monthly evolution of CH₄ as measured by CONTRAIL (dashed lines) and retrieved by IASI (full line) for 8 latitudinal bands of 10° each. The monthly evolution observed on both datasets is consistent whatever the latitude is, both in terms of seasonality and amplitude. Table 5 summarizes the statistics (mean and standard deviation) obtained within each 8 latitudinal bands for IASI, CONTRAIL and the difference between both. Both datasets are statistically in agreement. The standard deviations of IASI and CONTRAIL inside a given latitudinal band are noticeably close to each other.



Table 5: Mean and standard deviation of CH₄ (ppb): as measured by CONTRAIL aircrafts, as retrieved by IASI, and difference between the two over 7 latitudinal bands of 10° each. Statistics over July 2007-December 2017.

Latitudinal band	30S:40S	30S:20S	20S:10S	10S:EQ	EQ:10N	10N:20N	20N:30S	30N:40N
CONTRAIL	1807.98 ± 15.29	1795.43 ± 25.15	1792.49 ± 24.55	1810.47 ± 28.36	1827.10 ± 25.38	1830.52 ± 23.06	1835.80 ± 19.86	1807.98 ± 15.29
IASI A	1812.81 ± 15.61	1798.55 ± 20.94	1800.85 ± 22.32	1812.30 ± 22.83	1824.71 ± 24.85	1831.64 ± 24.12	1835.74 ± 29.09	1812.81 ± 15.61
IASI- CONTRAIL	-4.83 ± 18.05	-3.12 ± 12.87	-8.37 ± 11.68	-1.83 ± 15.40	2.38 ± 16.05	-1.11 ± 14.29	0.06 ± 20.08	-4.83 ± 18.05

Figure 7: Comparison between CONTRAIL and IASI CH₄ over July 2007-December 2017. Monthly evolution of CONTRAIL CH₄ (dashed line) and IASI CH₄ (full line) for 8 latitudinal bands of 10° each.



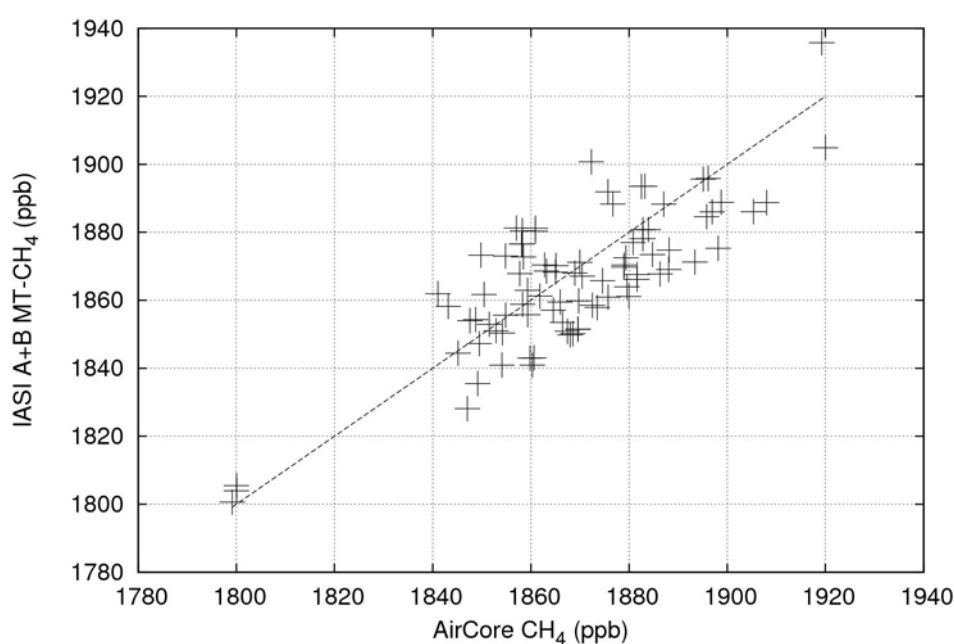


From Table 5, it is straightforward to compute the “relative spatial bias” of the “relative systematic error”, which is the standard deviation of the mean per-latitudinal band bias computed over the whole time series. The Accuracy is found to be 3.38 ppb. Due to several gaps in the time series, as can be seen in Figure 7, it is not possible to compute the “relative spatio-temporal bias” which is the standard deviation of the seasonal mean bias in each latitudinal band.

2.2.1.2 Validation with AirCore 0-30 km profiles

Here, IASI CH₄ retrievals are compared to several AirCore profiles from measurements made by the French AirCore program⁷ (*Membrive et al., 2017*). All IASI retrievals falling in a 5°x5° grid cell centered on each AirCore profile for the same day are averaged. Figure 8 shows the scatter plot of each pair of AirCore/IASI CH₄. Over the whole dataset (44 pairs for Metop-A and for Metop-B), the difference between AirCore and IASI CH₄ is -2.2 ± 13.2 ppb.

Figure 8: Comparison between IASI CH₄ v9.1 and AirCore CH₄. Correlation is 9.1.



⁷ <https://aircore.aeris-data.fr>



2.2.1.3 Comparison between CH₄_IASA_NLIS (Metop-A) and CH₄_IASB_NLIS (Metop-B)

A direct comparison between mid-tropospheric CH₄ fields retrieved from Metop-A and Metop-B (v9.1) yields a global difference of -3.43 ± 7.39 ppb. Figure 9 shows the seasonal maps (3 month average) of mid-tropospheric CH₄ retrieved from Metop-A and Metop-B. Figure 10 shows the difference between the two and the associated standard deviation, over the time period 2014-2020. The Metop-A and -B derived fields are close to each other. However, a small but positive bias at latitude higher than 60 degrees can be observed on the map. These biases appear to be constant throughout the year.



Figure 9: Seasonal maps (3 month average) of mid-tropospheric CH₄ as retrieved from Metop-A (left) and Metop-B (right), averaged over 2014-2021.

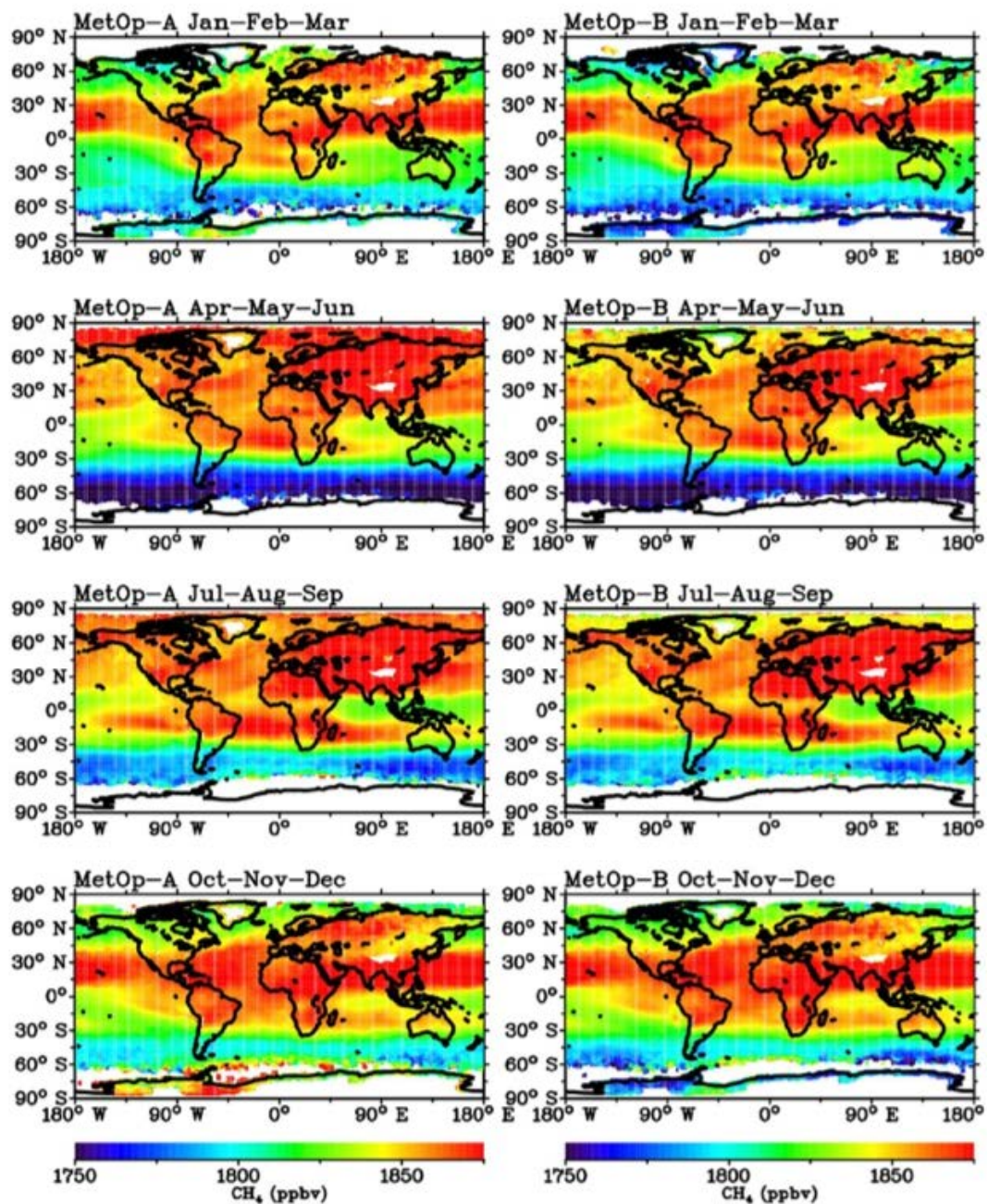
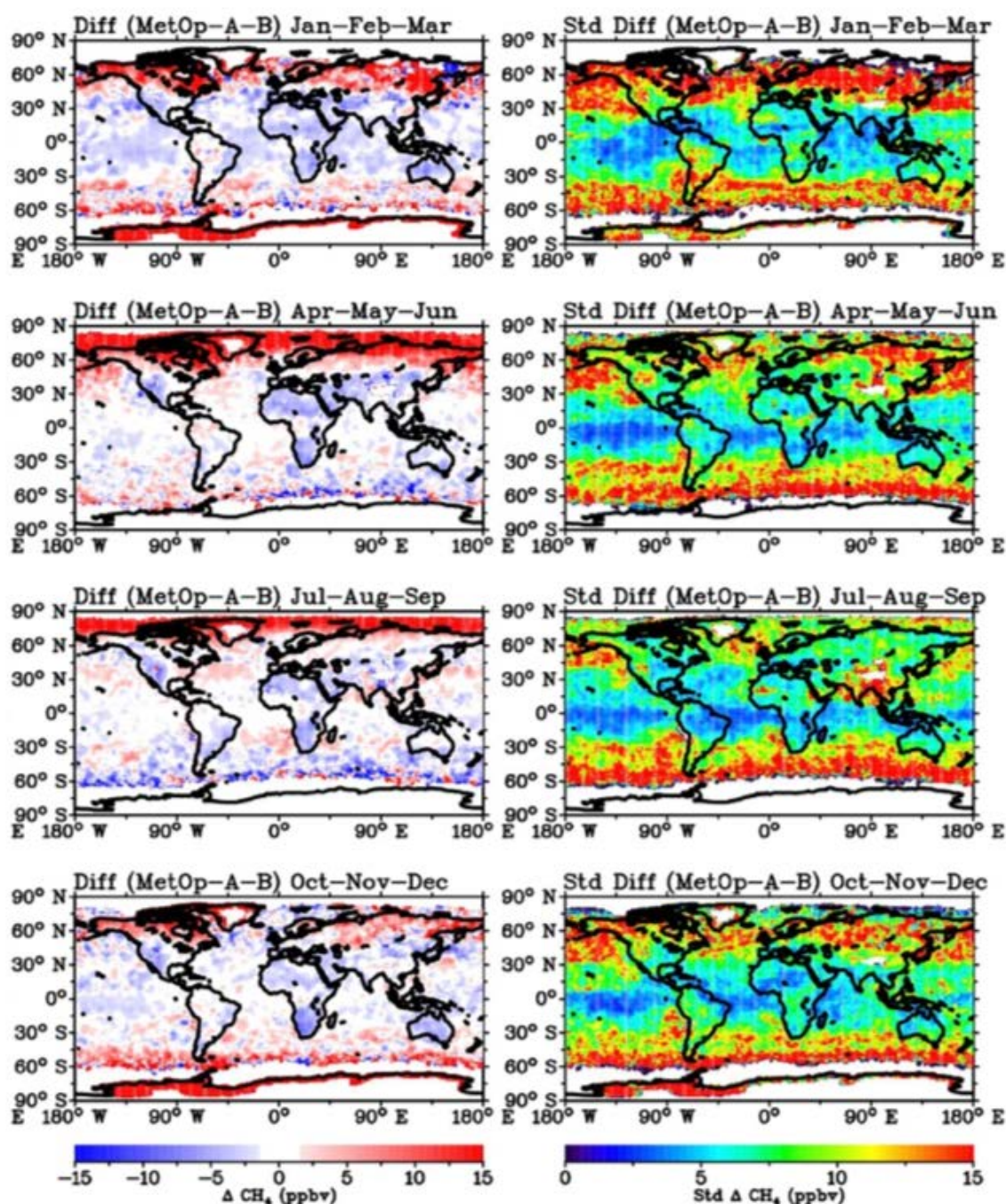




Figure 10: Seasonal maps (3 month average) of mid-tropospheric CH₄: Mean (left) and standard deviation (right) of the difference between Metop-A and Metop-B, averaged over 2014-2021.





2.2.2 Validation summary

The validation results are summarized in the table below for CH4_IASA_NLIS. Please refer to Section 2.2.1.3 for comparison between CH4_IASA_NLIS and CH4_IASB_NLIS.

Table 6: Product Quality Summary Table for products CH4_IASA_NLIS (NC stands for Not computed due to lack of available data). T means Threshold; B means Breakthrough; G means Goal.

Product Quality Summary Table for Product: CH4_IASA_NLIS Level: 2, Version: 9.1, Time period covered: 7.2007 – 12.2021				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Single measurement precision (1-sigma) in [ppb]	11.8	< 34 (T) < 17 (B) < 9 (G)	-	-
Mean bias [ppb]	-3.38	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: relative systematic error [ppb]	3.38	< 10	Probability that accuracy TR is met: 90%	-
Stability: Linear bias trend [ppb/year]	NC	< 3	NC	Time series of available aircraft/AirCore obs are not long enough to compute these 2 parameters
Stability: Year-to-year bias variability [ppb/year]	NC	< 3	-	



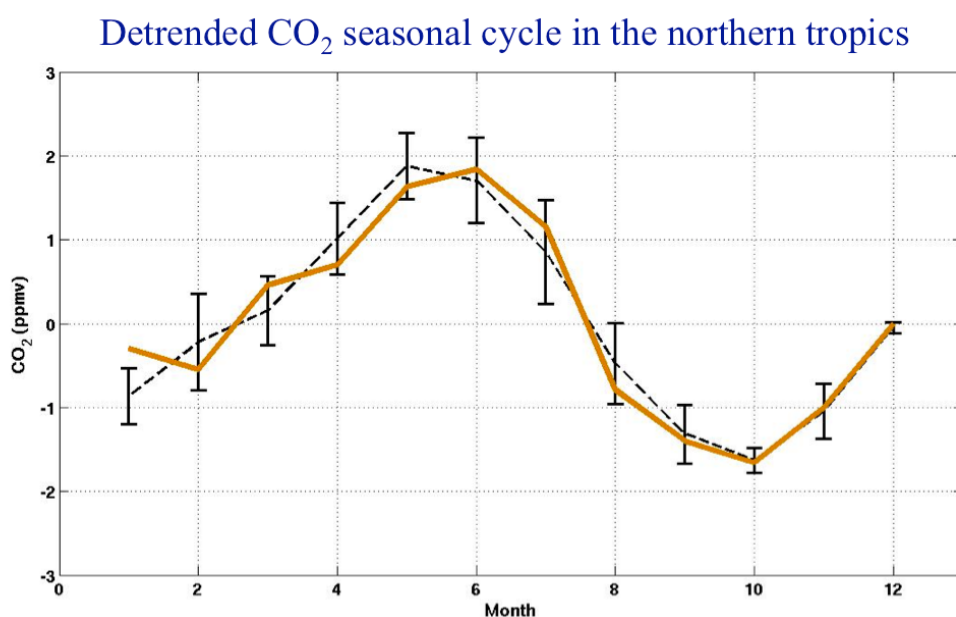
2.3 Product CO₂_AIRS_NLIS

2.3.1 Validation

The seasonal cycles of CO₂ measured by JAL are plotted in Fig. 11 for the period 2005-2006 (only period with full coverage). AIRS retrieved CO₂ cycle is also plotted in Fig. 11. There is a good agreement between both datasets in terms of the phase and amplitude of the seasonal cycle. Overall, the JAL – AIRS CO₂ difference is -0.43 ± 1.32 ppm.

Beginning of mid-2006, the bias between aircraft and AIRS CO₂ increases (negative sign), up to July 2007 when AIRS channels used to perform the retrievals were lost. This might be due to a non-corrected trend, which has affected either the AMSU observations in late 2006 and 2007, or some of the AIRS channels, which started exceeding radiometric specifications.

Figure 11: Detrended CO₂ seasonal cycle in the northern tropics as measured by JAL/CONTRAIL aircraft (black) and as retrieved from AIRS (brown).





2.3.2 Validation summary

Table 7: Product Quality Summary Table for products CO2_AIRS_NLIS. T means Threshold; B means Breakthrough; G means Goal.

Product Quality Summary Table for Product: CO2_AIRS_NLIS Level: 2, Version: 3.0, Time period covered: 4.2003 – 7.2007				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Single measurement precision (1-sigma) in [ppb]	1.32	< 8 (T) < 3 (B) < 1 (G)	-	-
Mean bias [ppb]	-0.43	-	-	No requirement but value close to zero expected for a high quality data product.



3. Application(s) specific assessments

The products can be used to monitor the evolution of major anthropogenic greenhouse gases in the atmosphere, by studying their trends, seasonality and geographical distributions (e.g., Crevoisier et al., 2013). They can also contribute to the characterization of specific emissions, such as those from rice paddies for methane or biomass burning (Thonat et al., 2015). They provide insight on global methane emissions by complementing observations of total columns of methane with observations only sensitive to the troposphere (Cressot et al., 2014).

4. Compliance with user requirements

Mid-tropospheric CO₂:

The single measurement precision of product CO2_IASA_NLIS (from IASI on Metop-A) is 1 ppm. The mean bias (global offset) is 0.96 ppm. The estimated relative accuracy is around 1 ppm. The probability that the < 0.5 ppm user requirement is met has been estimated to 50% taking into account the uncertainty of the reference data and assessment method. The product is also very stable (0.06 +/- 0.10 ppm/year (1-sigma)) meeting the requirement for long-term drift stability. The performance of product CO2_IASB_NLIS (from IASI on Metop-B) is similar.

Mid-tropospheric CH₄:

The single measurement precision of product CH4_IASA_NLIS (from IASI on Metop-A) is 12 ppb. The mean bias (global offset) is -3.4 ppb. The product appears to meet the “relative systematic error” requirement of better than 10 ppb: the estimated relative accuracy is 3.4 ppb. The product appears to be very stable but a quantitative analysis could not be carried out due to lack of reference data. The performance of product CH4_IASB_NLIS (from IASI on Metop-B) is similar.



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