ECMWF COPERNICUS REPORT

Copernicus Climate Change Service

Target Requirements and Gap Analysis Document

Greenhouse Gases (CO_2 & CH_4) ECV

Issued by: Michael Buchwitz, Germany, University of Bremen,

Institute of Environmental Physics (IUP)

Date: 19.02.2021

Ref: C3S_D312b_Lot2.1.0-2020(GHG)_TRD-GAD_v3.1

Official reference number service contract: 2018/C3S_312b_Lot2_DLR/SC1

Contributors

INSTITUTE OF ENVIRONMENTAL PHYSICS (IUP), UNIVERSITY OF BREMEN, BREMEN, GERMANY
(IUP)
M. Buchwitz
M. Reuter
O. Schneising-Weigel

SRON NETHERLANDS INSTITUTE FOR SPACE RESEARCH, UTRECHT, THE NETHERLANDS
(SRON)
I. Aben
L. Wu
O. P. Hasekamp

UNIVERSITY OF LEICESTER, LEICESTER, UK
(UoL)
H. Boesch
A. Di Noia

CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE (CNRS), LABORATOIRE DE METEOROLOGIE DYNAMIQUE (LMD), PALAISEAU, FRANCE
(LMD/CNRS)
C. Crevoisier
R. Armante

History of modifications

Version	Date	Description of modification	Chapters / Sections
1.0	11-Dec-2018	New document based on merging the following two separate Copernicus Climate Change Service (C3S) documents including (mostly minor) updates: • Target Requirement Document (TRD) C3S_312a_Lot6_IUP-UB – Greenhouse Gases, v1.3, 20-October-2017. • Gap Analysis Document (GAD) C3S_312a_Lot6_IUP-UB – Greenhouse Gases, v1.1, 1-March-2018.	All
1.1	25-Jan-2019	Correction of typos and broken links based on the review by ASSIMILA	Several
2.0	26-Feb-2020	Cross-harmonization within Lot2 Minor updates with respect to references etc. Updates with respect to identified gaps	All
2.1	30-Mar-2020	Corrections (mainly of cross reference errors) based on review by ASSIMILA	Several
2.11	9-Apr-2020	One minor correction (link to section specified)	-
3.0	30-Nov-2020	Several minor updates (esp. various links)	All
3.1	19-Feb-2021	Several improvements based on review by ASSIMILA	All

Related documents

Reference ID	Document
[D1]	**GCOS-154:** Global Climate Observing System (GCOS), SYSTEMATIC OBSERVATION REQUIREMENTS FOR SATELLITE-BASED PRODUCTS FOR CLIMATE, Supplemental details to the satellite-based component of the "Implementation Plan for the Global Observing System for Climate in Support of the UNFCCC (2010 update)", Prepared by World Meteorological Organization (WMO), Intergovernmental Oceanographic Commission, United Nations Environment Programme (UNEP), International Council for Science, Doc.: GCOS 154, link: http://cci.esa.int/sites/default/files/gcos-154.pdf, 2011.
[D2]	**GCOS-195:** Status of the Global Observing System for Climate. GCOS-195. Link: https://library.wmo.int/doc_num.php?explnum_id=7213, 2015.
[D3]	**GCOS-200:** The Global Observing System for Climate: Implementation Needs, GCOS 2016 Implementation Plan, World Meteorological Organization (WMO), GCOS-200 (GOOS-214), pp. 325, link: https://library.wmo.int/opac/doc_num.php?explnum_id=3417, 2016.
[D4]	**ESA-CCI-GHG-URDv3.0:** Chevallier, F., et al., User Requirements Document (URD), ESA Climate Change Initiative (CCI) GHG-CCI project, Version 3.0, 17 Feb 2020, pp.42, link: https://www.iup.uni-bremen.de/carbon_ghg/docs/GHG-CCIplus/URD/URDv3.0_GHG-CCIp_Final.pdf , 2020.
[D5]	**CMUG-RBD, 2012:** Climate Modelling User Group Requirements Baseline Document, Deliverable 1.2, Number D1.2, ESA Climate Change Initiative (CCI, https://earth.esa.int/documents/10174/1754357/RD-5-CMUG_D1.2_URD_v1.6.pdf/ef3b9619-e59c-4927-af8d-844924f15000;jsessionid=D85994FFED6AF216D1F203D3F8459EBB.eodisp-prod4040, Version 1.6, 17 Dec 2012, 2012.
[D6]	**PQAR GHG, 2020:** Buchwitz, M., Aben, I., Anand, J., Armante, R., Boesch, H., Crevoisier, C., Detmers, R. G., Hasekamp, O. P., Reuter, M., Schneising-Weigel, O., Product Quality Assessment Report (PQAR) – Main document for Greenhouse Gas (GHG: CO_2 & CH_4) data set CDR 4 (2003-2019), Copernicus Climate Change Service (C3S) project C3S_312b_Lot2), Version 4.0, 17-Sept-2020, pp. 104, link: https://www.iup.uni-bremen.de/carbon_ghg/docs/C3S/CDR4_2003-2019/C3S_D312b_Lot2.2.3.2-v2.0_PQAR-GHG_MAIN_v4.0.pdf, 2020.

Acronyms

Acronym	Definition
AIRS	Atmospheric Infrared Sounder
AMSU	Advanced Microwave Sounding Unit
ATBD	Algorithm Theoretical Basis Document
BESD	Bremen optimal EStimation DOAS
BRDF	Bidirectional reflectance distribution function
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
CO2M	CO_2 Monitoring (Mission)
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
FP	Full Physics retrieval method
FTIR	Fourier Transform InfraRed
FTS	Fourier Transform Spectrometer
GCOS	Global Climate Observing System
GDAS	GOSAT Data Archive Service
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
GPU	Graphic Processing Unit
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
LEO	Low Earth Orbit (satellite)
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 CO_2 and CH_4 retrieval algorithm
NOAA	National Oceanic and Atmospheric Administration
Obs4MIPs	Observations for Climate Model Intercomparisons
OCO	Orbiting Carbon Observatory
OCO-2	Orbiting Carbon Observatory 2
OE	Optimal Estimation
OPER	Operational (activity)
PBL	Planetary Boundary Layer
ppb	Parts per billion
PQAR	Product Quality Assessment Report
ppm	Parts per million
PR	(light path) PRoxy retrieval method
PVIR	Product Validation and Intercomparison Report
QA	Quality Assurance
QC	Quality Control
R&D	Research and Development
REQ	Requirement
RMS	Root-Mean-Square

RT	Radiative transfer
RTM	Radiative transfer model
S5	Sentinel 5
S5P	Sentinel 5 Precursor
SCIAMACHY	SCanning Imaging Absorption spectroMeter for Atmospheric ChartographY
SCIATRAN	SCIAMACHY radiative transfer model
SIF	Sun-Induced-Fluorescence
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
TRGAD	Target Requirements and Gap Analysis Document
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

Climate Data Record (CDR)	A (Thematic) Climate Data Record is derived from a FCDR and closely connected to an ECV but strictly covers one geophysical variable, whereas an ECV can encompass several geophysical variables. A (F)CDR can encompass several instruments.
Data Product (or: ECV product)	The geophysical product underlying a (I)CDR, characterized by product definition, product name, processing level, instruments used, processing algorithm (name and version), data provider, and data format.
Data Requirement	A quantitative requirement on spatio-temporal coverage and resolution, uncertainty and stability.
Essential Climate Variable (ECV)	A geophysical variable that is associated with climate variation and change as well as the impact of climate change onto Earth [GCOS-200]. ECVs might encompass a set of CDRs with associated Data Products.
Fundamental Climate Data Record (FCDR)	A well-characterized, long-term data record of, *e.g.*, calibrated radiances, with calibrations sufficient to allow the generation of a Data Product that is accurate and stable, in both space and time, to support climate applications. A FCDR includes the ancillary data used in the calibration [GCOS-200].
Gap	An unfulfilled (Target) User Requirement.
Gap Analysis	The assessment of Gaps, *i.e.*, an assessment of the differences between the (Target) User Requirements and their present-day fulfillment.
GCOS requirements	Quantitative Data Requirements for the ECVs on spatiotemporal resolution, accuracy and stability following the latest GCOS Implementation Plan, 2016 (GCOS-200). These are Target User requirements.
Interim Climate Data Record (ICDR)	A CDR which is regularly updated with an algorithm/system having maximum consistency to the CDR generation algorithm/system. The update cycle depends on the user requirements [GCOS-200].

Target User Requirement	A technology-aware potentially achievable User Requirement which could be regarded as the long-term development goal for an ECV.
User Requirement	A user need for (aspects of) a Data Product, including Data Requirements, metadata information, analysis tools, data formats, etc.
Level 1	Measured satellite data product: geolocated radiance (spectra)
Level 2	Satellite-derived data product: geolocated geophysical variables. Here: O3, aerosol or CO_2 and CH_4 information for each ground-pixel
Level 3	Aggregated satellite data product: gridded geophysical variables Here: Gridded O_3, aerosol or CO_2 and CH_4 information, e.g., 5 deg times 5 deg, monthly
Level 4	Satellite-derived data product: Here: Assimilated O3 columns or Surface fluxes (emission and/or uptake) of CO_2 and CH_4
Systematic error	Component of measurement error that in replicate measurements remains constant or varies in a predictable manner. “Systematic error” = “Absolute systematic error” (in contrast to “Relative systematic error”).
Relative systematic error	Identical with “Systematic error” but after bias correction. (especially important for satellite GHG ECV products).
Bias	Estimate of a systematic measurement error (*JCGM, 2008*).
Precision	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, 2012*). We quantify precision here with the standard deviation (1-sigma) of the error distribution.
Stability	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, 2012*). 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	How much a measured value represents the value over a grid cell of a model. It 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, 2012*).
Threshold requirement	The threshold is the limit at which the observation becomes ineffectual and is not of use for climate-related applications (*CMUG-RBD, 2012*). Threshold requirements are given for statistical quantities (average and standard deviation of an error distribution) rather than for individual soundings. This means that some sub-ensembles of a dataset can be useful and some others not. Threshold requirements are fully driven by the target application (here regional flux inversions), irrespective of available technology.
Goal requirement	The goal is an ideal requirement above which further improvements are not necessary (*CMUG-RBD, 2012*). This requirement is relative to a given state of the art for the target application. Indeed, the more accurate and precise the satellite data products are, the larger their information content is. However, other errors such as model transport errors do not allow exploiting the additional information content data have if they are more accurate than the specified goal requirement.
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, 2012*).
Horizontal resolution	Area over which one value of the variable is representative of (*CMUG-RBD, 2012*).

Vertical resolution	Height over which one value of the variable is representative of. Only used for profile data (*CMUG-RBD, 2012*).
Observing Cycle	Temporal frequency at which the measurements are required (*CMUG-RBD, 2012*). In this document also the term "Revisit time" is used. The definition is identical with the definition of "Observing cycle". Both terms refer to the (average) temporal frequency at a given location.

Table of Contents

Scope of the document

This document is the Target Requirements (TR) and Gap Analysis Document (TRGAD) for the Copernicus Climate Change Service (C3S, https://climate.copernicus.eu/) satellite-derived greenhouse gas (GHG) carbon dioxide (CO_2) and methane (CH_4) data products.

These satellite-derived CO_2 and CH_4 Essential Climate Variable (ECV) data products are generated for inclusion into the Copernicus Climate Data Store (CDS, https://cds.climate.copernicus.eu/), from where users can access the data products and their documentation.

The satellite-derived GHG data products are:
- Column-averaged dry-air mole fractions (molar mixing ratios) 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).

The main purpose of this document is to (i) define and formulate the (potentially evolving) target requirements (TR) for satellite-derived atmospheric CO_2 and CH_4 Climate Data Records (CDRs) based on C3S user needs, such as required precision (random error, scatter) and accuracy (systematic error, bias) and (ii) to report on identified service-related gaps including recommendations on how these gaps can be mitigated or entirely removed in the future in order to improve the C3S service.

Recommendations for service improvement are classified as either Research and Development (R&D) related activities or Operational (OPER) activities. R&D activities likely need to be funded by funding bodies outside Copernicus, for example, via ESA's Climate Change Initiative (CCI) and related follow-on activities.

Executive summary

This document is the Target Requirements (TR) and Gap Analysis Document (TRGAD) for the Copernicus Climate Change Service (C3S, https://climate.copernicus.eu/) satellite-derived greenhouse gas (GHG) carbon dioxide (CO_2) and methane (CH_4) data products.

These satellite-derived CO_2 and CH_4 Essential Climate Variable (ECV) data products are generated for inclusion into the Copernicus Climate Data Store (CDS, https://cds.climate.copernicus.eu/), from where users can access the data products and their documentation.

The satellite-derived GHG data products are:

- Column-averaged dry-air mole fractions (molar mixing ratios) 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).

The main purpose of this document is to (i) define and formulate the (potentially evolving) target requirements (TR) for satellite-derived atmospheric CO_2 and CH_4 Climate Data Records (CDRs) based on C3S user needs, such as required precision (random error, scatter) and accuracy (systematic error, bias) and (ii) to report on identified service-related gaps including recommendations on how these gaps can be mitigated or entirely removed in the future in order to improve the C3S service.

The satellite-derived GHG data products are generated from satellite instruments such as SCIAMACHY/ENVISAT and TANSO-FTS/GOSAT (XCO_2 and XCH_4 products) and AIRS and IASI (mid/upper troposphere products). All data products are available (via the CDS) as Level 2 (individual ground pixels / footprints) products in NetCDF format. The XCO_2 and XCH_4 Level 2 products are available for individual sensors but also as merged multi-sensor products. In addition, also merged Level 3 (i.e., gridded) products in Obs4MIPs format are available for the XCO2 and XCH_4 products. For the merged products also other satellites are planned to be used (initially XCO_2 from NASA's OCO-2 mission and in the future also XCH_4 from ESA's Sentinel-5-Precursor satellite and XCO_2 and XCH_4 from other satellites as soon as available and "good enough").

CO_2 and CH_4 are important climate-relevant atmospheric greenhouse gases. Because of their important role for climate, they have been included in the official list of Essential Climate Variables (ECVs). The ECV GHG as formulated by GCOS (Global Climate Observing System) is defined as: "Retrievals of greenhouse gases, such as CO_2 and CH_4, of sufficient quality to estimate regional sources and sinks". This definition contains already the main application of these atmospheric data products, namely to use them (in combination with appropriate modelling) to obtain (improved) information on their (primarily surface) sources and sinks.

Both gases, CO_2 and CH_4, have a long lifetime in the atmosphere. As a consequence of this fact - combined with human emissions - atmospheric concentrations of these gases are relatively high compared to other atmospheric trace gases. As a result of this even a moderate to strong (surface) source or sink typically only results in a relatively small local or regional change (enhancement or depletion relative to the surrounding region) in their vertical columns or their mid/upper tropospheric concentration. The observational requirements are therefore very demanding in particular with respect to random and systematic errors and stability.

Because of their long lifetime and atmospheric transport, elevated (or depleted) atmospheric CO_2 and CH_4 concentrations can be higher (or lower) relative to the background far away from the surface source (or sink), which has emitted (or taken up) these atmospheric gases. In order to obtain source/sink information from the atmospheric observations it is therefore required to take atmospheric transport (and in particular for methane also atmospheric chemistry) into account and to consider the exact time and location of the atmospheric observations. As a consequence, the most relevant data products are the Level 2 (L2) products, which contain detailed information (time, location, etc.) for each individual satellite ground pixel. The requirements as formulated in this document are, therefore, mostly L2 requirements. However, for XCO_2 and XCH_4 also (gridded) Level 3 (L3) products have been generated (in Obs4MIPs format).

The products are available as individual sensor Level 2 (L2) products, i.e., the CO_2 and CH_4 information is provided for each individual satellite ground pixel. For the XCO_2 and XCH_4 products also merged (multi sensor / multi algorithm) Level 2 and merged Level 3 (L3) products have been generated. The merged products are based on a small ensemble of L2 products, which have been generated using an ensemble of (Level 1 (radiances) to L2) retrieval algorithms.

The C3S GHG project (initially C3S_312a_Lot6, now the GHG component of project C3S_312b_Lot2) is essentially the operational continuation of the research and development (R&D) pre-cursor project GHG-CCI (https://climate.esa.int/en/projects/ghgs/) of ESA's Climate Change Initiative (CCI). The main goal of the C3S project is to extend (in time) the data base of GHG-CCI pre-cursor data products (however, also full reprocessing of the entire time series for certain products is possible, but this is not the baseline).

The main purpose of this document is to (i) define and formulate the (potentially evolving) target requirements for satellite-derived atmospheric CO_2 and CH_4 Climate Data Records (CDRs) based on C3S user needs, such as the required precision and accuracy and (ii) to identify service related gaps via gaps analysis.

The most challenging user requirements are those for systematic error and stability because very low biases are important as well as very high stability. As explained in this document, these requirements are:

- Systematic error CO_2: < 0.5 ppm (relative accuracy, 1-sigma)
- Stability CO_2: < 0.5 ppm/year
- Systematic error CH_4: < 10 ppb (relative accuracy, 1-sigma)
- Stability CH_4: < 3 ppb/year

These requirements are based on requirements which have been formulated by the Climate Research Group (CRG) of the GHG-CCI project of ESA's Climate Change Initiative (CCI) for XCO_2 and XCH_4 and they are also assumed to be applicable for the mid/upper tropospheric CO_2 and CH_4 data products.

The products are available in standard data format. The L2 product format is NetCDF format and the L3 products are in Obs4MIPs format. Furthermore, all products need to be properly documented in terms of algorithm description, product specification and User's guide and data quality documentation.

A gap analysis has been performed and the results are summarized in Table 2 including recommendations on how the service can be improved in the future. The recommendations are, in principle, classified as OPER (operational) or R&D (Research and Development). The latter likely requires funding by bodies outside Copernicus (e.g., ESA via CCI or follow-on or related programmes/projects).

As can be seen, essentially all listed recommendations are classified as R&D. No recommendation is classified as OPER for the following reason: Currently, no major gaps related to the operational service have been identified. This may be due to the fact that at the time of writing of this document the related service from a user point of view is quite new. Recommendations may be added in future updates of this document taking into account user feedback.

The following aspect is not addressed in this document: Costs, i.e., the needed financial resources. The following aspect is only briefly mentioned: Additional (i.e., not yet existing or planned) satellites (but activities related to the specification of future satellites are ongoing outside of this project).

Table 1: List of recommendations originating from the gap analysis.

C3S service component covered by the GHG component of project C3S_312b_Lot2 (satellite-derived CO_2 and CH_4 CDRs and related services): **List of identified gaps and recommendations on how to improve** *(not ordered by priority)*			
Rec. ID	**Type**	**Gap**	**Recommendation**
REC_ALG_001	R&D	Limited accuracy of data products – aerosols & clouds	Investigate alternative representations of light scattering (aerosols, cirrus) in the retrieval algorithms.
REC_ALG_002	R&D	Limited accuracy of data products – various items	-Implement and test Sun-Induced-Fluorescence (SIF) product for various datasets / missions -Fitting of intensity offsets to improve retrievals - Optimization of ancillary datasets used (e.g. prior CO_2, CH_4, etc.) - Surface treatment (e.g., BRDF) - Polarization radiative transfer - Sub-pixel cloud effects - other
REC_ALG_003	R&D	Limited accuracy of data products – input data	Improve spectroscopy of spectral bands used in the retrieval process, including proper aerosol spectral characterizations and solar spectrum characterization.
REC_ALG_004	R&D	Limited computational efficiency of L2 retrieval algorithms	Improvement of computational efficiency to enable processing of (not yet considered, e.g., OCO-2) current and future satellite data streams providing at least an order of magnitude more data. This includes, e.g., new RT methods and GPU processing.
REC_ALG_005	R&D	Limited number of data points (due to strict filtering)	Investigate to what extent the data yield can be improved including the use of (quasi) continuous quality indicator instead of binary flag (e.g. OCO-2 warn levels). Needs separate validation per warn level.
REC_ALG_006	R&D	Merging algorithms EMMA and Obs4MIPs not optimized for new sensors with large amounts of data (esp. OCO-2, S-5P)	Investigate how to optimally further develop the EMMA and Obs4MIPs merging algorithms. *Note: Since March 2019 partially addressed in GHG-CCI+ project (https://climate.esa.int/en/projects/ghgs/)*
REC_ERR_001	R&D	Lack of spatial coverage of TCCON	Use of in particular EM27Sun instruments for validation (approx. 15 instruments at the

		network limits validation and error characterization	moment) to fill up gaps in spatial coverage
REC_ERR_002	R&D or OPER or other	Risk of no or fewer TCCON validation data in the future	Insure continuity of TCCON network
REC_ERR_003	R&D	Limited validation due to small number of co-locations	Improve co-location method
REC_ERR_004	R&D	Unknown spatial and temporal error correlations	- Knowledge of error correlations is crucial for inverse modeling, therefore, it is important to investigate (by means of TCCON and model comparisons) spatial and temporal error correlations. - Improve validation of reported L2 errors
REC_ERR_005	R&D	Unknown systematic error functions	- Improved / extended investigation of error sources (e.g., how do systematic L2 errors depend on geophysical scene properties). -Improvement of L2 bias correction schemes.
REC_ERR_006	R&D	Lack of good vertical coverage of GHGs limits validation and characterization of total columns	- Development of atmospheric profiling 0-30 km such as AirCore or Amulse balloon-borne devices that could be flown at several TCCON/ICOS stations. - Use of IAGOS/CARIBIC/CONTRAIL aircraft 0-12 km profiles
REC_ERR_007	R&D	Lack of validation of mid/upper tropospheric columns retrieved from TIR observations	Investigate the use of NDACC FTIR observations to validate TIR retrievals.
REC_ERR_008	R&D	Lack of proper intercomparison between retrieval codes (both EU and non-EU)	Framework for comparison between various retrieval algorithms in order to establish the pros and cons of each approach
REC_INS_001	R&D	Currently no European OCO-2 XCO_2 Level 2 algorithm and corresponding data product mature enough (in terms of processing speed and/or accuracy and/or yield) for C3S	Further development of European XCO_2 retrievals algorithm(s) to generate Level 2 XCO_2 data product(s) from OCO-2 *Note: Since March 2019 partially addressed in GHG-CCI+ (https://climate.esa.int/en/projects/ghgs/) and other projects (EU H2020 CHE and VERIFY)*

REC_INS_002	R&D	Currently no European TanSat XCO_2 Level 2 algorithm and corresponding data product for C3S	Further development of European XCO_2 retrievals algorithm(s) to generate Level 2 XCO_2 data product(s) from TanSat *Note: Since March 2019 partially addressed in GHG-CCI+ (https://climate.esa.int/en/projects/ghgs/)*
REC_INS_003	R&D	Limited development of scientific S-5P methane retrieval algorithms to enable ensemble-based assessments and data product generation	Operational methane retrieval from S-5P is challenging and will highly benefit from parallel scientific algorithm development and comparisons of operational and scientific data products. *Note: Since March 2019 partially addressed in ESA projects GHG-CCI+ (https://climate.esa.int/en/projects/ghgs/) and Methane+ (https://methaneplus.eu/)*
REC_INS_004	R&D	Unclear to what extent GOSAT-1 XCO_2 and XCH_4 retrieval algorithms need to be adjusted for GOSAT-2 to achieve a similar or even better data quality	Adjust existing GOSAT-1 XCO_2 and XCH_4 Level 1 algorithms to GOSAT-2 and investigate the quality of the resulting data products. Develop methods for improvement, if necessary. *Note: Since March 2019 partially addressed in GHG-CCI+ (https://climate.esa.int/en/projects/ghgs/)*
REC_INS_005	R&D	Currently no European OCO-3 XCO_2 Level 2 algorithm and corresponding data product mature enough (in terms of processing speed and accuracy) for C3S	Further development of European XCO_2 retrievals algorithm(s) to generate Level 2 XCO_2 data product(s) from OCO-3
REC_INS_006	R&D	Currently no CO_2 and CH_4 C3S ECV products from IASI/MetOp-C	Assess the quality of IASI/MetOp-C mid/upper tropospheric CO_2 and CH_4 retrievals and generate and deliver also these products as C3S ECV products if the quality is high enough
REC_OTH_001	R&D	Currently, no algorithm for combined processing SWIR and TIR observation to increase vertical coverage	Design of new algorithms combining SWIR and TIR observations (which will be available with S-5/IASI-NG) in order to aim at having more than one degree of freedom on the vertical and to extract information near the surface. *Note: Now partially addressed in ESA project Methane+ (https://methaneplus.eu/)*

1. Product description

In this section, an overview of the satellite-derived GHG data products (specified in terms of variable, its property, processing level(s) and instrument(s)) is given to which the Target Requirements (TRs) as formulated in this document are compared.

The data products are (see also *Buchwitz et al., 2013a, 2016, 2017a, 2017b, 2018*):

- Column-averaged 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).
- Mid/upper tropospheric mixing ratios of CO_2 and CH_4.

Carbon dioxide and methane are important atmospheric greenhouse gases (e.g., *IPCC 2013*) but despite their importance our knowledge on their various and variable natural and anthropogenic sources and sinks has significant gaps (e.g., *IPCC 2013; Ciais et al., 2014; 2015; Kirschke et al., 2013; Nisbet et al., 2014*, and references given therein).

Carbon dioxide and methane are so-called Essential Climate Variables (ECVs) and the need to monitor them has been clearly identified including the definition of key requirements (e.g., *GCOS-154, GCOS-200*). In recent years several satellite-derived ECV data products have been generated in particular in the framework of the Climate Change Initiative (CCI) of ESA (e.g., *Hollmann et al., 2013, Merchant et al., 2017*) including CO_2 and CH_4 (e.g., *Buchwitz et al., 2013a, 2016, 2017a, 2017b, 2018*).

These satellite-derived CO_2 and CH_4 data products are used for a number of (primarily scientific) applications, e.g.,

- to improve our knowledge on the various natural and anthropogenic (surface) sources and sinks of these important greenhouse gases (GHG) (see, e.g., *Alexe et al., 2015; Bergamaschi et al., 2015; Chevallier et al., 2014, 2016; Cressot et al, 2014; ESA-CCI-GHG-URDv2.1; ESA-CCI-GHG-URDv3.0, Detmers et al., 2015; Guerlet et al., 2013; Houweling et al., 2015; Kaminski et al., 2017; McNorton et al., 2016; Pandey et al., 2016; Reuter et al., 2014b, 2017a; Schneising et al., 2014b; Scholze et al., 2017; Turner et al., 2015, 2016,* and references given therein)
- to monitor the global distribution of CO_2 and CH_4 (e.g., *Buchwitz et al., 2007, 2016b; Schneising et al., 2011; Frankenberg et al., 2011; Massart et al., 2016*)
- to improve our knowledge on emission ratios, e.g., for biomass burning (e.g., *Ross et al., 2013; Parker et al., 2016*)
- for comparisons with (chemistry) climate models (e.g., *Shindell et al., 2013; Hayman et al., 2014; Lauer et al., 2017*) and other models (e.g., *Schneising et al., 2014a; Parker et al., 2016*)

In the following sub-sections an overview about the satellite-derived CO_2 and CH_4 data products is given.

1.1 Column-averaged mixing ratios of CO_2 and CH_4 (XCO_2 and XCH_4)

1.1.1 Overview

Satellite radiance observations in the Near Infrared / Short Wave Infrared (NIR/SWIR) spectral region in nadir (downlooking) observation viewing mode are sensitive to atmospheric CO_2 and CH_4 concentration changes with good sensitivity down to the Earth's surface (because solar radiation reflected at the Earth's surface is observed). These measurements permit to obtain "total column information" but do not permit to obtain (detailed) information on the vertical profiles of CO_2 and CH_4. The CO_2 and CH_4 products derived from these satellites are column-averaged dry-air mixing ratios (more precisely: mole fractions) of CO_2 and CH_4 denoted XCO_2 (e.g., in ppm) and XCH_4 (e.g., in ppb). An overview about these data product is given in *Reuter et al., 2020*.

In the following, several satellite instruments are shortly described which are used / can be used to generate XCO_2 and/or XCH_4 data products.

1.1.2 Satellite Instruments

For satellite instruments which permit retrievals of XCO_2 and XCH_4 such as SCIAMACHY/ENVISAT, TANSO-FTS GOSAT and GOSAT-2, OCO-2 and TanSat see **Sect. 3.1**.

1.1.3 XCO_2

As explained, XCO_2 is the column-averaged dry-air mixing ratio (mole fraction) of atmospheric CO_2. A XCO_2 value of, for example, 400 ppm at a given location means that about 400 CO_2 molecules are present in the atmosphere above that location per one million air molecules excluding water molecules.

XCO_2 can be retrieved from instruments such as SCIAMACHY and TANSO-FTS/GOSAT using Optimal Estimation (*Rodgers, 2000*) or DOAS (*Buchwitz et al., 2000*) retrieval algorithms as shown in various publications (e.g., *Buchwitz et al., 2005; Butz et al., 2011; Cogan et al., 2011; Reuter et al., 2011; 2013; Schneising et al., 2011; Yoshida et al., 201*3).

These products have been validated using Total Carbon Column Observing Network (TCCON) (*Wunch et al., 2010, 2011*) XCO_2 ground based observations (e.g., *Dils et al., 2014*).

1.1.4 XCH_4

As explained, XCH_4 is the column-averaged dry-air mixing ratio (mole fraction) of atmospheric CH_4. A XCH_4 value of, for example, 1800 ppb at a given location means that about 1800 CH_4 molecules are present in the atmosphere above that location per one billion air molecules excluding water molecules.

XCH_4 can be retrieved from instruments such as SCIAMACHY and TANSO-FTS/GOSAT using Optimal Estimation (*Rodgers, 2000*) or DOAS (*Buchwitz et al., 2000*) retrieval algorithms as shown in various publications (e.g., *Buchwitz et al., 2005; Butz et al., 2011; Frankenberg et al., 2011; Schneising et al., 2011; Parker et al., 2011; Scheper et al., 2012; Yoshida et al., 201*3).

These products have been validated using Total Carbon Column Observing Network (TCCON) (*Wunch et al., 2010, 2011*) XCH_4 ground based observations (e.g., *Dils et al., 2014*).

1.2 Mid/upper tropospheric mixing ratios of CO_2 and CH_4

1.2.1 Overview

Satellite radiance observations in the thermal infrared (TIR) spectral region in nadir (downlooking) observation viewing mode are sensitive to atmospheric CO_2 and CH_4 mixing ratio changes in the mid/upper tropospheric region. They can thus be interpreted in terms of integrated mid/upper tropospheric columns, with typical sensitivity between 5 and 12 km. From C3S satellite-derived CO_2 and CH_4 data products are available primarily from the IASI instrument series (Metop-A and follow-on satellites) (also available is from AIRS as a brokered product from the GHG-CCI project).

1.2.2 Satellite Instruments

The relevant satellites instruments are IASI and AIRS. For details on IASI and AIRS see **Sect. 3.1**.

1.2.3 Mid/upper tropospheric CO_2

Mid/upper tropospheric columns of CO_2 can be retrieved from hyperspectral infrared sounders such as AIRS and IASI (*Chédin et al., 2003; Crevoisier et al., 2003*) using non-linear inference scheme (*Crevoisier et al., 2009a*).

Products have been validated using aircraft measurements, mostly from the Comprehensive Observation Network for TRace gases by AIrLiner (CONTRAIL) program (*Machida et al., 2008; Matsueda et al. 2008*).

1.2.4 Mid/upper tropospheric CH_4

Mid/upper tropospheric columns of CH_4 can be retrieved from the hyperspectral infrared sounder IASI (*Crevoisier et al., 2003, 2013*) using non-linear inference scheme (*Crevoisier et al., 2009b*).

Products have been validated using aircraft measurements, from the Comprehensive Observation Network for TRace gases by AIrLiner (CONTRAIL) program (*Machida et al., 2008; Matsueda et al. 2008*) and the HIAPER Pole-to-Pole Observations (HIPPO) project (*Wofsy et al., 2012*), as well as from balloon measurements from AirCores (*Membrive et al., 2016*).

2. Target Requirements

In this section the user requirements are given per product. Requirements for satellite-derived ECV GHG products are given in *GCOS-154* and *GCOS-200*. *GCOS-154* defines the ECV GHG as follows:

- ECV "Carbon Dioxide, Methane and other GHGs": Product number A.8.1: "Retrievals of greenhouse gases, such as CO_2 and CH_4, of sufficient quality to estimate regional sources and sinks".

Updated requirements are given in *GCOS-200*. They are listed in Table 3. For "Resolution" required values for horizontal and vertical resolution are given (NA = not applicable). The required measurement uncertainty is presented as 95% confidence interval (approx. 2 standard deviations or 2-sigma).

All (past, present and planned future) satellites dedicated to obtaining information on regional sources and sinks of CO_2 and CH_4 (see ECV definition) are optimized to deliver XCO_2 and XCH_4. However, no requirements for these quantities are given in *GCOS-200*. This means that the GCOS-200 requirements cannot be used directly but need "interpretation", e.g., to apply the GCOS requirements on "Tropospheric CO_2 column" for XCO_2 and the requirements for "Tropospheric CH_4 column" for XCH_4.

Unfortunately, this does not solve all problems. One reason is that GCOS does not specify the required "systematic error" (accuracy, bias) but "uncertainty", which is defined as follows:

- *GCOS-200*: "Uncertainty (of measurement): non-negative parameter, associated with the result of a measurement, that characterizes the dispersion of the values that could reasonably be attributed to the measurand."

This quantifies the "scatter of the data around a reference value" and is therefore a measure of random error (or "precision") but not a measure of systematic error (i.e., "accuracy" or "bias"). The "accuracy" and "bias" definitions are the following:

- *GCOS-200*: Accuracy is defined as the "closeness of the agreement between a measured quantity value and a true quantity value of the measurand". The concept 'measurement accuracy' is not a quantity and is not given a numerical quantity value.
- *GCOS-200*: Bias is defined as an estimate of the systematic measurement error.

The most critical parameter for the source/sink application (as well as for many other applications) for the satellite CO_2 and CH_4 products is low bias, i.e., low systematic error. Requirements for biases are however not defined by GCOS.

What is defined is the requirement for uncertainty = random error. The random error is however primarily determined by the instrument signal-to-noise performance (and only marginally affected by the retrieval method).

For these reasons the GCOS requirements cannot be used for the purpose of this document.

For completeness, however, we also list here the definition of the GCOS stability requirement:

- *GCOS-200*: “Stability may be thought of as the extent to which the uncertainty of measurement remains constant with time.”

Table 2: GCOS requirements for CO_2 and CH_4 (from *GCOS-200*, Table 23). (*) https://ensembles-eu.metoffice.gov.uk/cmug/index.html

ECV	Product	Frequency	Resolution	Required measurement uncertainty	Stability (per decade)	Standards / references
Carbon Dioxide, Methane and other Greenhouses gases	Tropospheric CO_2 column	4 hr	5-10km/NA	1 ppm	1.5 ppm/decade	ESA CCI CMUG tables (*)
	Tropospheric CO_2	4 hr	5-10km/5km	1 ppm	1.5 ppm	
	Tropospheric CH_4 column	4 hr	5-10km/NA	10 ppb	7 ppb	
	Tropospheric CH_4	4 hr	5-10km/5km	0.5 ppb	0.7 ppb	
	Stratospheric CH_4	daily	100-200km/ 5km	Max(2%, 5DU)	0.3%	

Instead, we use in this document (wherever possible) the requirements as have been formulated by the Climate Research Group (CRG) of the GHG-CCI project of ESA’s Climate Change Initiative. We use the latest version, which is the User Requirements Document (URD) referred to as *[D4]*.

2.1 Requirements for XCO_2 and XCH_4

In this section requirements for XCO_2 and XCH_4 are listed, which are based on the User Requirements Document (URD) *[D4]* as formulated by the Climate Research Group (CRG) of the GHG-CCI project of ESA's Climate Change Initiative.

2.1.1 Definitions

All definitions as relevant for the data products and their requirements covered by this part of the document are given in section "General definitions" on pages 9 - 12 of this document.

2.1.2 Horizontal resolution

The utility of satellite retrievals of CO_2 and CH_4 for the estimation of regional sources and sinks has been demonstrated using global model simulations made at resolution much coarser than current satellite soundings (see, e.g., *Houweling et al., 2004, Meirink et al., 2006*). Typically, model grid box in these studies span at least a couple of degrees in latitude and longitude, while the soundings that are available with the coarser resolution are from the SCIAMACHY nadir measurements with 60 km (across track) × 30 km (along track) footprint. Existing studies report a modest impact stemming from this "representation error" (e.g., *Corbin et al. 2008*). Furthermore, the purpose of this document is not to specify new satellite missions but to formulate requirements for generating useful data sets from existing or planned/approved satellites. Therefore, no requirements are formulated here.

2.1.3 Vertical resolution

Similarly, utility has been demonstrated for column-average measurements without any vertical resolution. Furthermore, the purpose of this document is not to specify a future satellite mission but to formulate requirements for existing missions with given characteristics. Therefore, no requirements are given here.

2.1.4 Observing cycle

Similarly, utility has been demonstrated for the observing cycle of existing satellites or irrespective of any specific observing cycle. The observing cycle does not seem to be a critical parameter for regional flux inversion as long as measurements are assimilated at appropriate time. Furthermore, the purpose of this document is not to specify a future satellite mission but to formulate requirements for existing missions with given characteristics. Therefore, no requirements are given here.

2.1.5 Random and systematic errors

In this section requirements for random errors (“precision”) and systematic errors (“bias”, “accuracy”) for satellite XCO_2 and XCH_4 retrievals are given. They are identical with the ones given in the ESA CCI URD *[D4]* and have been formulated in the context of regional flux inversions. It is assumed here that these requirements are also valid for most of the other climate-applications with the possible exception of climate model comparisons, where somewhat less stringent requirements may be acceptable (see *Lauer et al., 2017*) and future satellite missions optimized to monitor anthropogenic CO_2 emissions (e.g., *Bovensmann et al., 2010; Buchwitz et al., 2013b; Ciais et al., 2015*).

Precision requirements are given for single measurements but also for spatio-temporal averages (1000x1000 km^2, monthly). Requirements for spatio-temporal averages have been formulated to ensure that a significant number of measurements per month and region are available, at least on average. Alternatively, one could have formulated a requirement for the number of measurements for a given spatio-temporal interval. Note that the size of the region is given in km^2 and not in deg^2, i.e., refer to equal size areas on the Earth’s surface.

Single measurement precisions are determined by instrument noise plus likely additional “retrieval noise” contributions from random errors caused by, for example, variability of aerosols, (undetected) clouds and variations of the surface spectral reflectance.

Note: If the noise is really random, an instrument with low single measurement precision but a large number of (sufficiently cloud free) data can provide the same information content with respect to regional GHG sources and sinks as an instrument delivering fewer data but with higher single measurement precision. A stand-alone and instrument-independent single measurement precision requirement is therefore not very meaningful in itself but needs to be combined with (estimates of) the number of (useful) data in a given spatio-temporal interval. However, this requirements document gives single measurement precisions requirements because they offer the potential advantage of a straight forward verification incl. radiative transfer modelling for single observations and simulated retrievals. Further, a poor precision is usually accompanied with state-dependent systematic errors that cannot be damped by averages over many retrievals.

<u>*Random error (precision) requirements for XCO_2:*</u>

In *Rayner and O’Brien, 2001,* it has been shown that satellite retrievals of XCO_2 provide additional information on CO_2 surface fluxes if a precision of 2.5 ppm can be achieved for monthly averages in 8^o x 10^o large regions. This requirement has essentially been confirmed and refined in follow-on studies. For example, *Houweling et al., 2004*, showed that SCIAMACHY provides important information on CO_2 surface fluxes if a single measurement precision (defined in this report as the standard deviation, see above) of 1% (3.6 ppm) can be achieved and if approx. 10% of the measurements are sufficiently cloud free. *Hungershoefer et al., 2010,* showed that SCIAMACHY and TANSO have the potential to deliver data which result in significant uncertainty reduction of regional weekly and annual surface fluxes when used for inverse modelling. The uncertainty reductions for the weekly fluxes are about 70% for Europe and about 80% for South America for the two instruments. The assumed single measurement retrieval precisions depend on air mass factor, surface albedo at 1.6 µm and aerosol optical depth but are typically in the range 2-8 ppm. For example, for a solar zenith angle of 50°, a surface albedo at 1.6 µm of 0.1 (vegetation), and an aerosol optical depth of 0.2, the assumed single measurement precision for TANSO is 4.2 ppm (when computed using the formula given in *Hungershoefer et al., 2010*).

Approach to define the requirements for random errors: For this TRD single measurement precisions and precisions for spatio-temporal averages (1000x1000 km^2, monthly) have been formulated. The precisions for spatio-temporal averages are (mostly) a factor of 3 better compared to the single measurement precisions. If the achieved single measurement precision is identical with the required single measurement precision and if one assumes that the precision improves with the square root of the number of measurements added, this implies that at least 10 (uncorrelated) observations are available per month and per 1000x1000 km^2 large region.

For XCO_2 the threshold precision requirement for spatio-temporally averaged data has been set at 1.3 ppm (standard deviation), i.e. a twofold factor more demanding than the 2.5 ppm value of *Rayner and O'Brien, 2001*. The required single measurement precision is approximately a factor of 6 relaxed, i.e., 8 ppm (this implies that approx. 36 uncorrelated measurements per month and region have to be averaged to achieve the 1.3 ppm requirement if the single measurement precision is (only) 8 ppm (because $8/\sqrt{36} = 1.3$)). Note that the variability of XCO_2 at the global scale and along the year is less than 4 ppm (standard deviation, obtained from MACC-II global simulations run at 16-km resolution) so that the threshold requirement is very loose, even though it is tighter than *Rayner and O'Brien, 2001.* More demanding values have been chosen for the breakthrough and goal requirements.

Note: It is unlikely that the requirements can be met for all regions during all time periods. For example, the number of data products will be (very) sparse and noisy at high latitudes during winter (low sun, low snow/ice albedo, clouds, etc.). The precision requirements therefore refer to global long-term statistics. Sub-samples of lesser quality should be identified with appropriate quality flags and/or appropriate uncertainty values.

Random error (precision) requirements for XCH_4:

Meirink et al., 2006, showed that SCIAMACHY contributes significantly to CH_4 emission uncertainty reduction on monthly timescales for regions of size ~500 km assuming a single measurement precision of 1.5-2% (approx. 25-34 ppb). For the single measurement precision, a value of 34 ppb (2%) has therefore been chosen for the threshold requirement.

The XCH_4 precision requirements for spatio-temporal averages are chosen as for XCO_2, i.e., a factor 3 improvement compared to the single measurement precisions.

Systematic error requirements:

The requirements about systematic errors are based on studies using synthetic data (e.g., *Chevallier et al., 2005, 2007, 2009b; Meirink et al., 2006; Miller et al., 2007*) and analysis of real data (e.g., *Bergamaschi et al., 2009, 2013; Alexe et al., 2015*).

For example, it has been shown in *Chevallier et al., 2007*, that for CO_2 surface flux inverse modelling "regional biases of a few tenth of a parts per million in column-averaged CO_2 can bias the inverted yearly subcontinental fluxes by a few tenth of a gigaton of carbon". Similar conclusions have been drawn in *Miller et al., 2007*. Note that systematic errors can be tolerated as global offsets can be accounted for, e.g., via bias correction (e.g., using comparisons with calibrated reference data such TCCON FTS retrievals) or as part of the inverse modelling step as done by *Bergamaschi et al., 2009.* Low relative systematic errors are required however, see e.g., *Bergamaschi et al., 2009*, or *Miller et al., 2007*: "Coherent biases on 100–5000 km horizontal scales pose the greatest threat to the integrity of space-based XCO_2 data and must be corrected below detectable levels".

The CO_2 threshold requirement for systematic errors is based on an extension of *Chevallier et al., 2005a*, to TANSO (performed by F. Chevallier). The idea is to have the bias about one order of magnitude smaller than the model-minus-observation departures (computed from individual soundings). For TANSO the CO_2 departures are a few ppm, so the bias needs to be a few tenth of a ppm. Although very demanding from a remote sensing point of view, such requirements seem nevertheless justified by the results of *Houweling et al., 2010*, and *Chevallier et al., 2010*.

For XCH_4 the requirements are similar but somewhat relaxed, because XCH_4 is more variable compared to XCO_2 (of course in terms of percentage variations, not in terms of ppm). Nevertheless, also for methane, biases are critical and need to be as small as possible. As shown in *Meirink et al., 2006*, even systematic biases "well below 1%" may have a dramatic impact on the derived CH_4 emissions. They demonstrated that a systematic regional bias of 0.5% (e.g. caused by the presence of aerosols) may lead to an overestimate of regional emissions by ~60%. This strong dependence of the retrieved emissions on small changes of the retrieved XCH_4 has also been found when using real SCIAMACHY data (*Bergamaschi et al., 2007, 2009*). As a consequence, also the CH_4 bias threshold requirement is challenging.

The requirements are valid for observations over land, due to two main reasons: (i) The main application of the GHG ECV data products is to improve our knowledge of GHG sources and sinks located on land, most notably to reduce uncertainties of the CO_2 fluxes of the terrestrial biosphere and land-based sources of methane such as wetlands, rice paddies, ruminants, etc. and (ii) the low reflectivity of water in the 1.6 µm region used to retrieve the GHG columns typically results in low signal levels (with some exceptions, e.g., sun-glint observations) and therefore large noise.

Based on these considerations the requirements on random errors (precision) are:

REQ-XGHG-ERR-1	The XCO_2 and XCH_4 ECV data products over land shall meet the random error (precision) requirements given in Table 4. *The required thresholds refer to global long-term statistics (i.e., they refer to the ensemble of data products, i.e., of individual retrievals). Locally in space and time larger values may be acceptable.*

Based on these considerations the requirements on systematic errors are:

REQ-XGHG-ERR-2	The XCO_2 and XCH_4 ECV data products over land shall meet the systematic error requirements given in Table 4. *The required thresholds refer to global long-term statistics (i.e., they refer to the ensemble of data products, i.e., individual retrievals). Locally in space and time larger values may be acceptable.*

Correlations:

When the data products are used for inverse modelling purposes, assumptions have to be made concerning error correlations. Inverse modelling improves if information on error correlations is provided in addition to the uncertainty of the individual retrievals. Error correlation information can be used to deal with systematic observation errors (at least to some extent). How to reliably determine error correlations, i.e., to quantify how the errors of the single ground-pixel retrievals are correlated, has not yet been studied in detail but is an important (new) research topic. As error correlations are expected to depend on time and location (aerosols, residual clouds, surface reflectance, etc.) this is a complex issue. To consider this user need, the following requirement has been formulated:

REQ-XGHG-ERR-3	Estimates of the error correlations between the XCO_2 and XCH_4 values retrieved from individual ground-pixels shall be reported. *No requirement is given yet here on the actual values of these correlations*.

Note: It is unlikely that this information can be obtained for each single measurement but it may be possible to determine spatial and temporal error correlation lengths (which likely depend on spatial position and time). A possible approach could be to analyze differences with respect to accurate and precise TCCON FTS retrievals as a function of time/space lags. As this approach has limitations because the TCCON sites are sparse in space and the satellite retrievals are sparse in time, it needs to be studied to what extent state-of-the-art model data can be used to extend the analysis.

Table 3: XCO_2 and XCH_4 random ("precision") and systematic retrieval error requirements for measurements over land. 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 XCO_2 and XCH_4					
Parameter	**Req. type**	**Random error** ("Precision")		**Systematic error**	**Stability**
		Single obs.	1000^2 km^2 monthly		
XCO_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 #))	-"-
XCH_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 #))

2.1.6 Validation

Validation against high precision / low systematic error ground-based XCO_2 and XCH_4 retrievals is required.

The most appropriate network for this purpose is TCCON (Total Carbon Column Observing Network; http://www.tccon.caltech.edu/), which is a network of FTS sites designed for the purpose of validating satellite XCO_2 and XCH_4 retrievals.

As shown in *Wunch et al., 2010*, the uncertainty of the TCCON data products is typically 0.4 ppm for XCO_2 (1-sigma) and 4 ppb (1-sigma) for XCH_4 (see also the discussion of this in the context of validation of satellite retrievals as given in *Buchwitz et al., 2016, 2017a, 2017b*).

This indicates that TCCON has low errors and is therefore well suited for validation of the XCO_2 and XCH_4 satellite data products (nevertheless, there are limitations as the TCCON network is sparse, because TCCON retrievals are typically available only after one year of the observation and because the TCCON uncertainty is on the order of the systematic error and stability as required for the satellite data products).

REQ-XGHG-VAL-1	The XCO_2 and XCH_4 ECV data products shall be validated using TCCON. *Note: A proper validation requires to consider also the averaging kernels and a-priori profiles of the satellite AND FTS retrievals (see, e.g., Rodgers, 2000, and Rodgers and Connor, 2003). This information therefore needs to be provided as part of the data product(s) and used for validation.*

2.1.7 Observation operators

In order to construct appropriate observation operators for the XCO_2 and XCH_4 data products Averaging Kernels (AK) and (CO_2 and CH_4) *a-priori* profiles as used by the retrieval algorithms need to be made available to the users.

REQ-XGHG-OO-1	For each ECV data product all information needed to construct the corresponding observation operator such as Averaging Kernels (AK) and used CO_2 and CH_4 *a-priori* profiles needs to be made available.

2.1.8 Ancillary data

Various ancillary data are required to generate satellite CDRs such as the GHG ECV data products. This requires appropriate documentation.

REQ-XGHG-ANCIL-1	Each GHG ECV data product needs a proper documentation of which ancillary data have been used. This refers to information on the underlying Level 1 data product and auxiliary data products used such as meteorological data.

2.1.9 Data format

The Level 2 data products need to be properly documented. A dedicated document is required where the data products are described in detail. Consistent naming conventions shall be used across the different GHG ECV (sub)products but also, if possible, taking into account the naming conventions used within the other ECV projects.

REQ-XGHG-NCD-1	There shall be a document, which provides a detailed description of the GHG ECV data products. Consistent naming conventions shall be used for the different GHG ECV (sub)products but also, if possible, by adopting the naming conventions used for the other ECV projects and available standard naming conventions, most notably the naming conventions given in http://cfconventions.org/

In addition, the algorithms shall be described in sufficient detail.

REQ-XGHG-NCD-2	The retrieval algorithms shall be described in sufficient details via an Algorithm Theoretical Basis Document (ATBD) and/or peer-reviewed publications.

The users of the GHG ECV data products need data products which contain all the information required for surface flux inverse modelling such as retrieved XCO_2 and XCH_4 values for individual ground pixels, their errors, corresponding averaging kernels, used *a-priori* profiles, etc.

Most users need Level 2 data products (rather than Level 3) and most user are familiar with data products in NetCDF format.

Based on this the following requirements have been formulated:

REQ-GHG-META-1	The GHG ECV Level 2 data products shall contain in addition to the main parameter (e.g., XCO_2) all relevant meta data as needed for inverse modelling. This comprises at least the following information for each ground pixel: Latitude, longitude, time, main parameter uncertainty (e.g., XCO_2 uncertainty, 1-sigma), quality flag, averaging kernel and – if applicable for the used algorithm - the used *a-priori* profile for the main parameter. Note: If possible and appropriate (for the algorithm used to generate the product) the averaging kernels and *a-priori* profiles shall be reported on pressure levels (or pressure layers) and for all relevant levels (or layers) also the corresponding (effective) pressure differences (over the corresponding layer) shall be provided (e.g., as "pressure weights", i.e., normalized to surface pressure (with their sum being 1.0) or as absolute pressure differences). In any case the exact definitions need to be clearly explained in the product user guide.

REQ-GHG-DFO-1	The data products shall • be produced in netCDF-4 (classic) format (see http://www.unidata.ucar.edu/software/netcdf/) • be compliant with the CF (Climate and Forecasting) convention 3 • use CF standard names for the main variables (if possible, i.e., if an appropriate standard name exists) • include the global attributes listed in **/Bennett and James, 2013/** (if possible and appropriate)

2.1.10 Data access

The data products are made available via the C3S website. Nevertheless, a data access requirement has been added here.

REQ-XGHG-DA-1	The GHG ECV data products and all documents relevant for the users shall be made publicly available via a dedicated website and/or ftp server.

2.1.11 Level of processing

The data products needed to obtain information on (e.g., regional) CO_2 and CH_4 surface fluxes or for most other carbon or climate related applications (e.g., detailed comparisons with models) are the Level 2 data products as exact time and location information is needed as well as averaging kernels.

REQ-XGHG-PROC-1	All XCO_2 and XCH_4 product shall be available as Level 2 products.

For climate model comparisons (e.g., *Lauer et al., 2017*) also Level 3 data products are useful, in particular products in Obs4MIPs format (https://www.earthsystemcog.org/projects/obs4mips/).

REQ-XGHG-PROC-2	The XCO_2 and XCH_4 product shall also be available as Level 3 products in Obs4MIPs format.

2.2 Requirements for mid/upper tropospheric CO_2 and CH_4

In this section, requirements for mid/upper tropospheric CO_2 and CH_4 retrievals are listed.

2.2.1 Definitions

All definitions as relevant for the data products and their requirements covered by this part of the document are given in section “General definitions”.

2.2.2 Horizontal resolution

The mid/upper tropospheric CO_2 and CH_4 data products are Level 2 products generated from existing instruments (primarily IASI). Therefore, no requirements are formulated here.

2.2.3 Vertical resolution

The mid/upper tropospheric CO_2 and CH_4 data products are Level 2 products generated from existing instruments (primarily IASI). Therefore, no requirements are formulated here.

2.2.4 Observing cycle

The mid/upper tropospheric CO_2 and CH_4 data products are Level 2 products generated from existing instruments (primarily IASI). Therefore, no requirements are formulated here.

2.2.5 Random and systematic errors

In this section requirements for random errors (“precision”) and systematic errors (“bias”, “accuracy”) for satellite mid/upper tropospheric CO_2 and CH_4 retrievals are given. They are identical with the ones given in the ESA CCI URD *[D4]* and have been formulated in the context of regional flux inversions using XCO_2 and XCH_4. It is assumed here that these requirements are also valid for satellite mid/upper tropospheric CO_2 and CH_4 retrievals and for most of the other carbon or climate applications.

The requirements as given here are identical with the ones given in **Sect. 2.1**, where more details are given.

The requirements on random errors (precision) are:

REQ-MTGHG-ERR-1	The mid/upper tropospheric CO_2 and CH_4 ECV data products shall meet the random error (precision) requirements given in Table 5. *The required thresholds refer to global long-term statistics (i.e., they refer to the ensemble of data products, i.e., of individual retrievals). Locally in space and time larger values may be acceptable.*

The requirements on systematic errors are:

REQ-MTGHG-ERR-2	The mid/upper tropospheric CO_2 and CH_4 ECV data products shall meet the systematic error requirements given in Table 5. *The required thresholds refer to global long-term statistics (i.e., they refer to the ensemble of data products, i.e., individual retrievals). Locally in space and time larger values may be acceptable.*

Correlations:

When the data products are used for inverse modelling purposes, assumptions have to be made concerning error correlations. Inverse modelling improves if information on error correlations is provided in addition to the uncertainty of the individual retrievals. Error correlation information can be used to deal with systematic observation errors (at least to some extent). How to reliably determine error correlations, i.e., to quantify how the errors of the single ground-pixel retrievals are correlated, has not yet been studied in detail but is an important (new) research topic. As error correlations are expected to depend on time and location (aerosols, residual clouds, surface reflectance, etc.) this is a complex issue. To consider this user need, the following requirement has been formulated:

REQ-MTGHG-ERR-3	Estimates of the error correlations between the mid/upper tropospheric CO_2 and CH_4 values retrieved from individual ground-pixels shall be reported. *No requirement is given yet here on the actual values of these correlations.*

Table 4: 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”)		**Systematic error**	**Stability**
		Single obs.	1000^2 km^2 monthly		
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 #))

2.2.6 Validation

Validation against high precision / low systematic errors reference observations is required for the mid/upper troposphere CO_2 and CH_4 data products. Unfortunately, measurements of both gases in the free troposphere and stratosphere are every sparse. Validation thus mostly relies on existing aircraft measurements. A promising way consists in using 0-30 km profiles measured by balloon-borne AirCores (*Membrive et al., 2016*) to which averaging kernels can be applied to derive columns that can then be compared to those derived from space.

REQ-MTGHG-VAL-1	The mid/upper troposphere CO_2 and CH_4 data products shall be validated using available aircraft and balloon-borne (AirCore) measurements.

2.2.7 Observation operators

In order to construct appropriate observation operators for the mid/upper troposphere CO_2 and CH_4 data products Averaging Kernels (AK) as used by the retrieval algorithms need to be made available to the users.

REQ-MTGHG-OO-1	For each mid/upper troposphere CO_2 and CH_4 data product all information needed to construct the corresponding observation operator such as Averaging Kernels (AK) needs to be made available.

2.2.8 Ancillary data

Various ancillary data are required to generate satellite CDRs such as the GHG ECV data products. This requires appropriate documentation.

REQ-MTGHG-ANCIL-1	Each GHG ECV data product needs a proper documentation of which ancillary data have been used. This refers to information on the underlying Level 1 data product and auxiliary data products used such as meteorological data.

2.2.9 Data format

REQ-MTGHG-NCD-1	There shall be a document, which provides a detailed description of the GHG ECV data products. Consistent naming conventions shall be used for the different GHG ECV (sub)products but also, if possible, by adopting the naming conventions used for the other ECV projects and available standard naming conventions, most notably the naming conventions given in http://cfconventions.org/

REQ-MTGHG-NCD-2	The retrieval algorithms shall be described in sufficient details via an Algorithm Theoretical Basis Document (ATBD) and/or peer-reviewed publications.

The following requirements are also applicable for the CO_2 and CH_4 mid/upper troposphere Level 2 data products:

- **REQ-GHG-META-1**
- **REQ-GHG-DFO-1**

2.2.10 Data access

The data products are made available via the C3S website. Nevertheless, a data access requirement has been added here.

REQ-MTGHG-DA-1	The CO_2 and CH_4 mid/upper troposphere products and all documents relevant for the users shall be made publicly available via a dedicated website and/or ftp server.

2.2.11 Level of processing

The data products needed to obtain information on (e.g., regional) CO_2 and CH_4 surface fluxes or for most other carbon or climate related applications (e.g., detailed comparisons with models) are the Level 2 data products as exact time and location information is needed as well as averaging kernels.

REQ-MTGHG-PROC-1	The CO_2 and CH_4 mid/upper troposphere product shall be available as Level 2 products.

3. Gap Analysis

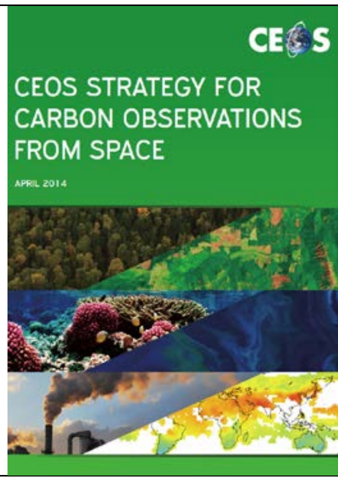
3.1 Description of past, current and future satellites

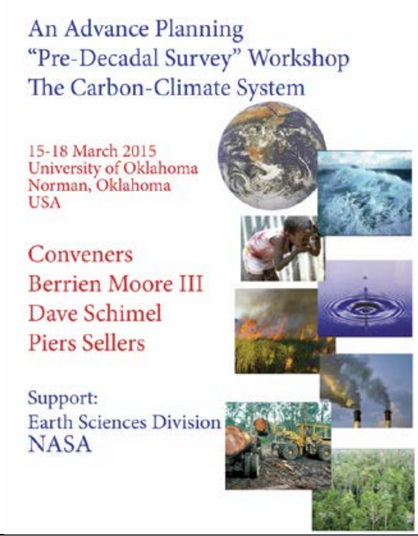
In this section the Earth Observation (EO) landscape relevant to the C3S_312b_Lot2 project satellite-derived GHG data products, i.e., CO_2 and CH_4 Climate Data Records (CDRs), is given, focusing on the temporal availability and coverage of the relevant measurements, including changes e.g. in the instrument specifications that could affect the long-term homogeneity of the CDR(s). The envisaged data availability for the next 10-15 years is also discussed in relation to possible data gaps.

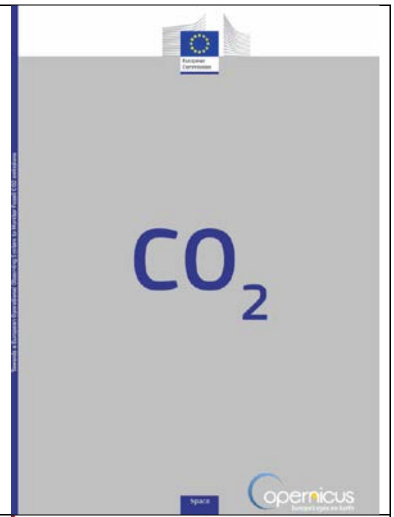
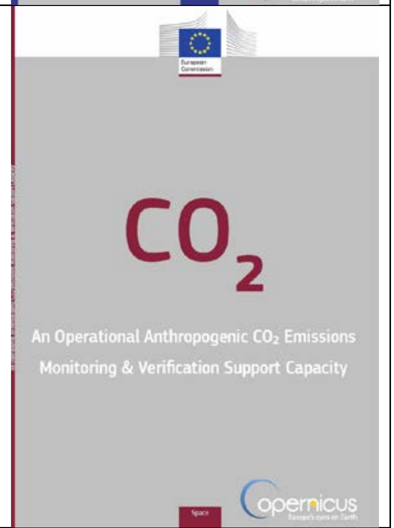
During recent years a large number of documents (including peer-reviewed publications) have been written where the following aspects are presented and discussed in detail:

- Need for space-based observations of CO_2 and/or CH_4
- Related observational requirements
- Overview past, present and planned satellites
- Recommendations for future improvements

Some of the key documents are listed here:

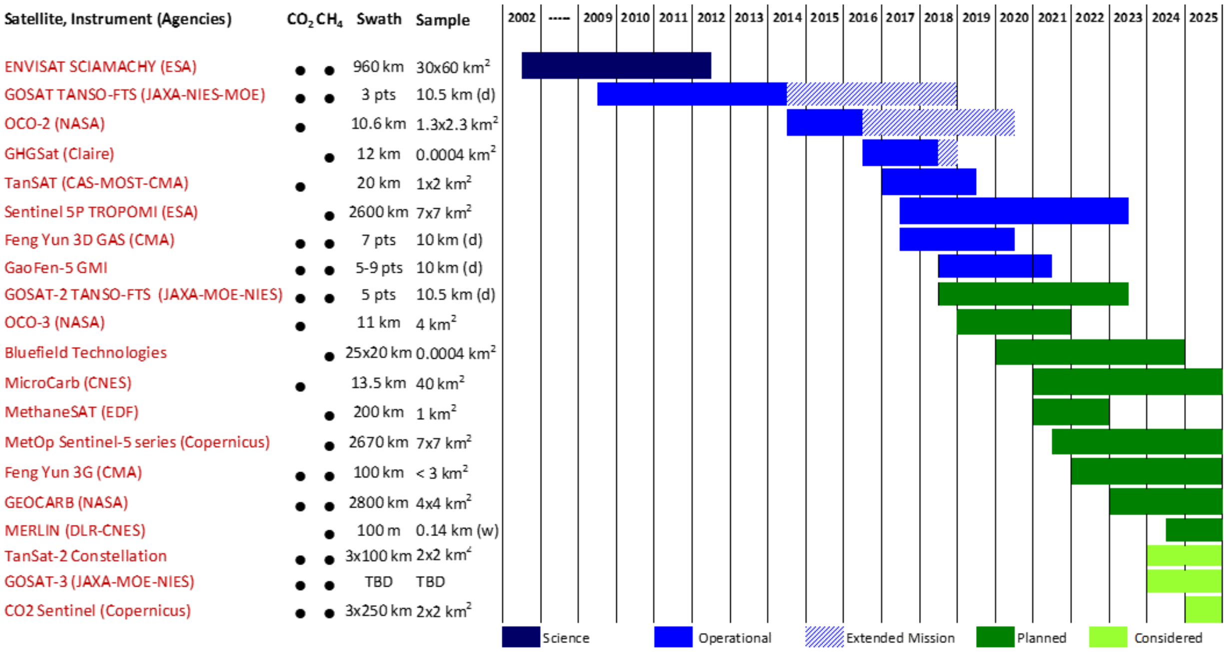
CEOS, 2014: CEOS Strategy for Carbon Observations from Space, The Committee on Earth Observation Satellites (CEOS) Response to the Group on Earth Observations (GEO) Carbon Strategy, April 2014. Link: http://ceos.org/document_management/Publications/WGClimate_CEOS-Strategy-for-Carbon-Observations-from-Space_Apr2014.pdf	
Ciais et al., 2014: Ciais, P., A. J. Dolman, A. Bombelli, et al., Current systematic carbon-cycle observations and the need for implementing a policy-relevant carbon observing system, Biogeosciences, 11, 3547-3602, 2014. Link: http://www.biogeosciences.net/11/3547/2014/bg-11-3547-2014.pdf	 Current systematic carbon-cycle observations and the need for implementing a policy-relevant carbon observing system

ESA 2015: Report for Mission Selection: CarbonSat, ESA SP-1330/1 (2 volume series), European Space Agency, Noordwijk, The Netherlands, 2015. Link: http://esamultimedia.esa.int/docs/EarthObservation/SP1330-1_CarbonSat.pdf	
Norman Report, 2015: An Advanced Planning “Pre-Decadal Survey” Workshop: The Carbon-Climate System, Workshop Report, Convenors B. Moore III, D. Schimel, P. Sellers, 15-178 March 2015, University of Oklahoma, Norman, Oklahoma, USA, 2015. Link: https://cce.nasa.gov/cce/pdfs/final_carbon_climate.pdf	
ESA-GCP-CEOS, 2016: Report of “3rd CARBON FROM SPACE WORKSHOP”, ESA-GCP-CEOS, University of Exeter, UK, 21st – 23rd January, 2016. Link: https://eo4society.esa.int/wp-content/uploads/2020/01/3rd-carbon-from-space-workshop-nbsp-report-.pdf	

(Blue) CO_2 Report, 2015: Ciais et al., Towards a European operational system to monitor fossil CO_2 emissions, Final Report from the expert group, October 2015, 2015. Link: http://edgar.jrc.ec.europa.eu/news_docs/CO2_report_22-10-2015.pdf	
(Red) CO_2 Report, 2017: Pinty B., G. Janssens-Maenhout, M. Dowell, H. Zunker, T. Brunhes, P. Ciais, D. Dee, H. Denier van der Gon, H. Dolman, M. Drinkwater, R. Engelen, M. Heimann, K. Holmlund, R. Husband, A. Kentarchos, Y. Meijer, P. Palmer and M. Scholze, An Operational Anthropogenic CO_2 Emissions Monitoring & Verification Support capacity - Baseline Requirements, Model Components and Functional Architecture, doi: 10.2760/39384, European Commission Joint Research Centre, EUR 28736 EN, 2017 Link: http://edgar.jrc.ec.europa.eu/news_docs/Report_Copernicus_CO2_Monitoring_TaskForce_2017.pdf	
CEOS, 2018: A CONSTELLATION ARCHITECTURE FOR MONITORING CARBON DIOXIDE AND METHANE FROM SPACE, Prepared by the CEOS Atmospheric Composition Virtual Constellation Greenhouse Gas Team Version 1.0 – 8 October 2018, 2018. Link: http://ceos.org/document_management/Virtual_Constellations/ACC/Documents/CEOS_AC-VC_GHG_White_Paper_Version_1_20181009.pdf	

Several of these documents also contain an overview about past, present and (possible) future missions (e.g., Figure 3).

Figure 1: Satellite CO_2 and CH_4 missions with sensitivity to the Planetary Boundary Layer (from: *CEOS, 2018*).



In this document, we present only a short overview of past, present and future satellites. Readers interested in more details are referred to the documents listed above.

Before this overview is presented, we first present a summary of the relevant GCOS ECV requirements in order to have a good understanding of which type of satellite observations are relevant for this climate-related service component.

3.1.1 Implications of GCOS ECV requirements for satellite instrumentation and related data products

Carbon dioxide (CO_2) and methane (CH_4) are Essential Climate Variables (ECVs) (e.g., *Bojinski et al., 2014*) and requirements for satellite-derived data sets have been formulated by GCOS (*GCOS-154*, *GCOS-195*, *GCOS-200*). According to *GCOS-154* the Essential Climate Variable Greenhouse Gases is defined as follows:

"Product Number A.8.1: Retrievals of greenhouse gases, such as CO_2 and CH_4, of sufficient quality to estimate regional sources and sinks".

The latest version of requirements for satellite-derived CO_2 and CH_4 data products are formulated in Annex A of *GCOS-200* (GCOS 2016 Implementation Plan) for the atmospheric ECV "Carbon dioxide, methane and other greenhouse gases".

The main goal of this project is to generate satellite-derived CO_2 and CH_4 ECV data products meeting GCOS and additional C3S service requirements. These data products and their corresponding documentation are available via the Copernicus Climate Data Store (CDS) (e.g., *Raoult et al., 2017*).

The GCOS CO_2 requirements are "Target Requirements" (in the sense of goal, i.e., ideal performance) to be achieved in the next 10 years. Some requirements cannot be met with current sensors or even future satellites (e.g., the 4 hour frequency requirement). Some important requirements are missing (especially a systematic error requirement, which is very important for this ECV). All current and near future CO_2 satellites aiming at improving our knowledge on CO_2 fluxes (e.g., GOSAT, GOSAT-2, OCO-2) are designed to provide column-average CO_2 (denoted XCO_2). The GCOS requirements are however only specified for "Tropospheric CO_2" currently (and in the near future) not available from satellites.

More specific requirements for current and (near) future CO_2 satellite observations have been formulated by the Climate Research Group (CRG) of the GHG-CCI project in the corresponding User Requirements Document (URD) *[D4]*. The most important (and challenging) requirements as formulated in the GHG-CCI URD are the systematic error requirement (< 0.5 ppm, 1-sigma) and the stability requirement (< 0.5 ppm/year).

The situation is essentially the same for methane and also for this gas detailed requirements have been formulated in *[D4].*

As a consequence, the C3S_312b_Lot2 project GHG requirements as formulated in **Sect. 2** are therefore largely based on *[D4]* taking into account all relevant GCOS requirements.

The most relevant satellite-derived data products for ECV greenhouse gases are the column average dry air mole fraction products XCO_2 and XCH_4 derived from satellite observations, which are sensitive to near-surface concentration variations (see **Sect. 2** for details). High near-surface sensitivity is important in order to use the data products for obtaining information on regional surface fluxes (as required for this ECV, see above), as the regional surface flux signal is largest near the ground.

Consequently, satellites providing near-surface sensitive XCO_2 and XCH_4 retrievals (e.g., GOSAT or OCO-2) are the focus of this document. With one exception (namely the future laser-based Merlin methane mission) these observations are based on reflected solar radiation in the near-infrared / short-wave infrared (NIR/SWIR) part of the electromagnetic spectrum.

Satellites performing observations in the relevant CO_2 and/or CH_4 sensitive parts of the thermal (or mid) infrared (TIR) parts of the electromagnetic spectrum typically have low sensitivity near the Earth's surface. Therefore, they typically can provide only limited information on regional surface fluxes. Their advantage is however that they provide data day and night, also at high latitudes throughout the year. The IASI instruments on the Metop satellite series provide long-term data sets of mid/upper tropospheric CO_2 and CH_4, that will be continued with IASI-NG onboard the Metop-SG-A platforms. These observations are highly complementary to the XCO_2 and XCH_4 observations and are important to monitor the concentration of these gases in higher atmospheric levels. Therefore, the IASI products are also covered via this document. Theoretically, NIR/SWIR and TIR measurements can also be combined to obtain information on sources and sinks but so far only little has been achieved in this area.

In the following sub-sections, focus is on satellites delivering XCO_2, XCH_4 and on IASI and follow-ons for mid/upper tropospheric CO_2 and CH_4 information.

3.1.2 Past satellites

SCIAMACHY/ENVISAT:

The first satellite which delivered XCO_2 and XCH_4 was ENVISAT thanks to its SCIAMACHY instrument (*Bovensmann et al., 1999*). Data product quality has been significantly improved during the GHG-CCI project of ESA's Climate Change Initiative (CCI) (https://climate.esa.int/en/projects/ghgs/) (*Buchwitz et al., 2015; 2016*). The latest version of these data products has been made available for C3S as "brokered products". SCIAMACHY (SCanning Imaging Absorption spectroMeter for Atmospheric ChartographY) was a spectrometer on ESA's ENVISAT satellite (2002-2012). SCIAMACHY (*Burrows et al., 2005; Bovensmann et al., 1999*) covered the spectral region from the ultra-violet to the SWIR spectral region (240 nm - 2380 nm) at moderate spectral resolution (0.2 nm - 1.5 nm) and was observing the Earth's atmosphere in various viewing geometries (nadir, limb and solar and lunar occultation). For a good general overview on SCIAMACHY see also https://en.wikipedia.org/wiki/SCIAMACHY. SCIAMACHY permits the retrieval of XCO_2 (e.g., *Reuter et al., 2011; Schneising et al., 2011*) and XCH_4 (e.g., *Schneising et al., 2011; Frankenberg et al., 2011*) from the appropriate spectral regions in the SWIR (around 1.6 µm) and the NIR (O_2 A-band at 760 nm used to obtain the dry-air column using the known dry-air mixing ratio of atmospheric oxygen). The ground pixel size is typically 30 km along track times 60 km across track and the swath width is about 960 km. There are no across-track gaps between the ground pixels but there are gaps along-track as SCIAMACHY operates only part of the time (approx. 50%) in nadir observation mode.

All other satellites are either current or future satellites and therefore described in the following sub-sections.

3.1.3 Current satellites

TANSO-FTS */GOSAT and GOSAT-2:*

TANSO-FTS is a Fourier-Transform-Spectrometer (FTS) onboard the Japanese GOSAT satellite (*Kuze et al., 2009, 2014, 2016*). The Greenhouse Gases Observing Satellite "IBUKI" (GOSAT) is the world's first spacecraft in orbit dedicated to measure the concentrations of carbon dioxide and methane from space. The spacecraft was launched successfully on January 23, 2009, and has been operating properly since then. GOSAT covers the relevant CO_2, CH_4 and O_2 absorption bands in the NIR and SWIR spectral region as needed for accurate XCO_2 and XCH_4 retrieval (in addition GOSAT also covers a large part of the Thermal Infrared (TIR) spectral region). The spectral resolution of TANSO-FTS is much higher compared to SCIAMACHY and also the ground pixels are smaller (10 km compared to several 10 km for SCIAMACHY). However, in contrast to SCIAMACHY, the GOSAT scan pattern consists of non-consecutive individual ground pixels, i.e., the scan pattern is not gap-free.
For a good general overview about GOSAT see also http://www.gosat.nies.go.jp/en/.

Recently, namely in October 2018, the follow-on mission GOSAT-2 was launched, which has similar characteristics as GOSAT but has been optimized for a higher yield of cloud-free observations and also permits the retrieval of carbon monoxide (CO).

OCO-2:

NASA’s Orbiting Carbon Observatory 2 (OCO-2) mission (*Crisp et al., 2004; Boesch et al., 2011*) was successfully launched in July 2014. The OCO-2 Project primary science objective is to collect space-based measurements of atmospheric carbon dioxide with the precision, resolution and coverage needed to characterize its sources and sinks and quantify their variability over the seasonal cycle. OCO-2 is in a sun-synchronous, near-polar orbit with a group of Earth-orbiting satellites with synergistic science objectives whose ascending node crosses the equator near 13:30 hours Mean Local Time (MLT). Near-global coverage of the sunlit portion of Earth is provided in this orbit over a 16-day (233-revolution) repeat cycle. OCO-2’s single instrument incorporates three high-resolution grating spectrometers, designed to measure the near-infrared absorption of reflected sunlight by carbon dioxide and molecular oxygen. OCO-2 covers similar spectral bands as SCIAMACHY and GOSAT but OCO-2 has much smaller ground pixels (km scale) but the swath width is much smaller (approx. 10 km) compared to SCIAMACHY. OCO-2 delivers XCO_2 but not XCH_4. Details on OCO-2 are also given on https://ocov2.jpl.nasa.gov/.

TanSat:

The Chinese TanSat satellite (https://www.wmo-sat.info/oscar/satellites/view/tansat) has been successfully launched in December 2016. The TanSat satellite and instrument is very similar to OCO-2. As OCO-2, TanSat delivers XCO_2 (*Yang et al. 2020*) but not XCH_4.

FY-3D:

The Chinese FY-3D satellite has been launched on 14-Nov-2017. The main mission is operational meteorology but there will also be substantial contribution to ocean and ice monitoring, climate monitoring, atmospheric chemistry and space weather. One of the instruments relevant for the service is the Greenhouse-gases Absorption Spectrometer (GAS), which permit to obtain information on CO_2 and CH_4. Details: https://www.wmo-sat.info/oscar/satellites/view/fy_3d

TROPOMI/Sentinel-5-Precursor (S5P):

ESA's Sentinel-5-Precursor (S5P) mission (*Veefkind et al, 2012*) has been successfully launch on 13-October-2017. S5P permits XCH_4 retrievals (*Butz et al., 2012; Hu et al., 2016, 2018; Schneising et al., 2019*) at about 7 km spatial resolution and using a wide swath of about 2600 km. Details on S5P can also be found on https://earth.esa.int/web/guest/missions/esa-future-missions/sentinel-5P.

OCO-3 (on the International Space Station (ISS)):
Similar as OCO-2 but with a different orbit and scan characteristics.
Details see: https://www.jpl.nasa.gov/missions/orbiting-carbon-observatory-3-oco-3/ and https://ocov3.jpl.nasa.gov/ where this information is given: "OCO-3, which launched to the International Space Station in May 2019, is tasked with continuing the CO_2 record of its still-operational predecessor OCO-2; however, there are some distinct differences between the two missions. The OCO-2 spacecraft was launched into a near-polar orbit, which means that every time is passes over a given point on Earth's surface, it does so at the same time of day. The space station, on the other hand, makes about 16 orbits of Earth per day, each shifting slightly to the west on its longitudinal axis. This orbit, combined with the fact that Earth itself is also rotating, allows OCO-3 to measure CO_2 over the same areas at different times of day."

AIRS:

The Atmospheric Infrared Sounder (AIRS) is a polar orbiting nadir-viewing high-resolution infrared sounder operating in a cross-track-scanning mode. It was launched onboard the EOS Aqua satellite in May 2002, with two operational microwave sounders, AMSU and HSB, and is operational since September 2002. It is a high-spectral resolution, grating multispectral infrared sounder with 2378 channels. Its spectral domain ranges from 650 cm^{-1} to 2665 cm^{-1} (15.4 µm and 3.8 µm), with a spectral resolving power of 1200 (i.e., a spectral resolution ranging from 0.5 cm^{-1} to 2 cm^{-1}). This domain is divided into three spectral bands, from 650 to 1135 cm^{-1}, from 1215 to 1615 cm^{-1} and from 2180 to 2665 cm^{-1}. AIRS cross-track scanning is 1650 km and covers 70% of the earth every day. The instantaneous field of view (IFOV) is sampled by 3×3 circular pixels whose ground resolution is 13 km at nadir. Measurements from the three instruments are analyzed jointly to filter out the effects of clouds from the IR data in order to derive clear-column air-temperature profiles and surface temperatures with high vertical resolution and accuracy (1 K per 1 km layer in the troposphere). The AIRS mid/upper tropospheric CO_2 product from GHG-CCI has been made available to C3S as a "brokered product".

IASI:

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. 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), and in September 2012 onboard Metop-B. A third IASI instrument has been launched onboard Metop-C on 7-November-2018. 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 apodisation ('Level 1c' spectra). 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. IASI has demonstrated the possibility to retrieve or detect several chemistry and climate variables from hyperspectral infrared observation: for instance, water vapour (H_2O), carbon dioxide (CO_2), carbon monoxide (CO), methane (CH_4), ozone (O_3), sulfur dioxide (SO_2), hydrogen sulfide (H_2S), ammonia (NH_3), nitric acid (HNO_3), volatile organic compounds (VOCs) and aerosols on regional and global scales. IASI enables the monitoring of key gases for climate and atmospheric chemistry in near real time and has also highlighted the benefit of high-performance infrared sounders for numerical weather prevision (NWP) applications.

3.1.4 Future satellites

For the reasons explained above only satellites providing near-surface sensitive XCO_2 or XCH_4 retrievals are mentioned in this sub-section (for the future IASI instrument on Metop-C see previous sub-section).

Relevant future LEO satellites are:

MicroCarb:
A dispersive spectrometer instrument that will be able to measure the total column concentration of CO_2 from 4 bands (0.76 and 1.27 O_2 bands and 1.6 and 2 µm CO_2 bands). Expected launch in 2021. Details see: https://microcarb.cnes.fr/en/MICROCARB/index.htm

UVNS/Sentinel-5 (S-5) on Metop-SG-A satellites:
Sentinel-5 is an atmospheric monitoring mission within the European Copernicus program, formerly the GMES (Global Monitoring for Environment and Security) program, jointly implemented by ESA and the EC (European Commission). The Sentinel-5 mission is a payload, consisting of a single instrument named UVNS. The main objective of the mission is the operational monitoring of trace gas concentrations for atmospheric chemistry and climate applications. It will provide accurate measurements of key atmospheric constituents such as ozone, nitrogen dioxide, sulphur dioxide, carbon monoxide, methane, formaldehyde, and aerosol properties. This means that S-5 is similar as S-5P but there are also differences. For example, S-5 includes a 1.6 µm band for improved XCH_4. This band also covers CO_2 absorption lines (but XCO_2 is not an official data product from S-5). Expected launch: Approx. 2022 on Metop-SG-A1, 2029 on Metop-SG-A2 and 2036 on Metop-SG_A3. Details see*:*
https://directory.eoportal.org/web/eoportal/satellite-missions/c-missions/copernicus-sentinel-5

IASI-NG:
A follow-on to the IASI mission, but with improved spectral resolution by a factor of 2 and improved radiometric noise by a factor 2 to 4 as compared to IASI. Will fly with UVMS/S-5 on the Metop-SG-A platforms. Expected launch in 2022, 2029 and 2036.
Details see: https://iasi-ng.cnes.fr/en/IASI-NG/index.htm

MERLIN:
First active (laser-based) satellite mission measuring XCH_4. Expected launch: 2024 (TBC).
Details see: https://merlin.cnes.fr/en/MERLIN/index.htm

CO_2 Monitoring (CO2M) Missions / Sentinel-7 (S-7):
The CO2M mission has been approved by ESA in 2019. CO2M will likely be a constellation of 2-3 satellites to measure XCO_2 (and XCH_4) at high spatial resolution (approx. 2x2 km^2) and good spatial coverage (approx. swath width 240 km). Expected launch: around 2025. See also *Pinty et al., 2017*, and *Janssens-Maenhout et al., 2020*.

Relevant future GEO satellites are:

GEOCARB mission:

Will measure XCO_2 and XCH_4 over parts of North or South America. Expected launch: early 2020s. Details see: https://www.wmo-sat.info/oscar/satellites/view/geocarb and http://scarbo-h2020.eu/news/19.

Conclusions future satellites:

Taking into account the ongoing and planned activities in Europe - in particular w.r.t. the atmospheric low Earth orbit (LEO) Sentinels (S-5P, S-5, S-7) and the IASI series - and elsewhere (in particular in the USA, Japan and China), no major gaps have been identified regarding the underlying satellite component of the Copernicus CO_2 and CH_4 service.

The most important application of the CO_2 and CH_4 satellites is to obtain information on (surface) sources and sinks of these greenhouse gases. This requires high sensitivity to concentration changes close to the Earth surface. This can be (and currently is) achieved via passive observations using reflected solar radiation (current default technique) or via active (laser-based) systems (in the future). Unfortunately, there is no single technique, which meets all requirements. Systems based on reflected solar radiation are limited to daytime observations and have poor coverage of the polar regions. These limitations can only be eliminated by complementary active (laser-based) observations (e.g., MERLIN), if this new technology turns out to be feasible / robust enough. Spatial coverage and along-track spatial resolution of the active sensors will however likely be very poor due to the narrow laser beam; furthermore, quite long integration times are needed to achieve sufficient signal to noise ratios, which also reduces the resolution along-track. Observations in the thermal infrared (e.g., IASI) can be performed day and night with good spatial coverage but sensitivity to the boundary layer is low. In summary, all techniques have advantages and disadvantages and requirements can only be met by an appropriate constellation of satellites. But even if all satellites listed above would be simultaneously in orbit, it is unlikely that all requirements can be met, especially not the GCOS "4 hour frequency requirement".

3.2 Development of processing algorithms

In this section aspect of the processing algorithms are described that limit the fitness-to-purpose of the current CDRs version compared to user requirements.

3.2.1 University of Bremen algorithms

For C3S currently two different types of algorithms are used:

- EMMA algorithm to generate merged Level 2 (L2) XCO_2 and XCH_4 products from the individual sensor Level 2 products of SCIAMACHY and GOSAT.
- OBS4MIPS algorithm, which generates merged Level 3 (L3) XCO_2 and XCH_4 products using the EMMA Level 2 products as input.

The algorithms are described in the Algorithm Theoretical Basis Document (ATBD) available from the C3S website. The data products are described in the Product User Guide and Specification (PUGS) available from the C3S website. The quality of the data products is described in the Product Quality Assessment Report (PQAR [D6]). Access to all these documents is also possible via this website: http://www.iup.uni-bremen.de/carbon_ghg/cg_data.html

It is planned for this service to include also existing individual sensor Level 2 products from OCO-2 and S5P for the generation of the merged L2 and L3 products in the (near) future. It requires some R&D in order to find out how to optimally implement this taking into account the large amounts of data these sensors deliver.

Identified aspects which limit the fitness of purpose for C3S:

- Merging algorithms EMMA and Obs4MIPs not optimized for new (not yet considered) sensors with large amounts of data (esp. S5P)

Recommendations on how to improve:

- See REC_ALG_006

3.2.2 University of Leicester algorithms

For C3S currently (year 2017) two different types of algorithms are used:

- Full physics (FP) algorithm to generate XCO_2 and XCH_4 from GOSAT.
- Proxy (PR) algorithm to generate XCH_4 from GOSAT.

The algorithms are described in the C3S_312a_Lot6 / C3S_312b_Lot2 document Algorithm Theoretical Basis Document (ATBD) (available from C3S website). The data products are described in the Product User Guide and Specification (PUGS) available from the C3S website. The quality of the data products is described in the Product Quality Assessment Report (PQAR [D6]). Access to all these documents is also possible via this website: http://www.iup.uni-bremen.de/carbon_ghg/cg_data.html

Identified aspects which limit the fitness of purpose for C3S:

- Limited accuracy (see requirements **(Sect. 2**) and achieved performance [D6])

Recommendations on how to improve:

- See REC_ALG_001, REC_ALG_002, REC_ALG_003

3.2.3 SRON algorithms

For C3S currently (year 2017) two different types of algorithms are used:

- Full physics (FP) algorithm to generate XCO_2 and XCH_4 from GOSAT.
- Proxy (PR) algorithm to generate XCH_4 from GOSAT.

The algorithms are described in the Algorithm Theoretical Basis Document (ATBD) available from the C3S website. The data products are described in the Product User Guide and Specification (PUGS) available from the C3S website. The quality of the data products is described in the Product Quality Assessment Report (PQAR [D6]). Access to all these documents is also possible via this website: http://www.iup.uni-bremen.de/carbon_ghg/cg_data.html

Identified aspects which limit the fitness of purpose for C3S:

- Limited accuracy (see requirements (**Sect. 2**) and achieved performance [D6])

Recommendations on how to improve:

- See REC_ALG_001, REC_ALG_002, REC_ALG_003

3.2.4 LMD/CNRS algorithms

For C3S currently (year 2017) the NLIS algorithm is used to retrieve mid/upper tropospheric CO_2 and CH_4 from the IASI instruments.

The algorithms are described in the Algorithm Theoretical Basis Document (ATBD) available from the C3S website. The data products are described in the Product User Guide and Specification (PUGS) available from the C3S website. The quality of the data products is described in the Product Quality Assessment Report (PQAR [D6]). Access to all these documents is also possible via this website: http://www.iup.uni-bremen.de/carbon_ghg/cg_data.html

Identified aspects which limit the fitness of purpose for C3S:

- Limited accuracy (see requirements (**Sect. 2**) and achieved performance [D6])

Recommendations on how to improve:

- See REC_ALG_003

3.3 Methods for estimating uncertainties

In this section it is briefly described how the uncertainties are estimated and how this compares with user requirements. The chapter is meant to highlight any aspect or obstacle that limits (the quality of) the current uncertainty estimates compared to the user requirements.

3.3.1 XCO_2 and XCH_4 products

In the following only a short description is given as assumed appropriate for the purpose of this document. For details please see the following C3S_312a_Lot6 / C3S_312b_Lot2 documents (available from C3S website):

- Algorithm Theoretical Basis Document (ATBD)
- Product Quality Assessment Report (PQAR [D6])

Individual sensor Level 2 products:

Uncertainties are reported for each single ground pixel (footprint). They are computed by error propagation from the uncertainties of the radiances as measured by the satellite instruments taking into account correlations of the Jacobians as used by the retrieval algorithms (see ATBD). The reported uncertainties are validated by comparisons with ground-based reference data (see PQAR [D6]).

Merged multi-sensor Level 2 products:

Uncertainties are taken from the individual sensor Level 2 products and validated using the same method as also used for the individual sensor Level 2 products. Additionally, the inter-algorithm spread is reported as an estimate for potential systematic uncertainties.

Level 3 products:

These products and their uncertainties are generated using the values and uncertainties of the merged multi-sensor Level 2 products.

Identified aspects which limit the fitness of purpose for C3S:

- Validation / data quality limitations (see requirements (**Sect. 2**) and achieved validation [D6])

Recommendations on how to improve:

- See REC_ERR_001 – REC_ERR_008

3.3.2 Mid/upper tropospheric CO_2 and CH_4 products

Please see the following C3S_312a_Lot6 / C3S_312b_Lot2 documents (available from C3S website and from http://www.iup.uni-bremen.de/carbon_ghg/cg_data.html):

- Algorithm Theoretical Basis Document (ATBD)
- Product Quality Assessment Report (PQAR [D6])

Identified aspects which limit the fitness of purpose for C3S:

- Validation / data quality limitations (see requirements (**Sect. 2**) and achieved validation [D6])

Recommendations on how to improve:

- See REC_ERR_003 – REC_ERR_008

3.4 Opportunities to improve quality and fitness-for-purpose of the CDRs

In this section opportunities are described to improve the current data version based on on-going research activities (e.g. improvements in the algorithm that are under testing) or on (improved) exploitation of existing measurements.

Reprocessing activities (where applicable) are also included.

Also mentioned are liaisons with the R&D community to address the identified needs.

3.4.1 Improvements based on ongoing R&D activities

R&D activities have been carried out in the past (until early 2017) within the framework of the GHG-CCI project (https://climate.esa.int/en/projects/ghgs/) of ESA's Climate Change Initiative (CCI). These R&D activities are currently partially considered via the follow-on project GHG-CCI+, which started in March 2019.

3.4.2 Reprocessing activities

Baseline for project C3S_312a_Lot6 / C3S_312b_Lot2 is to extend existing time series. Reprocessing activities may be carried out (if new algorithms are available and if schedule and funding permits) but this is not the current baseline.

It must be noted that, in order to provide CDRs that are compatible with climate studies, the homogeneity of the entire series is essential. In that sense, reprocessing activities should be envisioned and supported in the future in case of new R&D developments yielding improved accuracy of the datasets.

3.4.3 Liaisons with R&D community

The C3S_312a_Lot6 / C3S_312b_Lot2 project team consists of the European research institutions and corresponding scientists involved since the beginning (in 2010) of the GHG-CCI project (https://climate.esa.int/en/projects/ghgs/) of ESA's Climate Change Initiative (CCI). The C3S_312a_Lot6 / C3S_312b_Lot2 project essentially represents the (nearly entire) European research community working on the generation of satellite CO_2 and CH_4 ECV CDRs. On the level of satellite data providers of Level 2 and Level 3 data products there is no separation between R&D and operational activities. The liaison with the R&D community is therefore as close as possible.

3.5 Scientific research needs

In this section, any fundamental research need required to improve the processing algorithm, the error characterization and in general the CDR's fitness-for-purpose to be tackled at R&D level is described.

3.5.1 Processing algorithm research needs

The processing / retrieval algorithms must be accurate enough (low bias, low systematic error), fast enough and shall produce a large enough number of (high quality / quality filtered) observations with good enough precision (small enough random errors). The relevant TRs are described in **Sect. 2**. The following gaps and recommendations for improvement have been identified:

Rec. ID	Type	Gap	Recommendation
REC_ALG_001	R&D	Limited accuracy of data products – aerosols & clouds	Investigate alternative representations of light scattering (aerosols, cirrus) in the retrieval algorithms.
REC_ALG_002	R&D	Limited accuracy of data products – various items	-Implement and test Sun-Induced-Fluorescence (SIF) product for various datasets / missions -Fitting of intensity offsets to improve retrievals - Optimization of ancillary datasets used (e.g. prior CO_2, CH_4, etc.) - Surface treatment (e.g., BRDF) - Polarization radiative transfer - Sub-pixel cloud effects - other
REC_ALG_003	R&D	Limited accuracy of data products – input data	Improve spectroscopy of spectral bands used in the retrieval process, including proper aerosol spectral characterizations and solar spectrum characterization.
REC_ALG_004	R&D	Limited computational efficiency of L2 retrieval algorithms	Improvement of computational efficiency to enable processing of (not yet considered, e.g., OCO-2) current and future satellite data streams providing at least an order of magnitude more data. This includes, e.g., new RT methods and GPU processing.
REC_ALG_005	R&D	Limited number of data points (due to strict filtering)	Investigate to what extent the data yield can be improved including the use of (quasi) continuous quality indicator instead of binary flag (e.g. OCO-2 warn levels). Needs separate validation per warn level.
REC_ALG_006	R&D	Merging algorithms EMMA and	Investigate how to optimally further develop the EMMA and Obs4MIPs merging algorithms.

		Obs4MIPs not optimized for new sensors with large amounts of data (esp. OCO-2, S-5P)	*Note: Since March 2019 partially addressed in GHG-CCI+ project (https://climate.esa.int/en/projects/ghgs/)*

3.5.2 Error characterization research needs

The data products need to be well characterized w.r.t. their errors. The relevant TRs are described in **Sect. 2**. The following gaps and recommendations for improvement have been identified:

Rec. ID	Type	Gap	Recommendation
REC_ERR_001	R&D	Lack of spatial coverage of TCCON network limits validation and error characterization	Use of in particular EM27Sun instruments for validation (approx. 15 instruments at the moment) to fill up gaps in spatial coverage
REC_ERR_002	R&D or OPER or other	Risk of no or fewer TCCON validation data in the future	Insure continuity of TCCON network
REC_ERR_003	R&D	Limited validation due to small number of co-locations	Improve co-location method
REC_ERR_004	R&D	Unknown spatial and temporal error correlations	- Knowledge of error correlations is crucial for inverse modeling, therefore, it is important to investigate (by means of TCCON and model comparisons) spatial and temporal error correlations. - Improve validation of reported L2 errors
REC_ERR_005	R&D	Unknown systematic error functions	- Improved / extended investigation of error sources (e.g., how do systematic L2 errors depend on geophysical scene properties). -Improvement of L2 bias correction schemes.
REC_ERR_006	R&D	Lack of good vertical coverage of GHGs limits validation and characterization of total columns	- Development of atmospheric profiling 0-30 km such as AirCore or Amulse balloon-borne devices that could be flown at several TCCON/ICOS stations. - Use of IAGOS/CARIBIC/CONTRAIL aircraft 0-12 km profiles
REC_ERR_007	R&D	Lack of validation of	Investigate the use of NDACC FTIR

		mid/upper tropospheric columns retrieved from TIR observations	observations to validate TIR retrievals.
REC_ERR_008	R&D	Lack of proper intercomparison between retrieval codes (both EU and non-EU)	Framework for comparison between various retrieval algorithms in order to establish the pros and cons of each approach

3.5.3 Research needs related to not yet included satellite instruments

3.5.3.1 OCO-2

OCO-2 provides XCO_2 since 2014 as retrieved by the NASA OCO-2 team. Level 2 version 8 products have been released in October 2017.

Project C3S_312b_Lot2 is using this operational OCO-2 data product from NASA for the generation of the merged XCO_2 Level 2 and Level 3 products (see *Reuter et al., 2020*).

A dedicated European XCO_2 Level 2 retrieval effort for OCO-2 is highly recommended for the following reasons:

- To establish (at least a small) ensemble of OCO-2 XCO_2 products as needed for improved error assessment / sensitivity analysis to ensure robustness of results
- Capacity building for future European CO_2 missions (“Sentinel 7”)

This is a challenging activity as OCO-2 delivers 2 orders of magnitude more data as the currently used sensors SCIAMACHY and GOSAT (but about one order of magnitude less than CO2M).

The following gaps and recommendations for improvement have been identified (see also REC_ALG_004):

Rec. ID	Type	Gap	Recommendation
REC_INS_001	R&D	Currently no European OCO-2 XCO_2 Level 2 algorithm and corresponding data product mature enough (in terms of processing speed and/or accuracy and/or yield) for C3S	Further development of European XCO_2 retrievals algorithm(s) to generate Level 2 XCO_2 data product(s) from OCO-2 *Note: Since March 2019 partially addressed in GHG-CCI+ and other projects (EU H2020 CHE and VERIFY)*

3.5.3.2 TanSat

TanSat delivers XCO_2 with a similar characteristics as OCO-2 (*Yang et al., 2020*) in terms of spatial resolution and coverage.

Adding TanSat XCO_2 to C3S would result in additional (improved) spatio-temporal coverage.

The following gaps and recommendations for improvement have been identified:

Rec. ID	Type	Gap	Recommendation
REC_INS_002	R&D	Currently no European TanSat XCO_2 Level 2 algorithm and corresponding data product for C3S	Further development of European XCO_2 retrievals algorithm(s) to generate Level 2 XCO_2 data product(s) from TanSat *Note: Since March 2019 partially addressed in GHG-CCI+*

3.5.3.3 Sentinel-5-Precursor (S-5P)

S-5P delivers XCH_4 with high spatial resolution (7 x 7 km^2) and very good spatial coverage (daily) (e.g., *Lorente et al., 2021*). Using S-5P XCH_4 for C3S is expected to result in a wealth of additional information on atmospheric methane not currently available in particular with respect to localized methane emission sources (e.g., *Schneising et al., 2020*).

The following gaps and recommendations for improvement have been identified:

Rec. ID	Type	Gap	Recommendation
REC_INS_003	R&D	Limited development of scientific S-5P methane retrieval algorithms to enable ensemble-based assessments and data product generation	Operational methane retrieval from S-5P is challenging and will highly benefit from parallel scientific algorithm development and comparisons of operational and scientific data products. *Note: Since March 2019 partially addressed in ESA projects GHG-CCI+ and Methane+*

3.5.3.4 GOSAT-2

GOSAT-2 aims at delivering XCO_2 and XCH4 with similar characteristics as GOSAT-1 apart from the improved coverage (e.g., because of "intelligent pointing").

Adding GOSAT-2 XCO_2 and XCH4 to C3S would result in additional (improved) spatio-temporal coverage and (in case of GOSAT-1 failure or switch-off) continuation of the GOSAT-1 time series.

The following gaps and recommendations for improvement have been identified:

Rec. ID	Type	Gap	Recommendation
REC_INS_004	R&D	Unclear to what extent GOSAT-1 XCO_2 and XCH_4 retrieval algorithms need to be adjusted for GOSAT-2 to achieve a similar or even better data quality	Adjust existing GOSAT-1 XCO_2 and XCH_4 Level 1 algorithms to GOSAT-2 and investigate the quality of the resulting data products. Develop methods for improvement, if necessary. *Note: Since March 2019 partially addressed in GHG-CCI+*

3.5.3.5 OCO-3

OCO-3 (*Taylor et al., 2020*) delivers XCO_2 with similar characteristics as OCO-2 apart from the spatio-temporal coverage, which will be different (because of the different orbit).

Adding OCO-3 XCO_2 to C3S would result in additional (improved) spatio-temporal coverage.

The following gaps and recommendations for improvement have been identified:

Rec. ID	Type	Gap	Recommendation
REC_INS_005	R&D	Currently no European OCO-3 XCO_2 Level 2 algorithm and corresponding data product mature enough (in terms of processing speed and accuracy) for C3S	Further development of European XCO_2 retrievals algorithm(s) to generate Level 2 XCO_2 data product(s) from OCO-3

3.5.3.6 IASI on Metop-C

IASI/MetOp-C will permit continuation of the mid/upper tropospheric CO_2 and CH_4 time series of IASI/MetOp-B, so long as both IASI and AMSU instruments on Metop-C are spectrally and radiometrically characterized and compared to their predecessors on Metop-A and B.

It is recommended to also include mid/upper tropospheric CO_2 and CH_4 retrievals from IASI/MetOp-C in the future:

Rec. ID	Type	Gap	Recommendation
REC_INS_006	R&D	Currently no CO_2 and CH_4 C3S ECV products from IASI/MetOp-C	Assess the quality of IASI/MetOp-C mid/upper tropospheric CO_2 and CH_4 retrievals and generate and deliver also these products as C3S ECV products if the quality is high enough

3.5.4 Other research needs

As stated above, NIR/SWIR and TIR measurements could be combined to obtain information on sources and sinks, by providing a means to increase the vertical resolution of the retrieval and allowing for the separation between the lower-troposphere, mid/upper troposphere and stratosphere. So far, only little has been achieved in this area.

Rec. ID	Type	Gap	Recommendation
REC_OTH_001	R&D	Currently, no algorithm for combined processing SWIR and TIR observation to increase vertical coverage	Design of new algorithms combining SWIR and TIR observations (which will be available with S-5/IASI-NG) in order to aim at having more than one degree of freedom on the vertical and to extract information near the surface. *Note: Now partially addressed in ESA project Methane+*

3.6 Opportunities from exploiting the Sentinels and any other relevant satellite

In this section it is discussed what impact the envisaged future instruments' availability relevant to the CDR(s) discussed in **Sect. 1** could make.

It is considered that this impact could be on various aspects, for instance, differences in the instrument specifications that could provide better or more accurate measurements.

3.6.1 OCO-2

Gaps and recommended solutions on how to improve: See **Sect. 3.5.3**.

3.6.2 TanSat

Gaps and recommended solutions on how to improve: See **Sect. 3.5.3**.

3.6.3 Sentinel-5-Precursor (S-5P)

Gaps and recommended solutions on how to improve: See **Sect. 3.5.3**.

3.6.4 GOSAT-2

Gaps and recommended solutions on how to improve: See **Sect. 3.5.3**.

3.6.5 OCO-3

Gaps and recommended solutions on how to improve: See **Sect. 3.5.3**.

3.6.6 IASI on Metop-C

Gaps and recommended solutions on how to improve: See **Sect. 3.5.3**.

3.6.7 MERLIN

Recommendations for C3S: Currently: None.

3.6.8 MicroCarb

Recommendations for C3S: Currently: None.

3.6.9 Sentinel-5 (S-5)

Recommendations for C3S: Currently: None.

3.6.10 GEOCARB

Recommendations for C3S: Currently: None.

3.6.11 Improved future satellite instruments

3.6.11.1 CarbonSat

CarbonSat (Bovensmann et al., 2010; Buchwitz et al., 2013b) has been proposed to ESA as Earth Explorer 8 Satellite (EE8) (ESA 2015) in order to significantly improve the capability of measuring CO_2 and CH_4 from space in the future. CarbonSat but has not been selected for EE8 but see **Sect. 3.6.11.2**.

Recommendations for C3S: None.

3.6.11.2 Anthropogenic CO_2 Monitoring (CO2M) mission ("Sentinel-7")

Currently, the European Commission in cooperation with ESA and other institutions are aiming at a system for better monitoring anthropogenic CO_2 emissions in the future. The space component will likely be a constellation of CO2M satellites similar to CarbonSat. It is likely that such a constellation will be launched around 2025.

Recommendations for C3S: Currently: None.

References

Alexe et al., 2015: Alexe, M., P. Bergamaschi, A. Segers, R. Detmers, A. Butz, O. Hasekamp, S. Guerlet, R. Parker, H. Boesch, C. Frankenberg, R. A. Scheepmaker, E. Dlugokencky, C. Sweeney, S. C. Wofsy, and E. A. Kort, Inverse modeling of CH4 emissions for 2010–2011 using different satellite retrieval products from GOSAT and SCIAMACHY, Atmos. Chem. Phys., 15, 113–133, doi:10.5194/acp-15-113-2015, 2015.

Bennett and James, 2013: Bennett, V. and James, S., Data Standards Requirements for CCI Data Producers, ESA Technical Note, Reference: CCI-PRGM-EOPS-TN-13-0009, Issue 1, Revision 1, Date of Issue 24/05/2013, 2013.

Bergamaschi et al., 2009: Bergamaschi, P., Frankenberg, C., Meirink, J. F., Krol, M., Villani, M. G., Houweling, S., Dentener, F., Dlugokencky, E. J., Miller, J. B., Gatti, L. V., Engel, A., and Levin, I.: Inverse modeling of global and regional CH_4 emissions using SCIAMACHY satellite retrievals, J. Geophys. Res., 114, D22301, doi:10.1029/2009JD012287, 2009.

Bergamaschi et al., 2013: Bergamaschi, P., Houweling, H., Segers, A., et al., Atmospheric CH4 in the first decade of the 21st century: Inverse modeling analysis using SCIAMACHY satellite retrievals and NOAA surface measurements, J. Geophys. Res., 118, 7350-7369, doi:10.1002/jrgd.50480, 2013.

Boesch et al., 2011: Boesch, H., D. Baker, B. Connor, D. Crisp, and C. Miller, Global characterization of CO_2 column retrievals from shortwave-infrared satellite observations of the Orbiting Carbon Observatory-2 mission, Remote Sensing, 3 (2), 270-304, 2011.

Bojinski et al., 2014: Bojinski, S., M. Verstraete, T.C. Peterson, C. Richter, A. Simmons, M. Zemp, The Concept of Essential Climate Variables in Support of Climate Research, Applications, and Policy. Bull. Amer. Meteor. Soc., 95, 1431–1443. Available at http://journals.ametsoc.org/doi/pdf/10.1175/BAMS-D-13-00047.1, 2014.

Bovensmann et al., 1999: Bovensmann, H., Burrows, J. P., Buchwitz, M., Frerick, J., Noël, S., Rozanov, V. V., Chance, K. V., Goede, A. H. P. (1999), SCIAMACHY - Mission objectives and measurement modes, J. Atmos. Sci., 56 (2), 127-150, 1999.

Bovensmann et al., 2010: Bovensmann, H., Buchwitz, M., Burrows, J. P., Reuter, M., Krings, T., Gerilowski, K., Schneising, O., Heymann, J., Tretner, A., and Erzinger, J.: A remote sensing technique for global monitoring of power plant CO_2 emissions from space and related applications, Atmos. Meas. Tech., 3, 781-811, 2010.

Buchwitz et al., 2000: Buchwitz, M., Rozanov, V. V., and Burrows, J. P.: A near-infrared optimized DOAS method for the fast global retrieval of atmospheric CH_4, CO, CO_2, H_2O, and N_2O total column amounts from SCIAMACHY Envisat-1 nadir radiances, J. Geophys. Res. 105, 15,231-15,245, 2000.

Buchwitz et al., 2005: Buchwitz, M., R. de Beek, J. P. Burrows, H. Bovensmann, T. Warneke, J. Notholt, J. F. Meirink, A. P. H. Goede, P. Bergamaschi, S. Körner, M. Heimann, and A. Schulz, Atmospheric methane and carbon dioxide from SCIAMACHY satellite data: Initial comparison with chemistry and transport models, Atmos. Chem. Phys., 5, 941-962, 2005.

Buchwitz et al., 2007: Buchwitz, M., O. Schneising, J. P. Burrows, H. Bovensmann, M. Reuter, J. Notholt, First direct observation of the atmospheric CO_2 year-to-year increase from space, Atmos. Chem. Phys., 7, 4249-4256, 2007.

Buchwitz et al., 2013a: Buchwitz, M., M. Reuter, O. Schneising, H. Boesch, S. Guerlet, B. Dils, I. Aben, R. Armante, P. Bergamaschi, T. Blumenstock, H. Bovensmann, D. Brunner, B. Buchmann, J. P. Burrows, A. Butz, A. Chédin, F. Chevallier, C. D. Crevoisier, N. M. Deutscher, C. Frankenberg, F. Hase, O. P. Hasekamp, J. Heymann, T. Kaminski, A. Laeng, G. Lichtenberg, M. De Mazière, S. Noël, J. Notholt, J. Orphal, C. Popp, R. Parker, M. Scholze, R. Sussmann, G. P. Stiller, T. Warneke, C. Zehner, A. Bril, D. Crisp, D. W. T. Griffith, A. Kuze, C. O'Dell, S. Oshchepkov, V. Sherlock, H. Suto, P. Wennberg, D. Wunch, T. Yokota, Y. Yoshida, The Greenhouse Gas Climate Change Initiative (GHG-CCI): comparison and quality assessment of near-surface-sensitive satellite-derived CO_2 and CH_4 global data sets, *Remote Sensing of Environment*, doi:10.1016/j.rse.2013.04.024, http://authors.elsevier.com/sd/article/S0034425713003520, 2013.

Buchwitz et al., 2013b: Buchwitz, M., Reuter, M., Bovensmann, H., Pillai, D., Heymann, J., Schneising, O., Rozanov, V., Krings, T., Burrows, J. P., Boesch, H., Gerbig, C., Meijer, Y., and Loescher, A.: Carbon Monitoring Satellite (CarbonSat): assessment of atmospheric CO_2 and CH_4 retrieval errors by error parameterization, Atmos. Meas. Tech., 6, 3477-3500, 2013.

Buchwitz et al., 2015: Buchwitz, M., Reuter, M., Schneising, O., Boesch, H., Guerlet, S., Dils, B., Aben, I., Armante, R., Bergamaschi, P., Blumenstock, T., Bovensmann, H., Brunner, D., Buchmann, B., Burrows, J.P., Butz, A., Chédin, A., Chevallier, F., Crevoisier, C.D., Deutscher, N.M., Frankenberg, C., Hase, F., Hasekamp, O.P., Heymann, J., Kaminski, T., Laeng, A., Lichtenberg, G., De Mazière, M., Noël, S., Notholt, J., Orphal, J., Popp, C., Parker, R., Scholze, M., Sussmann, R., Stiller, G.P., Warneke, T., Zehner, C., Bril, A., Crisp, D., Griffith, D.W.T., Kuze, A., O'Dell, C., Oshchepkov, S., Sherlock, V., Suto, H., Wennberg, P., Wunch, D., Yokota, T., Yoshida, Y., The Greenhouse Gas Climate Change Initiative (GHG-CCI): comparison and quality assessment of near-surface-sensitive satellite-derived CO2 and CH4 global data sets. Remote Sens. Environ. 162:344–362, http://dx.doi.org/10.1016/j.rse.2013.04.024, 2015.

Buchwitz et al., 2016: Buchwitz, M., Reuter, M., Schneising, O., Hewson, W., Detmers, R. G., Boesch, H., Hasekamp, O. P., Aben, I., Bovensmann, H., Burrows, J. P., Butz, A., Chevallier, F., Dils, B., Frankenberg, C., Heymann, J., Lichtenberg, G., De Mazière, M., Notholt, J., Parker, R., Warneke, T., Zehner, C., Griffith, D. W. T., Deutscher, N. M., Kuze, A., Suto, H., and Wunch, D.:, Global satellite observations of column-averaged carbon dioxide and methane: The GHG-CCI XCO_2 and XCH_4 CRDP3 data, Remote Sensing of Environment (in press), Special Issue on Essential Climate Variables, DOI: 10.1016/j.rse.2016.12.027, link: http://dx.doi.org/10.1016/j.rse.2016.12.027, 2016.

Buchwitz et al., 2017a: ESA Climate Change Initiative (CCI) Product Validation and Intercomparison Report (PVIR) for the Essential Climate Variable (ECV) Greenhouse Gases (GHG) for data set Climate Research Data Package No. 4 (CRDP#4), Version 5.0, 9. Feb. 2017, 2017.

Buchwitz et al., 2017b: Buchwitz, M.; Reuter, M.; Aben, I.; Boesch, H.; Butz, A.; Detmers, R.G.; Frankenberg, C.; Hasekamp, O.P.; Parker, R.; Schneising, O.; Somkuti, P., ESA Greenhouse Gases Climate Change Initiative (GHG-CCI): Merged SCIAMACHY and GOSAT Level 3 gridded atmospheric column-average methane (XCH_4) product in Obs4MIPs format version 2 (CRDP#4), Technical Note, pp. 11, 1 February 2017, 2017.

Buchwitz et al., 2017c: Buchwitz, M., Schneising, O., Reuter, M., Heymann, J., Krautwurst, S., Bovensmann, H., Burrows, J. P., Boesch, H., Parker, R. J., Somkuti, P., Detmers, R. G., Hasekamp, O. P., Aben, I., Butz, A., Frankenberg, C., Turner, A. J., Satellite-derived methane hotspot emission estimates using a fast data-driven method, Amos. Chem. Phys., 17, 5751-5774, doi:10.5194/acp-17-5751-2017, 2017.

Buchwitz et al., 2018: Buchwitz, M., Reuter, M., Schneising, O., Bovensmann, H., Burrows, J. P., Boesch, H., Anand, J., Parker, R., Detmers, R. G., Aben, I., Hasekamp, O. P., Crevoisier, C., Armante, R., Zehner, C., Schepers, D., Copernicus Climate Change Service (C3S) Global Satellite Observations of Atmospheric Carbon Dioxide and Methane, Adv. Astronaut. Sci. Technol., https://doi.org/10.1007/s42423-018-0004-6, 2018.

Burrows et al., 1995: Burrows, J. P., Hölzle, E., Goede, A. P. H., Visser, H., and Fricke, W., SCIAMACHY—Scanning Imaging Absorption Spectrometer for Atmospheric Chartography, Acta Astronaut., 35(7), 445–451, doi:10.1016/0094-5765(94)00278-t, 1995.

Butz et al., 2011: Butz, A., Guerlet, S., Hasekamp, O., et al., Toward accurate CO_2 and CH_4 observations from GOSAT, *Geophys. Res. Lett.*, doi:10.1029/2011GL047888, 2011.

Butz et al., 2012: Butz, A., Galli, A., Hasekamp, O., Landgraf, J., Tol, P., and Aben, I.: Remote Sensing of Environment, TROPOMI aboard Sentinel-5 Precursor : Prospective performance of CH_4 retrievals for aerosol and cirrus loaded atmospheres, 120, 267-276, doi:10.1016/j.rse.2011.05.030, 2012.

CEOS, 2014: CEOS Strategy for Carbon Observations from Space, The Committee on Earth Observation Satellites (CEOS) Response to the Group on Earth Observations (GEO) Carbon Strategy, April 2014. Link: http://ceos.org/document_management/Publications/WGClimate_CEOS-Strategy-for-Carbon-Observations-from-Space_Apr2014.pdf

Chédin et al. 2003: Chédin, A., Saunders, R., Hollingsworth, A., Scott, N. A., Matricardi, M., Etcheto, J., Clerbaux, C., Armante, R. and Crevoisier, C.: The feasibility of monitoring CO_2 from high resolution infrared sounders. J. Geophys. Res., 108, ACH 6-1–6-19, doi: 10.1029/2001JD001443, 2003.

Chevallier et al., 2005: Chevallier, F., R. J. Engelen, and P. Peylin, The contribution of AIRS data to the estimation of CO2 sources and sinks. Geophys. Res. Lett., 32, L23801, doi:10.1029/ 2005GL024229, 2005.

Chevallier et al., 2007: Chevallier, F., F.-M. Bréon, and P. J. Rayner, Contribution of the Orbiting Carbon Observatory to the estimation of CO_2 sources and sinks: Theoretical study in a variational data assimilation framework. J. Geophys. Res., 112, D09307, doi:10.1029/2006JD007375, 2007.

Chevallier et al., 2009a: Chevallier, F., R. J. Engelen, C. Carouge, T. J. Conway, P. Peylin, C. Pickett-Heaps, M. Ramonet, P. J. Rayner and I. Xueref-Remy, AIRS-based vs. surface-based estimation of carbon surface fluxes. J. Geophys. Res., 114, D20303, doi:10.1029/2009JD012311, 2009.

Chevallier et al., 2009b: Chevallier, F., S. Maksyutov, P. Bousquet, F.-M. Bréon, R. Saito, Y. Yoshida, and T. Yokota, On the accuracy of the CO_2 surface fluxes to be estimated from the GOSAT observations. Geophys. Res. Lett., 36, L19807, doi:10.1029/2009GL040108, 2009.

Chevallier et al., 2010: Chevallier, F., Feng, L., Boesch, H. Palmer, P., and Rayner, P., On the impact of transport model errors for the estimation of CO_2 surface fluxes from GOSAT observations, Geophys. Res. Let., 37, L21803, 2010.

Chevallier et al., 2014: Chevallier, F., Palmer, P.I., Feng, L., Boesch, H., O'Dell, C.W., Bousquet, P., Towards robust and consistent regional CO2 flux estimates from in situ and space-borne measurements of atmospheric CO_2, Geophys. Res. Lett., 41, 1065-1070, DOI: 10.1002/2013GL058772, 2014.

Chevallier et al., 2016: Chevallier, F., et al., Climate Assessment Report (CAR), ESA Climate Change Initiative (CCI) GHG-CCI project, Version 3, 3 May 2016, 2016.

Ciais et al., 2014: Ciais, P., Dolman, A. J., Bombelli, A., et al.: Current systematic carbon cycle observations and needs for implementing a policy-relevant carbon observing system, Biogeosciences, 11, 3547-3602, www.biogeosciences.net/11/3547/2014/, doi:10.5194/bg-11-3547-2014, 2014.

Ciais et al., 2015: Ciais, P., et al.: Towards a European Operational Observing System to Monitor Fossil CO_2 emissions - Final Report from the expert group, http://www.copernicus.eu/main/towards-european-operational-observing-system-monitor-fossil-co2-emissions, pp. 68, October 2015, 2015.

CMUG-RBD, 2012: Climate Modelling User Group Requirements Baseline Document, Deliverable 1.2, Number D1.2, ESA Climate Change Initiative (CCI, https://earth.esa.int/documents/10174/1754357/RD-5-CMUG_D1.2_URD_v1.6.pdf/ef3b9619-e59c-4927-af8d-844924f15000;jsessionid=D85994FFED6AF216D1F203D3F8459EBB.eodisp-prod4040?version=1.0), Version 1.6, 17 Dec 2012, 2012.

CO_2 Report 2015: Ciais et al., Towards a European operational system to monitor fossil CO2 emissions, Final Report from the expert group, October 2015, 2015
Link: http://www.copernicus.eu/sites/default/files/library/CO2_Report_22Oct2015.pdf

CO_2 Report 2017: Pinty B., G. Janssens-Maenhout, M. Dowell, H. Zunker, T. Brunhes, P. Ciais, D. Dee, H. Denier van der Gon, H. Dolman, M. Drinkwater, R. Engelen, M. Heimann, K. Holmlund, R. Husband, A. Kentarchos, Y. Meijer, P. Palmer and M. Scholze, An Operational Anthropogenic CO_2 Emissions Monitoring & Verification Support capacity - Baseline Requirements, Model Components and Functional Architecture, doi: 10.2760/39384, European Commission Joint Research Centre, EUR 28736 EN, 2017 Link:
http://copernicus.eu/sites/default/files/documents/News/Report_Copernicus_CO2_Monitoring_TaskForce_21122017.pdf

Cogan et al., 2011: Cogan, A. J., Boesch, H., Parker, R. J., et al., Atmospheric carbon dioxide retrieved from the Greenhouse gases Observing SATellite (GOSAT): Comparison with ground-based TCCON observations and GEOS-Chem model calculations, *J. Geophys. Res.*, 117, D21301, doi:10.1029/2012JD018087, 2012.

Corbin et al., 2008: Corbin, K. D., A. S. Denning, L. Lu, J.-W. Wang, and I. T. Baker, Possible representation errors in inversions of satellite CO_2 retrievals, J. Geophys. Res., 113, D02301, doi:10.1029/2007JD008716, 2008.

Cressot et al., 2014: Cressot, C., F. Chevallier, P. Bousquet, et al., On the consistency between global and regional methane emissions inferred from SCIAMACHY, TANSO-FTS, IASI and surface measurements, Atmos. Chem. Phys., 14, 577-592, 2014.

Crevoisier et al. 2003: Crevoisier, C., Chédin, A., and Scott, N. A., AIRS channel selection for CO_2 and other trace-gas retrievals, Q. J. Roy. Meteorol. Soc., 129, 2719–2740, 2003a.

Crevoisier et al., 2009: Crevoisier, C., Chédin, A., Matsueda, H., et al., First year of upper tropospheric integrated content of CO_2 from IASI hyperspectral infrared observations, *Atmos. Chem. Phys.*, 9, 4797-4810, 2009.

Crevoisier et al. 2009b: Crevoisier, C., Nobileau, D., Fiore, A., Armante, R., Chédin, A., and Scott, N. A.: Tropospheric methane in the tropics – first year from IASI hyperspectral infrared observations, Atmos. Chem. Phys., 9, 6337–6350, doi:10.5194/acp-9-6337-2009, 2009b.

Crevoisier et al., 2013: Crevoisier, C., Nobileau, D., Armante, R., et al., The 2007–2011 evolution of tropical methane in the mid/upper troposphere as seen from space by MetOp-A/IASI, *Atmos. Chem. Phys.*, 13, 4279-4289, 2013.

Crisp et al., 2004: Crisp, D., Atlas, R. M., Breon, F.-M., Brown, L. R., Burrows, J. P., Ciais, P., Connor, B. J., Doney, S. C., Fung, I. Y., Jacob, D. J., Miller, C. E., O'Brien, D., Pawson, S., Randerson, J. T., Rayner, P., Salawitch, R. S., Sander, S. P., Sen, B., Stephens, G. L., Tans, P. P., Toon, G. C., Wennberg, P. O., Wofsy, S. C., Yung, Y. L., Kuang, Z., Chudasama, B., Sprague, G., Weiss, P., Pollock, R., Kenyon, D., and Schroll, S.: The Orbiting Carbon Observatory (OCO) mission, Adv. Space Res., 34, 700-709, 2004.

Dee et al., 2011: Dee, D. P., et al.: The ERA-Interim reanalysis: Configuration and performance of the data assimilation system, Q. J. R. Meteorol. Soc., 137(656), 553–597, doi:10.1002/qj.828, 2011.

Detmers et al., 2015: Detmers, R. G., O. Hasekamp, I. Aben, S. Houweling, T. T. van Leeuwen, A. Butz, J. Landgraf, P. Koehler, L. Guanter, and B. Poulter, Anomalous carbon uptake in Australia as seen by GOSAT, Geophys. Res. Lett., 42, doi:10.1002/2015GL065161, 2015.

Dils et al., 2014: B. Dils, M. Buchwitz, M. Reuter, O. Schneising, H. Boesch, R. Parker, S. Guerlet, I. Aben, T. Blumenstock, J. P. Burrows, A. Butz, N. M. Deutscher, C. Frankenberg, F. Hase, O. P. Hasekamp, J. Heymann, M. De Mazière, J. Notholt, R. Sussmann, T. Warneke, D. Griffith, V. Sherlock, D. Wunch :The Greenhouse Gas Climate Change Initiative (GHG-CCI): Comparative validation of GHG-CCI SCIAMACHY/ENVISAT and TANSO-FTS/GOSAT CO_2 and CH_4 retrieval algorithm products with measurements from the TCCON network, Atmos. Meas. Tech., 7, 1723-1744, 2014.

ESA 2015: Report for Mission Selection: CarbonSat, ESA SP-1330/1 (2 volume series), European Space Agency, Noordwijk, The Netherlands, 2015. Link: http://esamultimedia.esa.int/docs/EarthObservation/SP1330-1_CarbonSat.pdf

ESA-CCI-GHG-URDv2.1: Chevallier, F., et al., User Requirements Document (URD), ESA Climate Change Initiative (CCI) GHG-CCI project, Version 2.1, 19 Oct 2016, 2016.

ESA-CCI-GHG-URDv3.0: Chevallier, F., et al., User Requirements Document (URD), ESA Climate Change Initiative (CCI) GHG-CCI project, Version 3.0, 17 Feb 2020, pp.42, link: https://www.iup.uni-bremen.de/carbon_ghg/docs/GHG-CCIplus/URD/URDv3.0_GHG-CCIp_Final.pdf , 2020.

ESA-GCP-CEOS, 2016: Report of “3rd CARBON FROM SPACE WORKSHOP”, ESA-GCP-CEOS, University of Exeter, UK, 21st – 23rd January, 2016. Available from: http://www.carbonfromspace.info/ (-> Reports Download)

Frankenberg et al., 2011: Frankenberg, C., Aben, I., Bergamaschi, P., et al., Global column-averaged methane mixing ratios from 2003 to 2009 as derived from SCIAMACHY: Trends and variability, *J. Geophys. Res.*, doi:10.1029/2010JD014849, 2011.

GCOS-154: Global Climate Observing System (GCOS), SYSTEMATIC OBSERVATION REQUIREMENTS FOR SATELLITE-BASED PRODUCTS FOR CLIMATE, Supplemental details to the satellite-based component of the "Implementation Plan for the Global Observing System for Climate in Support of the UNFCCC (2010 update)", Prepared by World Meteorological Organization (WMO), Intergovernmental Oceanographic Commission, United Nations Environment Programme (UNEP), International Council for Science, Doc.: GCOS 154, ink: https://www.wmo.int/pages/prog/gcos/Publications/gcos-154.pdf, 2010.

GCOS-195: Status of the Global Observing System for Climate. GCOS-195. Link: https://library.wmo.int/pmb_ged/gcos_195_en.pdf, 2015.

GCOS-200: The Global Observing System for Climate: Implementation Needs, World Meteorological Organization (WMO), GCOS-200 (GOOS-214), pp. 325, link: http://unfccc.int/files/science/workstreams/systematic_observation/application/pdf/gcos_ip_10oct2016.pdf, 2016.

Guerlet et al., 2013: Guerlet, S., S. Basu, A. Butz, M. Krol, P. Hahne, S. Houweling, O. P. Hasekamp and I. Aben, Reduced carbon uptake during the 2010 Northern Hemisphere summer from GOSAT, Geophys. Res. Lett., doi: 10.1002/grl.50402, 2013.

Hayman et al., 2014: Hayman, G. D., O'Connor, F. M., Dalvi, M., Clark, D. B., Gedney, N., Huntingford, C., Prigent, C., Buchwitz, M., Schneising, O., Burrows, J. P., Wilson, C., Richards, N., Chipperfield, M., Comparison of the HadGEM2 climate-chemistry model against in-situ and SCIAMACHY atmospheric methane data, Atmos. Chem. Phys., 14, 13257-13280, doi:10.5194/acp-14-13257-2014, 2014.

Hollmann et al., 2013: Hollmann, C.J. Merchant, R. Saunders, C. Downy, M. Buchwitz, A. Cazenave, E. Chuvieco, P. Defourny, G. de Leeuw, R. Forsberg, T. Holzer-Popp, F. Paul, S. Sandven, S. Sathyendranath, M. van Roozendael, W. Wagner, The ESA Climate Change Initiative: satellite data records for essential climate variables, Bulletin of the American Meteorological Society (BAMS), 0.1175/BAMS-D-11-00254.1, pp. 12, 2013.

Houweling et al., 2004: Houweling, S., Breon, F.-M., Aben, I., Rödenbeck, C., Gloor, M., Heimann, M. and Ciais, P.: Inverse modeling of CO_2 sources and sinks using satellite data: A synthetic inter-comparison of measurement techniques and their performance as a function of space and time, Atmos. Chem. Phys., 4, 523-538, 2004.

Houweling et al., 2005: Houweling, S., Hartmann, W., Aben, I., Schrijver, H., Skidmore, J., Roelofs, G.-J., and Breon, F.-M.: Evidence of systematic errors in SCIAMACHY-observed CO_2 due to aerosols, Atmos. Chem. Phys., 5, 3003–3013, 2005.

Houweling et al., 2015: Houweling, S., D. Baker, S. Basu, H. Boesch, A. Butz, F. Chevallier, F. Deng, E. J. Dlugokencky, L. Feng, A. Ganshin, O. Hasekamp, D. Jones, S. Maksyutov, J. Marshall, T. Oda, C.W. O'Dell1, S. Oshchepkov, P. I. Palmer, P. Peylin, Z. Poussi, F. Reum, H. Takagi, Y. Yoshida, and R. Zhuravlev, An intercomparison of inverse models for estimating sources and sinks of CO_2 using GOSAT measurements, J. Geophys. Res. Atmos., 120, 5253–5266, doi:10.1002/2014JD022962, 2015.

Hu et al., 2016: Hu, H., O. Hasekamp, A. Butz, et al., The operational methane retrieval algorithm for TROPOMI, Atmos. Meas. Tech., 9, 5423-5440, doi:10.5195/amt-9-5423-2016, 2016.

Hu et al., 2018: Hu, H., J. Landgraf, R. Detmers, et al., Towards global mapping of methane with TROPOMI : first results and intersatellite comparison to GOSAT, Geophys. Res. Lett., doi:10.1002/2018GL077259, 2018.

Hungershoefer et al., 2010: Hungershoefer, K., Breon, F.-M., Peylin, P., Chevallier, F., Rayner, P., Klonecki, A., Houweling, S., and Marshall, J., Evaluation of various observing systems for the global monitoring of CO_2 surface fluxes, Atmos. Chem. Phys., 10, 10503-10520, 2010.

IPCC, 2013: Climate Change 2013: The Physical Science Basis, Working Group I Contribution to the Fifth Assessment Report of the Intergovernmental Report on Climate Change, http://www.ipcc.ch/report/ar5/wg1/, 2013.

Janssens-Maenhout et al., 2020: Janssens-Maenhout, G., B. Pinty, M. Dowell, H. Zunker, E. Andersson, G. Balsamo, J.-L. Bezy, T. Brunhes, H. Boesch, B. Bojkov, D. Brunner, M. Buchwitz, D. Crisp, P. Ciais, P. Counet, D. Dee, H. Denier van der Gon, H. Dolman, M. Drinkwater, O. Dubovik, R. Engelen, T. Fehr, V. Fernandez, M. Heimann, K. Holmlund, S. Houweling, R. Husband, O. Juvyns, A. Kentarchos, J. Landgraf, R. Lang, A. Loescher, J. Marshall, Y. Meijer, M. Nakajima, P.I. Palmer, P. Peylin, P. Rayner, M. Scholze, B. Sierk, J. Tamminen, and P. Veefkind, Towards an operational anthropogenic CO_2 emissions monitoring and verification support capacity, Bulletin of the American Meteorological Society (BAMS), 10.1175/BAMS-D-19-0017.1, https://doi.org/10.1175/BAMS-D-19-0017.1, pp. 13, 2020.

JCGM, 2008: JCGM/WG 1, Working Group 1 of the Joint Committee for Guides in Metrology, Evalutation of measurement data – Guide to the expression of uncertainty in measurement, http://www.bipm.org/utils/common/documents/jcgm/JCGM_100_2008_E.pdf, 2008.

Kaminski et al., 2017: Kaminski, T., Scholze, M., Vossbeck, M., Knorr, W., Buchwitz, M., and Reuter, M.: Constraining a terrestrial biosphere model with remotely sensed atmospheric carbon dioxide, Remote Sensing of Environment 203, 109-124, http://dx.doi.org/10.1016/j.rse.2017.08.017, 2017.

Kirschke et al., 2013: Kirschke, S., Bousquet, P., Ciais, P., et al.: Three decades of global methane sources and sinks, Nat. Geosci., 6, 813–823, doi:10.1038/ngeo1955, 2013.

Kuze et al., 2009: Kuze, A., Suto, H., Nakajima, M., and Hamazaki, T. (2009), Thermal and near infrared sensor for carbon observation Fourier-transform spectrometer on the Greenhouse Gases Observing Satellite for greenhouse gases monitoring, Appl. Opt., 48, 6716–6733, 2009.

Kuze et al., 2014: Kuze, A., Taylor, T., Kataoka, F., Bruegge, C., Crisp, D., Harada, M., Helmlinger, M., Inoue, M., Kawakami, S., Kikuchi, N., Mitomi, Y., Murooka, J., Naitoh, M., O'Brien, D., O'Dell, C., Ohyama, H., Pollock, H., Schwandner, F., Shiomi, K., Suto, H., Takeda, T., Tanaka, T., Urabe, T., Yokota, T., and Yoshida, Y. (2014), Long-term vicarious calibration of GOSAT short-wave sensors: techniques for error reduction and new estimates of radiometric degradation factors, IEEE T. Geosci. Remote, 52, 3991–4004, doi:10.1109/TGRS.2013.2278696, 2014.

Kuze et al., 2016: Kuze, A., Suto, H., Shiomi, K., Kawakami, S., Tanaka, M., Ueda, Y., Deguchi, A., Yoshida, J., Yamamoto, Y., Kataoka, F., Taylor, T. E., and Buijs, H. L.: Update on GOSAT TANSO-FTS performance, operations, and data products after more than 6 years in space, Atmos. Meas. Tech., 9, 2445-2461, doi:10.5194/amt-9-2445-2016, 2016.

Lauer et al., 2017: Lauer, A., V. Eyring, M. Righi, M. Buchwitz, P. Defourny, M. Evaldsson, P. Friedlingstein, R. de Jeu, G. de Leeuw, A. Loew, C. J. Merchant, B. Müller, T. Popp, M. Reuter, S.

Sandven, D. Senftleben, M. Stengel, M. Van Roozendael, S. Wenzel, U, Willén, Benchmarking CMIP5 models with a subset of ESA CCI Phase 2 data using the ESMValTool, Remote Sensing of Environment, DOI: 10.1016/j.rse.2016.12.027, in press, pp. 31, 2017.

Lorente et al. 2021: Lorente, A., Borsdorff, T., Butz, A., Hasekamp, O., aan de Brugh, J., Schneider, A., Wu, L., Hase, F., Kivi, R., Wunch, D., Pollard, D. F., Shiomi, K., Deutscher, N. M., Velazco, V. A., Roehl, C. M., Wennberg, P. O., Warneke, T., and Landgraf, J.: Methane retrieved from TROPOMI: improvement of the data product and validation of the first 2 years of measurements, Atmos. Meas. Tech., 14, 665–684, https://doi.org/10.5194/amt-14-665-2021, 2021.

Machida et al. 2008: Machida, T., Matsueda, H., Sawa, Y., Nakagawa, Y., Hirotani, K., Kondo, N., Goto, K., Nakazawa, T., Ishikawa, K., and Ogawa, T.: Worldwide measurements of atmospheric CO_2 and other trace gas species using commercial airlines, J. Atmos. Ocean. Tech., 25(10), 1744–1754, doi:10.1175/2008JTECHA1082.1, 2008.

Massart et al., 2016: Massart, S., A. Agustí-Panareda, J. Heymann, M. Buchwitz, F. Chevallier, M. Reuter, M. Hilker, J. P. Burrows, N. M. Deutscher, D. G. Feist, F. Hase, R. Sussmann, F. Desmet, M. K. Dubey, D. W. T. Griffith, R. Kivi, C. Petri, M. Schneider, V. A. Velazco, Ability of the 4-D-Var analysis of the GOSAT BESD XCO2 retrievals to characterize atmospheric CO2 at large and synoptic scales, Atmos. Chem. Phys., 16, 1653-1671, doi:10.5194/acp-16-1653-2016, 2016.

Matsueda et al. 2008: Matsueda, H., Machida, T., Sawa, Y., Nakagawa, Y., Hirotani, K., Ikeda, H., Kondo, N., and Goto, K.: Evaluation of atmospheric CO_2 measurements from new flask air sampling of JAL airliner observation, Pap. Meteorol. Geophys., 59, 1–17, 2008.

McNorton et al., 2016: McNorton, J., E. Gloor, C. Wilson, G. D. Hayman, N. Gedney, E. Comyn-Platt, T. Marthews, R. J. Parker, H. Boesch, and M. P. Chipperfield, Role of regional wetland emissions in atmospheric methane variability, Geophys. Res. Lett., 43, doi:10.1002/2016GL070649, 2016.

Meirink et al., 2006: Meirink, J.-F., Eskes, H. J., and Goede, A. P. H., Sensitivity analysis of methane emissions derived from SCIAMACHY observations through inverse modelling, Atmos. Chem. Phys., 6, 1275-1292, 2006.

Membrive et al., 2016: Membrive, O., Crevoisier, C., Sweeney, C., Danis, F., Hertzog, A., Engel, A., Bönisch, H., and Picon, L.: AirCore-HR: A high resolution column sampling to enhance the vertical description of CH_4 and CO_2, Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2016-236, 2016.

Merchant et al., 2017: Merchant, C. J., Paul, F., Popp, T., Ablain, M., Bontemps, S., Defourny, P., Hollmann, R., Lavergne, T., Laeng, A., de Leeuw, G., Mittaz, J., Poulsen, C., Povey, A. C., Reuter, M., Sathyendranath, S., Sandven, S., Sofeiva, V. F. and Wagner, W., Uncertainty information in climate data records from Earth observation. Earth System Science Data, 9 (2), pp. 511-527, ISSN 1866-3516, 2017.

Miller et al., 2007: Miller, C. E., Crisp, D., DeCola, P. L., et al.: Precision requirements for space-based XCO2 data, J. Geophys. Res., 112, D10314, doi:10.1029/2006JD007659, 2007.

Nisbet et al., 2014: Nisbet, E., Dlugokencky, E., and Bousquet, P.: Methane on the rise – again, Science, 343, 493–495, doi:10.1126/science.1247828, 2014.

Norman Report, 2015: An Advanced Planning “Pre-Decadal Survey” Workshop: The Carbon-Climate System, Workshop Report, Convenors B. Moore III, D. Schimel, P. Sellers, 15-178 March 2015, University of Oklahoma, Norman, Oklahoma, USA, 2015. Link: https://cce.nasa.gov/cce/pdfs/final_carbon_climate.pdf

Pandey et al., 2016: Pandey, S., S. Houweling, M. Krol, I. Aben, F. Chevallier, E. J. Dlugokencky, L. V. Gatti, E. Gloor, J. B. Miller, R. Detmers, T. Machida, T. Roeckmann, Inverse modeling of GOSAT-retrieved ratios of total column CH4 and CO2 for 2009 and 2010, Atmos. Chem. Phys., 16, 5043–5062, doi:10.5194/acp-16-5043-2016, 2016.

Parker et al., 2011: Parker, R., Boesch, H., Cogan, A., et al., Methane Observations from the Greenhouse gases Observing SATellite: Comparison to ground-based TCCON data and Model Calculations, *Geophys. Res. Lett*., doi:10.1029/2011GL047871, 2011.

Parker et al., 2016: Parker, R. J., H. Boesch, M. J. Wooster, D. P. Moore, A. J. Webb, D. Gaveau, and D. Murdiyarso, Atmospheric CH4 and CO2 enhancements and biomass burning emission ratios derived from satellite observations of the 2015 Indonesian fire plumes, Atmos. Chem. Phys., Atmos. Chem. Phys., 16, 10111-10131, doi:10.5194/acp-16-10111-2016, 2016.

Peters et al., 2007: Peters, W., A. R. Jacobson, C. Sweeney, A. E. Andrews, T. J. Conway, K. Masarie, J. B. Miller, L. M. P. Bruhwiler, G. Pétron, A. I. Hirsch, D. E. J. Worthy, G. R. van derWerf, J. T. Randerson, P. O. Wennberg, M. C. Krol, and P. P. Tans (2007), An atmospheric perspective on North American carbon dioxide exchange: CarbonTracker, Proceedings of the National Academy of Sciences (PNAS) of the United States of America, 27 November 2007, 104(48), 18 925–18 930, 2007.

Pillai et al., 2016: Pillai, D., Buchwitz, M., Gerbig, C., Koch, T., Reuter, M., Bovensmann, H., Marshall, J., and Burrows, J. P.: Tracking city CO_2 emissions from space using a high resolution inverse modeling approach: A case study for Berlin, Germany, Atmos. Chem. Phys., 16, 9591-9610, doi:10.5194/acp-16-9591-2016, 2016.

Pinty et al., 2017: Pinty, B., et al., An Operational Anthropogenic CO_2 Emissions Monitoring & Verification Support capacity - Baseline Requirements, Model Components and Functional Architecture, doi: 10.2760/39384, European Commission Joint Research Centre, EUR 28736 EN, 2017.

PQAR GHG, 2017: Buchwitz, M., Aben, I., Anand, J., Armante, R., Boesch, H., Crevoisier, C., Detmers, R. G., Hasekamp, O. P., Reuter, M., Schneising-Weigel, O., Product Quality Assessment Report, Copernicus Climate Change Service (C3S) project on satellite-derived Essential Climate Variable (ECV) Greenhouse Gases (CO_2 and CH_4) data products (project C3S_312a_Lot6), Version 1.1, 20-October-2017, pp. 103, 2017.

PQAR GHG, 2018: Buchwitz, M., Aben, I., Anand, J., Armante, R., Boesch, H., Crevoisier, C., Detmers, R. G., Hasekamp, O. P., Reuter, M., Schneising-Weigel, O., Product Quality Assessment Report, Copernicus Climate Change Service (C3S) project on satellite-derived Essential Climate Variable (ECV) Greenhouse Gases (CO_2 and CH_4) data products (project C3S_312a_Lot6), Version 2.0, 16-October-2018, pp. 99, 2018.

PQAR GHG, 2020: Buchwitz, M., Aben, I., Anand, J., Armante, R., Boesch, H., Crevoisier, C., Detmers, R. G., Hasekamp, O. P., Reuter, M., Schneising-Weigel, O., Product Quality Assessment Report (PQAR) – Main document for Greenhouse Gas (GHG: CO_2 & CH_4) data set CDR 4 (2003-2019), Copernicus Climate Change Service (C3S) project C3S_312b_Lot2), Version 4.0, 17-Sept-2020, pp.

104, link: https://www.iup.uni-bremen.de/carbon_ghg/docs/C3S/CDR4_2003-2019/C3S_D312b_Lot2.2.3.2-v2.0_PQAR-GHG_MAIN_v4.0.pdf, 2020.

Raoult et al., 2017: Raoult, B., C. Bergeron, A. López Alós, J-N. Thépaut, D. Dee, Climate service develops user-friendly data store. ECMWF Newsletter No. 151, 22-27. Available at https://www.ecmwf.int/sites/default/files/elibrary/2017/17181-newsletter-no-151-spring-2017.pdf, 2017.

Rayner and O'Brien, 2001: Rayner, P. J., and O'Brien, D.M.: The utility of remotely sensed CO_2 concentration data in surface inversions, Geophys. Res. Lett., 28, 175-178, 2001.

Reuter et al., 2010: Reuter, M., Buchwitz, M., Schneising, O., Heymann, J., Bovensmann, H., and Burrows, J. P., A method for improved SCIAMACHY CO_2 retrieval in the presence of optically thin clouds, Atmos. Meas. Tech., 3, 209-232, 2010.

Reuter et al. 2011: Reuter, M., Bovensmann, H., Buchwitz, M., Burrows, J. P., Connor, B. J., Deutscher, N. M., Griffith, D.W. T., Heymann, J., Keppel-Aleks, G., Messerschmidt, J., and et al.: Retrieval of atmospheric CO_2 with enhanced accuracy and precision from SCIAMACHY: Validation with FTS measurements and comparison with model results., Journal of Geophysical Research, 116, doi:10.1029/2010JD015047, URL http://dx.doi.org/10.1029/2010JD015047, 2011.

Reuter et al., 2013: Reuter, M. H. Bösch, H. Bovensmann, A. Bril, M. Buchwitz, A. Butz, J. P. Burrows, C. W. O'Dell, S. Guerlet, O. Hasekamp, J. Heymann, N. Kikuchi, S. Oshchepkov, R. Parker, S. Pfeifer, O. Schneising, T. Yokota, and Y. Yoshida, A joint effort to deliver satellite retrieved atmospheric CO_2 concentrations for surface flux inversions: The ensemble median algorithm EMMA, Atmos. Chem. Phys., 13, 1771-1780, 2013.

Reuter et al., 2014a: Reuter, M., M. Buchwitz, A. Hilboll, A. Richter, O. Schneising, M. Hilker, J. Heymann, H. Bovensmann and J. P. Burrows, Decreasing emissions of NOx relative to CO_2 in East Asia inferred from satellite observations, Nature Geoscience, 28 Sept. 2014, doi:10.1038/ngeo2257, pp.4, 2014.

Reuter et al., 2014b: Reuter, M., M. Buchwitz, M. Hilker, J. Heymann, O. Schneising, D. Pillai, H. Bovensmann, J. P. Burrows, H. Bösch, R. Parker, A. Butz, O. Hasekamp, C. W. O'Dell, Y. Yoshida, C. Gerbig, T. Nehrkorn, N. M. Deutscher, T. Warneke, J. Notholt, F. Hase, R. Kivi, R. Sussmann, T. Machida, H. Matsueda, and Y. Sawa, Satellite-inferred European carbon sink larger than expected, Atmos. Chem. Phys., 14, 13739-13753, doi:10.5194/acp-14-13739-2014, 2014.

Reuter et al., 2016: Reuter, M.; Buchwitz, M.; Aben, I.; Boesch, H.; Butz, A.; Detmers, R.G.; Hasekamp, O.P.; Heymann, J.; Parker, R.; Schneising, O.; Somkuti, P., ESA Greenhouse Gases Climate Change Initiative (GHG_cci): Merged SCIAMACHY and GOSAT Level 3 gridded atmospheric column-average carbon dioxide (XCO_2) product in Obs4MIPs format. Centre for Environmental Data Analysis, 10 October 2016, doi:10.5285/3FAE8371-0CBB-4B21-9EA6-7A1FC293C4A2, pp. 11, 2016.

Reuter et al., 2017a: Reuter, M., M. Buchwitz, M. Hilker, J. Heymann, H. Bovensmann, J. Burrows, S. Houweling, Y. Liu, R. Nassar, F. Chevallier, P. Ciais, J. Marshall, and M. Reichstein, 2016: How much CO2 is taken up by the European terrestrial biosphere ?, Bull. Amer. Meteor. Soc. (BAMS), doi:10.1175/BAMS-D-15-00310.1, 24 April 2017, 665-671, 2017.

Reuter et al., 2017b: Reuter, M., M. Buchwitz, O. Schneising, S. Noel, H. Bovensmann, J. P. Burrows, A Fast Atmospheric Trace Gas Retrieval for Hyperspectral Instruments Approximating Multiple

Scattering - Part 2: Application to XCO_2 Retrievals from OCO-2, Remote Sens., 9, 1102, doi:10.3390/rs9111102, 2017.

Reuter et al., 2020: Reuter, M., Buchwitz, M., Schneising, O., Noel, S., Bovensmann, H., Burrows, J. P., Boesch, H., Di Noia, A., Anand, J., Parker, R. J., Somkuti, P., Wu, L., Hasekamp, O. P., Aben, I., Kuze, A., Suto, H., Shiomi, K., Yoshida, Y., Morino, I., Crisp, D., O'Dell, C. W., Notholt, J., Petri, C., Warneke, T., Velazco, V. A., Deutscher, N. M., Griffith, D. W. T., Kivi, R., Pollard, D. F., Hase, F., Sussmann, R., Te, Y. V., Strong, K., Roche, S., Sha, M. K., De Maziere, M., Feist, D. G., Iraci, L. T., Roehl, C. M., Retscher, C., and Schepers, D.: Ensemble-based satellite-derived carbon dioxide and methane column-averaged dry-air mole fraction data sets (2003-2018) for carbon and climate applications, Atmos. Meas. Tech., 13, 789-819, https://doi.org/10.5194/amt-13-789-2020, 2020.

Rodgers, 2000: Rodgers C. D.: Inverse Methods for Atmospheric Sounding: Theory and Practice, World Scientific Publishing, 2000.

Ross et al., 2013: Ross, A. N., Wooster, M. J., Boesch, H., Parker, R., First satellite measurements of carbon dioxide and methane emission ratios in wildfire plumes, Geophys. Res. Lett., 40, 1-5, doi:10.1002/grl.50733, 2013.

Schaefer et al., 2016: Schaefer, H., Mikaloff Fletcher, S. E., Veidt, C., Lassey, K. R., Brailsford, G. W., Bromley, T. M., Dlugokencky, E. J., Michel, S. E., Miller, J. B., Levin, I., Lowe, D. C., Martin, R. J., Vaughn, B. H., and White, J. W. C.: A 21st-century shift from fossil-fuel to biogenic methane emissions indicated by $^{13}CH_4$, Science, Vol. 352, Issue 6281, pp. 80-84, doi 10.1126/science.aad2705, 2016.

Schepers et al., 2012: Schepers, D., Guerlet, S., Butz, A., Landgraf, J., Frankenberg, C., Hasekamp, O., Blavier, J.-F., Deutscher, N. M., Griffith, D. W. T., Hase, F., Kyro, E., Morino, I., Sherlock, V., Sussmann, R., Aben, I. (2012), Methane retrievals from Greenhouse Gases Observing Satellite (GOSAT) shortwave infrared measurements: Performance comparison of proxy and physics retrieval algorithms, J. Geophys. Res., 117, D10307, doi:10.1029/2012JD017549, 2012.

Schneising et al., 2011: Schneising, O., Buchwitz, M., Reuter, M., et al., Long-term analysis of carbon dioxide and methane column-averaged mole fractions retrieved from SCIAMACHY, *Atmos. Chem. Phys*., 11, 2881-2892, 2011.

Schneising et al., 2014a: Schneising, O., Reuter, M., Buchwitz, M., Heymann, J., Bovensmann, H., and Burrows, J. P., Terrestrial carbon sink observed from space: variation of growth rates and seasonal cycle amplitudes in response to interannual surface temperature variability, Atmos. Chem. Phys., 14, 133-141, 2014.

Schneising et al., 2014b: Schneising, O., Burrows, J. P., Dickerson, R. R., Buchwitz, M., Reuter, M., Bovensmann, H., Remote sensing of fugitive methane emissions from oil and gas production in North American tight geologic formations, Earth's Future, 2, DOI: 10.1002/2014EF000265, pp. 11, 2014.

Schneising et al., 2019: Schneising, O., Buchwitz, M., Reuter, M., Bovensmann, H., Burrows, J. P., Borsdorff, T., Deutscher, N. M., Feist, D. G., Griffith, D. W. T., Hase, F., Hermans, C., Iraci, L. T., Kivi, R., Landgraf, J., Morino, I., Notholt, J., Petri, C., Pollard, D. F., Roche, S., Shiomi, K., Strong, K., Sussmann, R., Velazco, V. A., Warneke, T., and Wunch, D.: A scientific algorithm to simultaneously retrieve carbon monoxide and methane from TROPOMI onboard Sentinel-5 Precursor, Atmos.

Meas. Tech., 12, 6771-6802, https://doi.org/10.5194/amt-12-6771-2019, https://doi.org/10.5194/amt-12-6771-2019, 2019.

Schneising et al., 2020: Schneising, O., Buchwitz, M., Reuter, M., Vanselow, S., Bovensmann, H., and Burrows, J. P.: Remote sensing of methane leakage from natural gas and petroleum systems revisited, Atmos. Chem. Phys., 20, 9169-9182, https://doi.org/10.5194/acp-20-9169-2020, 2020.

Shindell et al., 2013: Shindell, D. T., Pechony, O., Voulgarakis, A., et al. (2013), Interactive ozone and methane chemistry in GISS-E2 historical and future climate simulations, Atmos. Chem. Phys., 13, 2653–2689, doi:10.5194/acp-13-2653-2013, 2013.

Scholze et al., 2017: Scholze, M., M. Buchwitz, W. Dorigo, L. Guanter, S. Quegan, Reviews and syntheses: Systematic Earth observations for use in terrestrial carbon cycle data assimilation systems, Biogeosciences, 14, 3401-3429, 2017.

Taylor et al., 2020: Taylor, T. E., et al.: OCO-3 early mission operations and initial (vEarly) XCO_2 and SIF retrievals, Remote Sensing of Environment, Volume 251, 112032, ISSN 0034-4257, pp. 27, https://doi.org/10.1016/j.rse.2020.112032 (https://www.sciencedirect.com/science/article/pii/S0034425720304028), 2020.

TRD GHG, 2017: Buchwitz, M., Aben, I., Anand, J., Armante, R., Boesch, H., Crevoisier, C., Detmers, R. G., Hasekamp, O. P., Reuter, M., Schneising-Weigel, O., Target Requirement 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_312a_Lot6), Version 1.3, 20-October-2017, pp. 53, 2017.

Turner et al., 2015: Turner, A. J., D. J. Jacob, K. J. Wecht, J. D. Maasakkers, S. C. Biraud, H. Boesch, K. W. Bowman, N. M. Deutscher, M. K. Dubey, D. W. T. Griffith, F. Hase, A. Kuze, J. Notholt, H. Ohyama, R. Parker, V. H. Payne, R. Sussmann, V. A. Velazco, T. Warneke, P. O. Wennberg, and D. Wunch, Estimating global and North American methane emissions with high spatial resolution using GOSAT satellite data, Atmos. Chem. Phys., 15, 7049-7069, doi:10.5194/acp-15-7049-2015, 2015.

Turner et al., 2016: Turner, A. J., D. J. Jacob, J. Benmergui, S. C. Wofsy, J. D. Maasakkers, A. Butz, O. Hasekamp, and S. C. Biraud, A large increase in U.S. methane emissions over the past decade inferred from satellite data and surface observations, Geophys. Res. Lett., 43, 2218–2224, doi:10.1002/2016GL067987, 2016.

Veefkind et al. 2012: Veefkind, J. P., Aben, I., McMullan, K., Förster, H., De Vries, J., Otter, G., Claas, J., Eskes, H. J., De Haan, J. F., Kleipool, Q., Van Weele, M., Hasekamp, O., Hoogeveen, R., Landgraf, J., Snel, R., Tol, P.,Ingmann, P., Voors, R., Kruizinga, B., Vink, R., Visser, H., and Levelt, P. F.: TROPOMI on the ESA Sentinel-5 Precursor: A GMES mission for global observations of the atmospheric composition for climate, air quality and ozone layer applications. Rem. Sens. Environment, 120:70–83, 2012.

Velazco et al. 2011: Velazco, V. A., Buchwitz, M., Bovensmann, H., Reuter, M., Schneising, O., Heymann, J., Krings, T., Gerilowski, K., and Burrows, J. P.: Towards space based verification of CO2 emissions from strong localized sources: fossil fuel power plant emissions as seen by a CarbonSat constellation, Atmos. Meas. Tech., 4, 2809-2822, 2011.

Wofsy et al. 2012: Wofsy, S. C., Daube, B. C., Jimenez, R., et al.: HIPPO Merged 10-second Meteorology, Atmospheric Chemistry, Aerosol Data (R 20121129), Carbon Dioxide Information

Analysis Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA, release 29 November 2012, 2012.

Wunch et al. 2010: Wunch, D., Toon, G. C., Wennberg, P. O., Wofsy, S. C., Stephens, B. B., Fischer, M. L., Uchino, O., Abshire, J. B., Bernath, P., Biraud, S. C., Blavier, J.-F. L., Boone, C., Bowman, K. P., Browell, E. V., Campos, T., Connor, B. J., Daube, B. C., Deutscher, N. M., Diao, M., Elkins, J. W., Gerbig, C., Gottlieb, E., Griffith, D. W. T., Hurst, D. F., Jiménez, R., Keppel-Aleks, G., Kort, E. A., Macatangay, R., Machida, T., Matsueda, H., Moore, F., Morino, I., Park, S., Robinson, J., Roehl, C. M., Sawa, Y., Sherlock, V., Sweeney, C., Tanaka, T., and Zondlo, M. A.: Calibration of the Total Carbon Column Observing Network using aircraft profile data, Atmospheric Measurement Techniques, 3, 1351–1362, doi:10.5194/amt-3-1351-2010, URL http://www.atmos-meas-tech.net/3/1351/2010/, 2010.

Wunch et al. 2011: Wunch, D., Toon, G. C., Blavier, J.-F. L., Washenfelder, R. A., Notholt, J., Connor, B. J., Griffith, D. W. T., Sherlock, V., and Wennberg, P. O.: The Total Carbon Column Observing Network (TCCON), Philosophical Transactions of the Royal Society of London, Series A: Mathematical, Physical and Engineering Sciences, 369, 2087–2112, doi:10.1098/rsta.2010.0240, 2011.

Yang et al. 2020: Yang, D., H. Boesch, Y. Liu, P. Somkuti, Z. Cai, X. Chen, A. Di Noia, C. Lin, N. Lu, D. Lyu, R. J. Parker, L. Tian, M. Wang, A. Webb, L. Yao, Z. Yin, Y. Zheng, N. M. Deutscher, D. W. T. Griffith, F. Hase, R. Kivi, I. Morino, J. Notholt, H. Ohyama, D. F. Pollard, K. Shiomi, R. Sussmann, Y. Te, V. A. Velazco, T. Warneke, D. Wunch: Toward high precision XCO_2 retrievals from TanSat observations: Retrieval improvement and validation against TCCON measurements, Journal of Geophysical Research: Atmospheres, 125, e2020JD032794, https://doi.org/10.1029/2020JD032794, 2020.

Yoshida et al. 2013: Yoshida, Y., Kikuchi, N., Morino, I., Uchino, O., Oshchepkov, S., Bril, A., Saeki, T., Schutgens, N., Toon, G. C., Wunch, D., Roehl, C. M., Wennberg, P. O., Griffith, D. W. T, Deutscher, N. M., Warneke, T., Notholt, J., Robinson, J., Sherlock, V., Connor, B., Rettinger, M., Sussmann, R., Ahonen, P., Heikkinen, P., Kyrö, E., Mendonca, J., Strong, K., Hase, F., Dohe, S., and Yokota, T.: Improvement of the retrieval algorithm for GOSAT SWIR XCO_2 and XCH_4 and their validation using TCCON data, Atmos. Meas. Tech., 6, 1533–1547, doi:10.5194/amt-6-1533-2013, 2013.

Copernicus Climate Change Service

ECMWF - Shinfield Park, Reading RG2 9AX, UK

Contact: info@copernicus-climate.eu