Copernicus Climate Change Service

Product User Guide and Specification (PUGS) – ANNEX E for IASI CO_2 and CH_4 (v9.1) and AIRS CO_2 mid-tropospheric products

C3S_312b_Lot2_DLR – Atmosphere

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Contributors

INSTITUTE OF ENVIRONMENTAL PHYSICS (IUP), UNIVERSITY OF BREMEN, BREMEN, GERMANY

(IUP)

M. Buchwitz

CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE (CNRS), LABORATOIRE DE METEOROLOGIE DYNAMIQUE (LMD), PALAISEAU, FRANCE

(LMD/CNRS)

C. Crevoisier

R. Armante

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History of modifications

Version	Date	Description of modification	Chapters / Sections
1.3	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) with additional information on Metop-C	All, esp. Sects. 1.1 and 1.2
3.1	03-November-2019	Update after review by Assimila: Correction of typos and broken links. Improved typesetting of equations.	All
4.0	18-August-2020	Update for CRD4 (until 2019) with new version of the retrieval code	All

Related documents

Reference ID	Document
D1	**Main PUGS:** Buchwitz, M., et al., Product User Guide and Specification (PUGS) – Main document for Greenhouse Gas (GHG: CO2 & CH4) data set CDR 4 (2003-2019), project C3S_312b_Lot2_DLR – Atmosphere, 4.0, 2020. *(this document is an ANNEX to the Main PUGS)*
D2	**TRD GAD GHG, 2020:** Buchwitz, M., Aben, I., Armante, R., Boesch, H., Crevoisier, C., Hasekamp, O. P., Wu, L.., Reuter, M., Schneising-Weigel, O., Target Requirement and Gap Analysis Document, Copernicus Climate Change Service (C3S) project on satellite-derived Essential Climate Variable (ECV) Greenhouse Gases (CO_2 and CH_4) data products (project C3S_312b_Lot2), Version 2.11, 9-April-2020, pp. 80, 2020.
D3	**Related PQAR:** Crevoisier, C., et al.: Product Quality Assessment Report (PQAR) – ANNEX E for IASI CO_2 and CH_4 and AIRS CO_2 mid-tropospheric products, C3S project C3S_312b_Lot2_DLR, v4.0, 2020.

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)
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
GOSAT	Greenhouse Gases Observing Satellite
IASI	Infrared Atmospheric Sounding Interferometer

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 *neuronal* network mid/upper tropospheric CO2 and CH4 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

Table 1 lists some general definitions relevant for this document.

Table 1: General definitions.

Item	Definition
XCO_2	Column-averaged dry-air mixing ratios (mole fractions) of CO_2
XCH_4	Column-averaged dry-air mixing ratios (mole fractions) of CH_4
L1	Level 1 satellite data product: geolocated radiance (spectra)
L2	Level 2 satellite-derived data product: Here: CO_2 and CH_4 information for each ground-pixel
L3	Level 3 satellite-derived data product: Here: Gridded CO_2 and CH_4 information, e.g., 5 deg times 5 deg, monthly
L4	Level 4 satellite-derived data product: Here: Surface fluxes (emission and/or uptake) of CO_2 and CH_4

Scope of document

This document is a Product User Guide and Specification (PUGS) for the Copernicus Climate Change Service (C3S, https://climate.copernicus.eu/) greenhouse gas (GHG) component as covered by project C3S_312b_Lot2.

Within this project satellite-derived atmospheric carbon dioxide (CO_2) and methane (CH_4) Essential Climate Variable (ECV) data products have been 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-average dry-air mixing ratios (mole fractions) of CO_2 and CH_4, denoted XCO_2 (in parts per million, ppm) and XCH_4 (in parts per billion, ppb), respectively.
- Mid/upper tropospheric mixing ratios of CO_2 (in ppm) and CH_4 (in ppb).

This document describes the C3S products CO2_IASA_NLIS (v8.0), CH4_IASA_NLIS (v8.4), CO2_IASB_NLIS (v4.2), CH4_IASB_NLIS (v8.1), CO2_AIRS_NLIS (v3.0).

These products are mid-tropospheric CO_2 and CH_4 Level 2 products as retrieved from the IASI sensors on Metop-A and Metop-B and mid-tropospheric CO_2 from AIRS using algorithms developed at CNRS-LMD, France.

Executive summary

This document describes the data and metadata delivered to the Copernicus Climate Change Service (C3S) for the Level 2 CO_2 and CH_4 data products retrieved from IASI and AIRS observations at CNRS-LMD. These products are mid-tropospheric-averaged dry-air mixing ratios (mole fractions) of CH_4 and CO_2, retrieved at 9:30 am/pm (local time) from observations made by the IASI and AMSU instruments onboard the European Metop-A (since July 2006) and Metop-B (since February 2013) platforms. They also include CO_2 mid-tropospheric-averaged dry-air mixing ratios derived from observations made by AIRS and AMSU instruments flying onboard Aqua for the period 2003-2005.

Data are provided as daily netCDF files available at the C3S website. Their content (data format, averaging kernels, geolocation information, etc.) as well as information on performances and limitations will be given.

1. Product description

1.1 The IASI instrument onboard the Metop platforms

The Infrared Atmospheric Sounding Interferometer (IASI) is a high resolution Fourier Transform Spectrometer based on a Michelson Interferometer coupled to an integrated imaging system that measures infrared radiation emitted from the Earth (https://iasi.cnes.fr/en/IASI/index.htm). Developed by the Center National d'Etudes Spatiales (CNES) in collaboration with the European Organisation for the Exploitation of Meteorological Satellites (EUMETSAT), IASI was launched in October 2006 onboard the polar orbiting Meteorological Operational Platform (Metop-A), in September 2012 onboard Metop-B and in October 2018 onboard Metop-C. The 3 instruments have been declared operational in July 2007, February 2013 and July 2019, respectively.

IASI provides 8461 spectral samples, ranging from 645 cm^{-1} to 2760 cm^{-1} (15.5 µm and 3.6 µm), with a spectral sampling of 0.25 cm^{-1}, and a spectral resolution of 0.5 cm^{-1} after apodization. IASI is an across track scanning system, whose swath width is of 2200 km, allowing global coverage twice a day. The IFOV is sampled by 2×2 circular pixels whose ground resolution is 12 km at nadir at 9:30 am/pm local time.

The combined use of both Metop satellites, which are flying on the same orbit but with nearly half an orbit out of phase, yields a complete coverage of the Earth in one day. With the recent launch of Metop-C, in 2018, these time series will cover about 20 years. In order to be useful for climate studies, it is mandatory that the time series derived from the 3 successive platforms are consistent in order to allow studying trends and growth rates.

1.2 CH_4 and CO_2 mid-tropospheric column averaged mole fractions

Four Level 2 products are described in this document:
- CH4_IASA_NLIS: mid-tropospheric column averaged mole fractions of CH_4 retrieved from IASI onboard Metop-A.
- CH4_IASB_NLIS: mid-tropospheric column averaged mole fractions of CH_4 retrieved from IASI onboard Metop-B.
- CO2_IASA_NLIS: mid-tropospheric column averaged mole fractions of CO_2 retrieved from IASI onboard Metop-A.
- CO2_IASB_NLIS: mid-tropospheric column averaged mole fractions of CO_2 retrieved from IASI onboard Metop-B.

Each of these products have been are retrieved from simultaneous observations of the IASI and AMSU instruments flying together onboard the Metop satellites using a non-linear inference scheme using Multi-Layer Perceptrons with 2 hidden layers. IASI hyperspectral observations in the thermal infrared at 7.7 µm (resp. 15 µm), which are sensitive to both temperature and gas concentrations of CH_4 (resp. CO_2) are used in conjunction with microwave observations form the AMSU instruments, only sensitive to temperature, to decorrelate both signals (*Crevoisier et al., 2009a, 2009b, 2013*).

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 model (Scott and Chédin, 1981; https://4aop.noveltis.com/), which is based on the updated 2011 version of the GEISA spectroscopic database (available at https://geisa.aeris-data.fr) (Jacquinet-Husson et al., 2011), and radiosonde measurements from the Analyzed RadioSoundings Archive database (available at http://ara.lmd.polytechnique.fr). IASI calibrated radiance spectra (level1c) are received through the EUMETCast near real time data distribution service via the French Ether center (https://www.aeris-data.fr/).

The retrieved CO_2 and CH_4 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 CO_2 retrievals are limited to the tropical region (30N:30S) because of the greater stability of the temperature atmospheric profile, which helps decorrelating temperature from gas in the observed radiances, yielding a much better precision compared to the extratropics.

Through comparisons with regular aircraft (*Machida et al., 2008)* or balloon *(Membrive et al., 2017*) measurements as well as observations made at the surface, it has been shown that, once the radiometric characterization of the instruments is performed, IASI and AMSU capture well the trend and interannual variation of CH_4, with an excellent agreement with the rate of increase measured at the surface, giving confidence in the ability of IASI to follow its evolution over the 20 years of the Metop program.

Figure 1 shows the daily coverage provided by the use of both Metop-A and Metop-B in terms of mid-tropopsheric CH_4. Figures 2 shows the monthly time series of mid-tropospheric CO_2 as retrieved from IASI onboard Metop-A.

Figure 1: Daily maps of CH_4 mid-tropospheric column averaged mole fraction retrieved from Metop-A, from Metop-B and from both platforms for September, 15th, 2013.

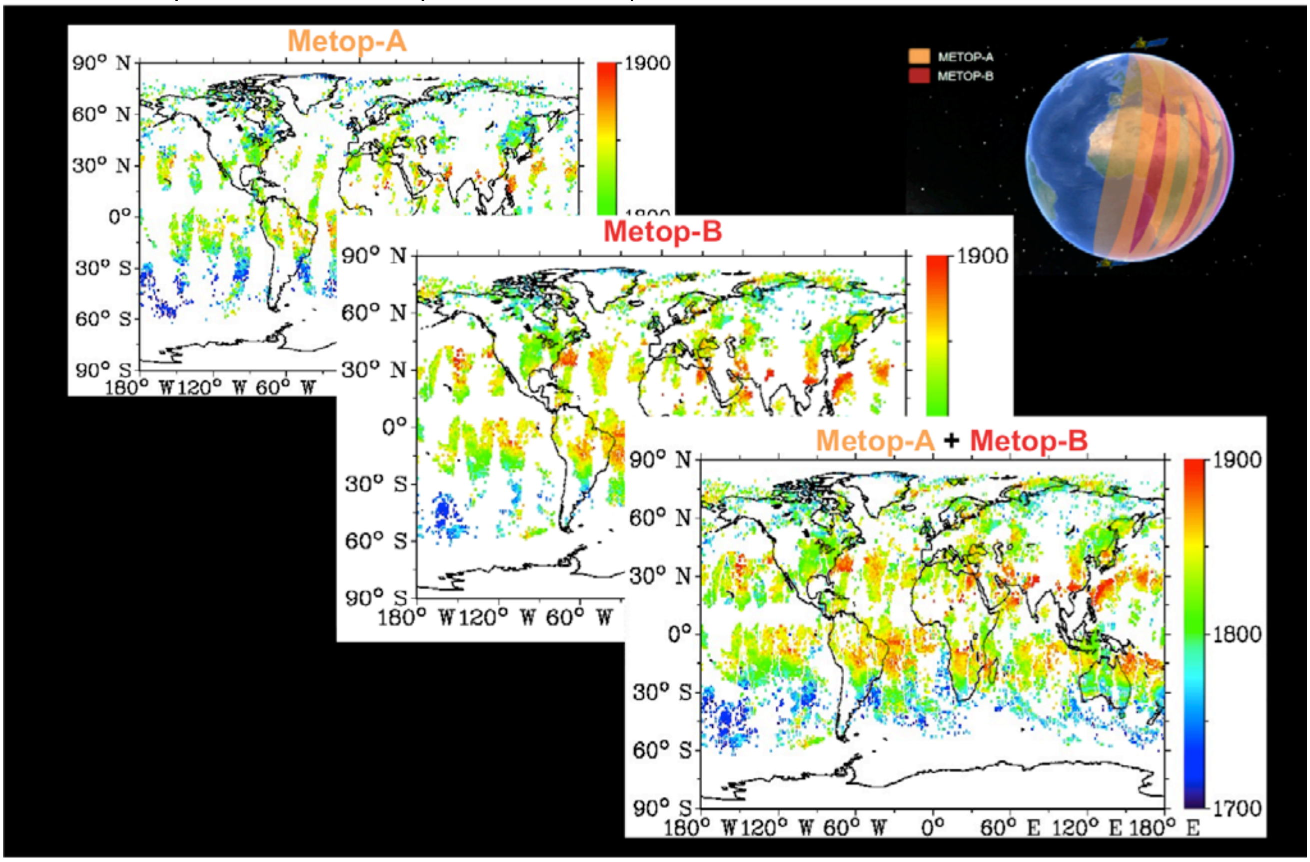


Figure 2: Seasonal maps of mid-tropospheric CH_4 (v9.1) retrieved from Metop-A only (JAS 2007-OND 2012), from Metop-A and Metop-B (JFM 2013-OND 2019).

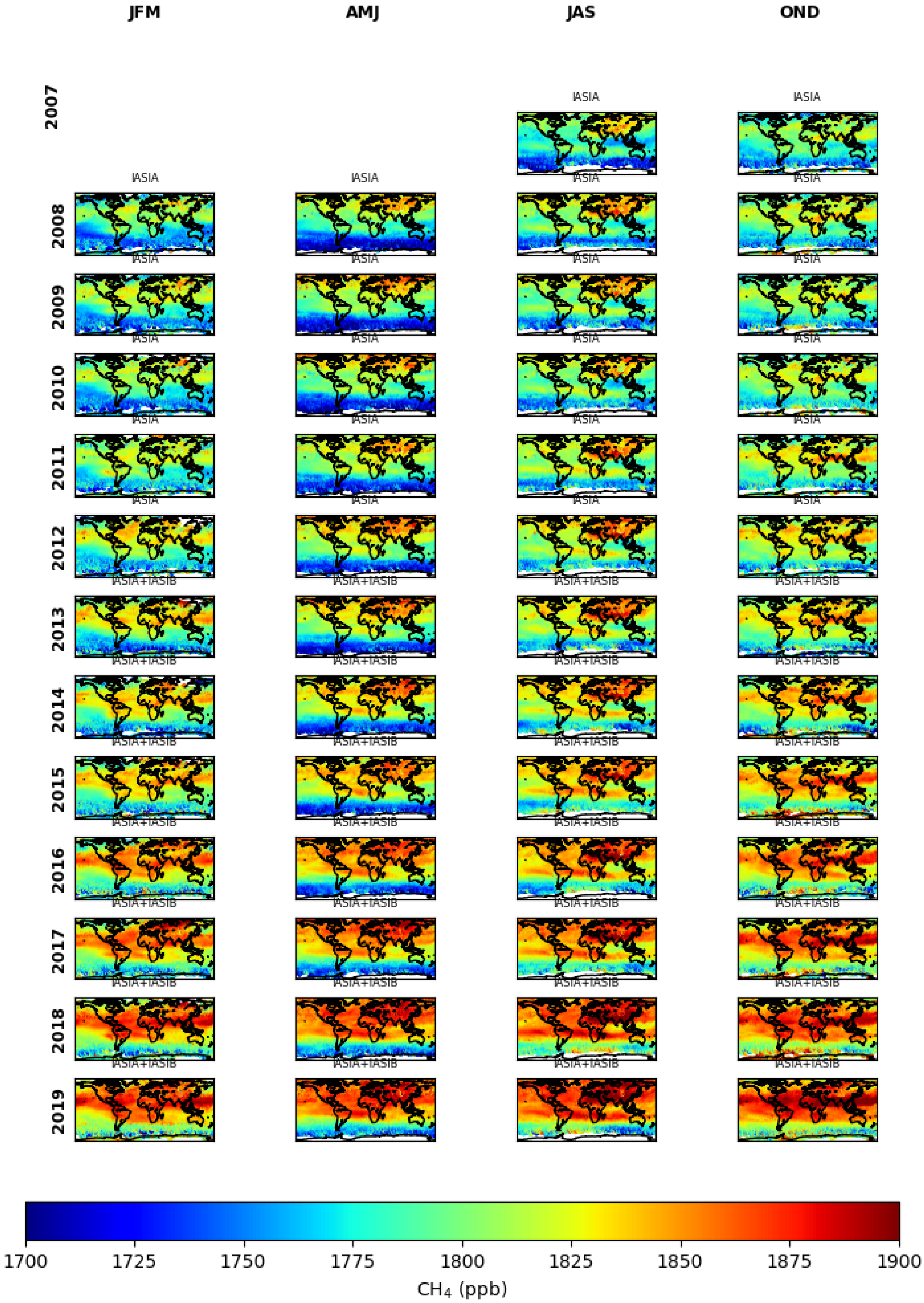


Figure 3: Same as Fig. 2 but mid-tropospheric CO_2 (v9.1).

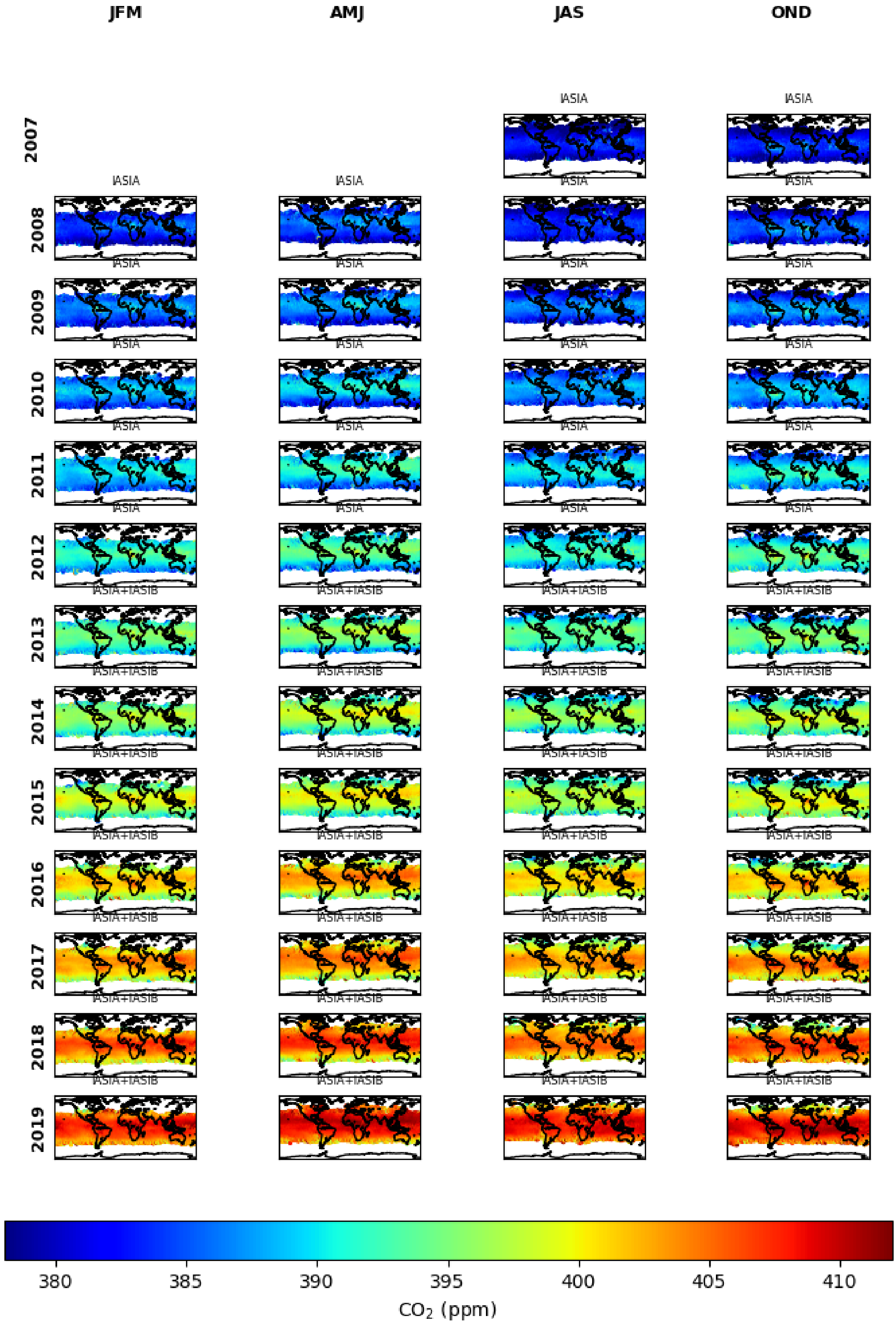


Figure 4. Monthly evolution displayed as a function of latitude of CO_2 mid-tropospheric column averaged mole fraction retrieved from Metop-A and Metop-B combined (version 9.1).

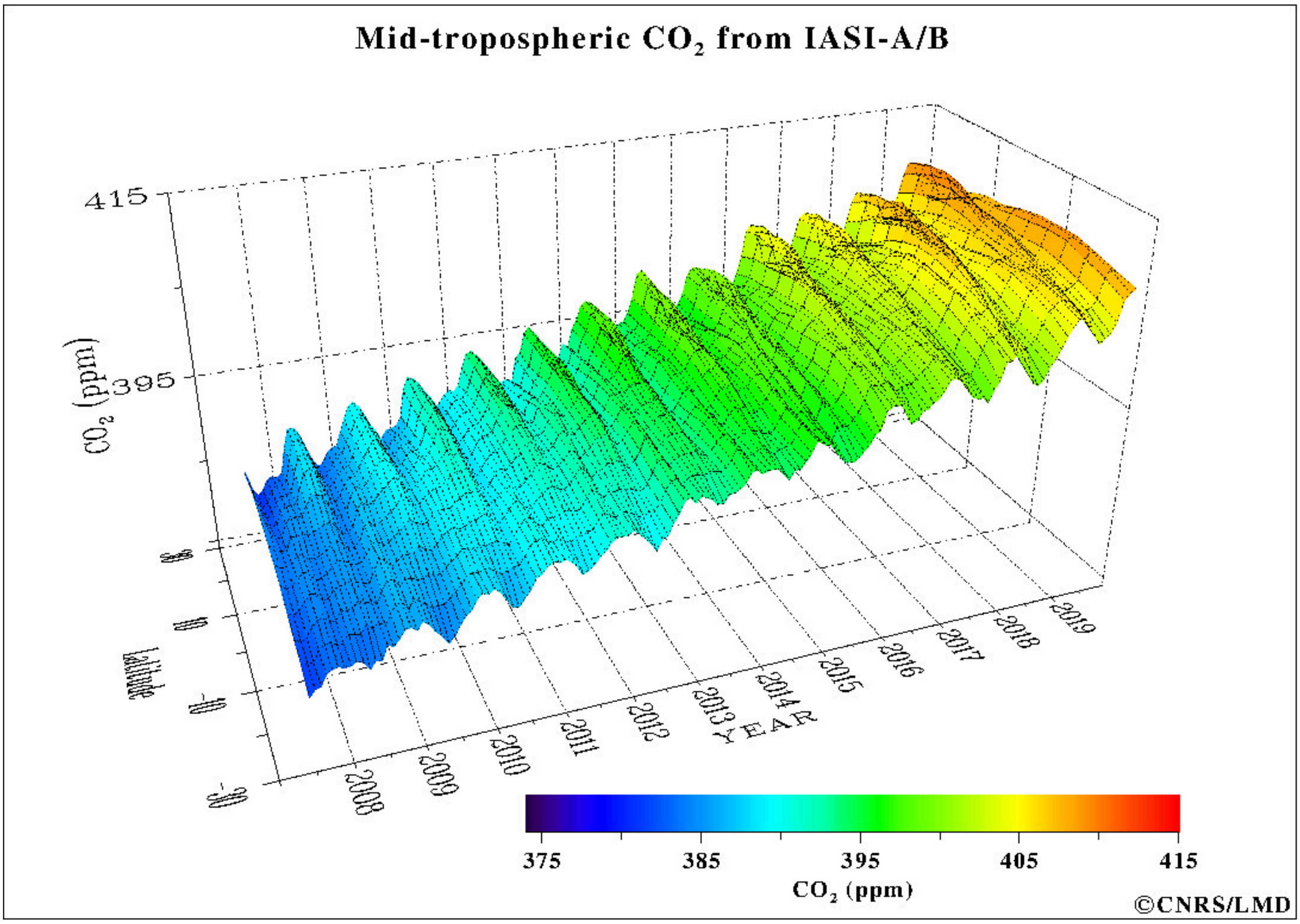
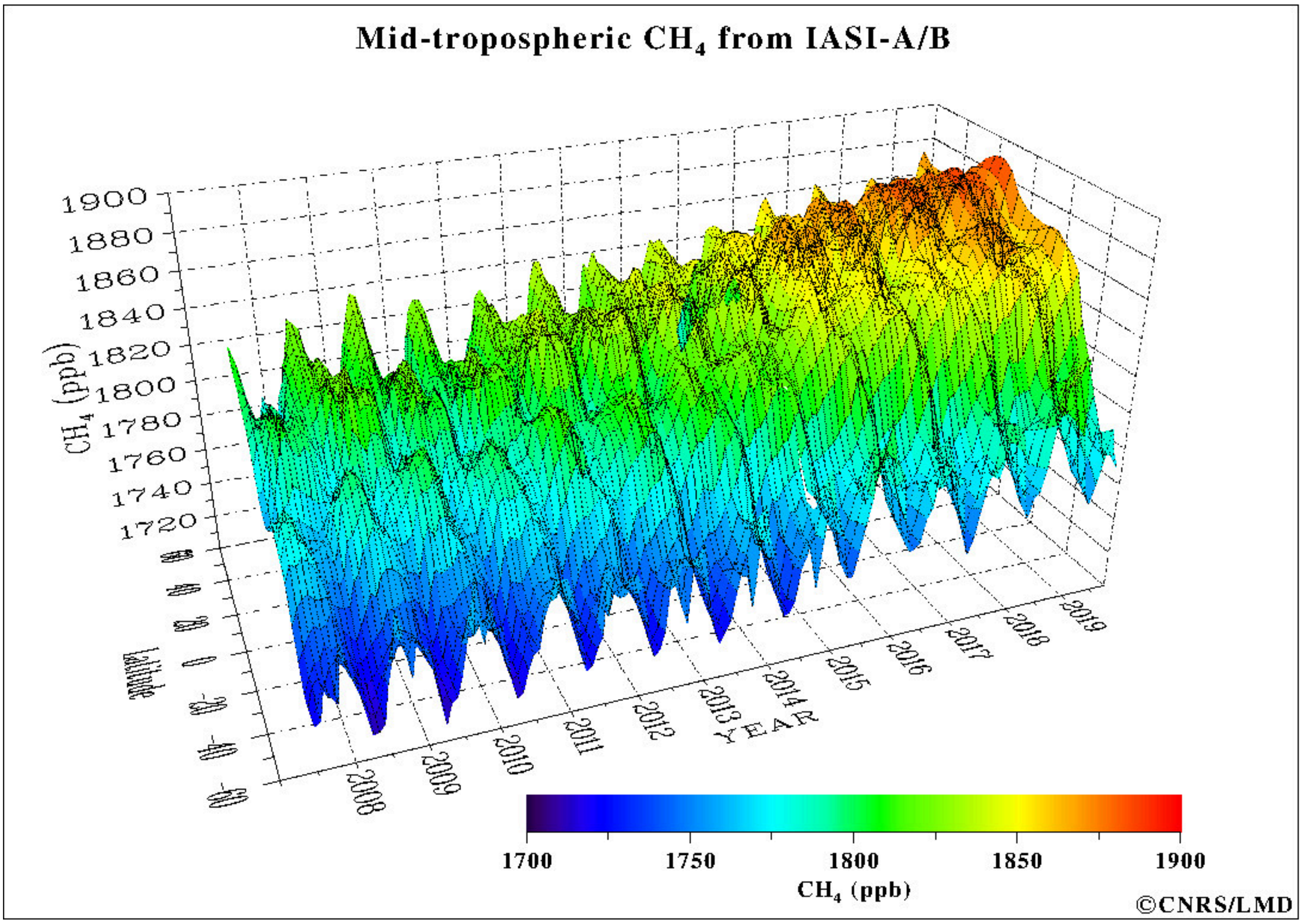


Figure 5. Monthly evolution displayed as a function of latitude of CH_4 mid-tropospheric column averaged mole fraction retrieved from Metop-A and Metop-B combined (version 9.1).



1.3 AIRS CO_2 mid-tropospheric column averaged mole fractions

Also described in this document is the Level 2 mid-tropospheric column averaged mole fractions retrieved from simultaneous observations of the AIRS and AMSU instruments flying together onboard the Aqua satellite since 2002 using a non-linear inference scheme (*Crevoisier et al., 2003*). This dataset covers the period January 2003-June 2006. Although AIRS is still in operation, the loss of several channels that were used in the retrieval has stopped the generation of retrievals. As part of C3S, the dataset generated during the ESA-CCI-GHG initiative has been rewritten in daily netcdf files, following the same structure as for the other products.

2. Target requirements

Quality requirements for Level 2 products generated from IASI and delivered to C3S are discussed in the Target Requirements Document (TRD) (*D2*). Table 1 shows the random and systematic errors stated in the TRD. The evaluation itself of our products is described in the PQAR document (*D3*).

Table 1: Mid/upper tropospheric CO_2 and CH_4 random ("precision") and systematic retrieval error requirements. Abbreviations: G=Goal, B=Breakthrough, T=Threshold requirement. §) Required systematic

error after an empirical bias correction, that does not use the verification data. #) Required systematic error and stability after bias correction, where bias correction is not limited to the application of a constant offset / scaling factor.

Random and systematic error requirements for mid/upper tropospheric CO_2 and CH_4					
Parameter	**Req. type**	**Random error** ("Precision") Single obs.	**Random error** ("Precision") 1000^2 km^2 monthly	**Systematic error**	**Stability**
CO_2	G	< 1 ppm	< 0.3 ppm	< 0.2 ppm (absolute)	As systematic error but per year
	B	< 3 ppm	< 1.0 ppm	< 0.3 ppm (relative §))	-"-
	T	< 8 ppm	< 1.3 ppm	< 0.5 ppm (relative #))	-"-
CH_4	G	< 9 ppb	< 3 ppb	< 1 ppb (absolute)	< 1 ppb/year (absolute)
	B	< 17 ppb	< 5 ppb	< 5 ppb (relative §))	< 2 ppb/year (relative §))
	T	< 34 ppb	< 11 ppb	< 10 ppb (relative #))	< 3 ppb/year (relative #))

3. Data usage information

3.1 Product content and format

The daily Netcdf files contain all of the common parameters for the C3S data products. The mid-tropospheric column averaged mole fractions of CH_4 (ppb) and CO_2 (ppm) are stored in the ch4 and co2 variables. The quality flags (0=good) must be applied before use. Averaging kernels are provided on pressure layers (pressure-weight), as opposed to layers. A dimension of *n* refers to the number of retrievals per file. A dimension of *m* refers to the number of levels used in the radiative transfer retrieval process.

Table 2: Variables present in the Netcdf file for the CH4_IASA_NLIS and CH4_IASB_NLIS products.

Name	Type	Dimension	Units	Description
latitude	float	n	degrees_north	Center latitude of the measurement
longitude	float	n	degrees_east	Center longitude of the measurement
time	float	n	seconds since 1970-1-1 0:0:0	Measurement time
solar_zenith_angle	float	n	degrees	Angle between line of sight to the sun and local vertical
sensor_zenith_angle	float	n	degrees	Angle between the line of sight to the sensor and the local vertical
ch4_quality_flag	byte	n		0=good, 1=bad
ch4	float	n	1e-9	Retrieved mid-tropopsheric column of atmospheric methane (CH_4) in ppb
ch4_uncertainty	float	n	1e-9	1-sigma uncertainty of the retrieved Mid-tropospheric-CH_4 in ppb
ch4_averaging_kernel	float	n, m		Normalized column-averaging kernel, which represents the sensitivity of the retrieved mid-tropospheric CH_4 to the atmospheric methane mole fraction depending on pressure (height). All values represent layer averages within the corresponding pressure levels.
pressure_levels	float	n, m	hPa	Pressure levels define the boundaries of the averaging kernel. Surface pressure is represented by the 1st element, i.e., profiles are ordered from surface to top of atmosphere.
pressure_weight	float	n, m	hPa	Layer dependent weights corresponding to pressure levels

Table 3: Variables present in the Netcdf file for the CO2_IASA_NLIS, CO2_IASB_NLIS and CO2_AIRS_NLIS products.

Name	Type	Dimension	Units	Description
latitude	float	n	degrees_north	Center latitude of the measurement
longitude	float	n	degrees_east	Center longitude of the measurement
time	float	n	seconds since 1970-1-1 0:0:0	Measurement time
solar_zenith_angle	float	n	degrees	Angle between line of sight to the sun and local vertical
sensor_zenith_angle	float	n	degrees	Angle between the line of sight to the sensor and the local vertical
co2_quality_flag	byte	n		0=good, 1=bad
co2	float	n	1e-6	Retrieved mid-tropopsheric column of atmospheric methane (CO_2) in ppm
co2_uncertainty	float	n	1e-6	1-sigma uncertainty of the retrieved Mid-tropospheric-CO_2 in ppm
co2_averaging_kernel	float	n, m		Normalized column-averaging kernel, which represents the sensitivity of the retrieved mid-tropospheric CO_2 to the atmospheric methane mole fraction depending on pressure (height). All values represent layer averages within the corresponding pressure levels.
pressure_levels	float	n, m	hPa	Pressure levels define the boundaries of the averaging kernel. Surface pressure is represented by the 1st element, i.e., profiles are ordered from surface to top of atmosphere.
pressure_weight	float	n, m	hPa	Layer dependent weights corresponding to pressure levels

3.2 Tools for reading data

Data are provided in Netcdf files that can easily be read with standard tools in any common programming languages.

3.3 Recommended data usage

For model comparison or for intercomparison with in-situ or remote-sensing measurements for which vertical profile information is available, use should be made of the provided normalized-column averaging kernels, denoted *G*. The 40 G_i values are independent of the layer thickness and can be interpolated to any vertical layer distribution. Note that they are normalized so that the sum of the G_i, weighted by layer pressure thickness, is 1. The simulated integrated content of the consider gas, denoted q_{gas}^{other}, is finally given by

$$q_{gas}^{other} = \frac{\sum_{i=1}^{M_{lay}} H_i \Delta p_i q_i}{\sum_{i=1}^{M_{lay}} H_i \Delta p_i}$$

where H_i is the vertical weighting function G_i interpolated on the M_{lay} pressure layers Δp_i used by the other product for which the gas mixing ratio q_i at level P_i is given in ppb.

3.4 Known limitations and issues

- From beginning of 2015, AMSU channel 7 has started degrading and then exceeding specifications. Retrievals performed from IASI/AMSU onboard Metop-A have thus been stopped in August 2015, and more 'bad quality' retrievals have been flagged in the first half of 2015 than the years before. The regeneration of the full dataset without the information given by AMSU7 is planned for the next release.
- For high scan angles (between 10th and 15th angle), the retrievals display a variation with the scan angle that depends on the year, and that can reach quite high values at the edges of the orbits. For these reasons, only retrievals for scan angles lower than the 10th angle are provided.
- A 2 ppm bias was found in CO_2 retrieved from Metop-B with version V4.1. An update of the computation of radiative biases characterizing IASI and AMSU Metop-B channels has been removed it in version V4.2.
- Differences in CO_2 partial columns (v9.1) larger than 2 ppm have been observed between Metop-A and Metop-B for latitudes higher than 25°N/S larger.
- Differences in CH_4 partial columns (v9.1) larger than 10 ppb have been observed between Metop-A and Metop-B for latitudes higher than 60°N/S larger.

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Copernicus Climate Change Service

ECMWF - Shinfield Park, Reading RG2 9AX, UK

Contact: info@copernicus-climate.eu