ESA Climate Change Initiative (CCI)

User Requirements Document (URD)

for the Essential Climate Variable (ECV)

Greenhouse Gases (GHG)

Written by:

GHG-CCI project team

Lead author for Version 1: M. Buchwitz, IUP, Univ. Bremen, Germany

Lead author for Version 2: F. Chevallier, LSCE, France

Lead author for Version 3: J. Marshall, MPI-BGC, Germany

Other contributors:

- P. Bergamaschi, EC-JRC-IES, Italy
- S. Houweling and T. van Leeuwen, SRON, the Netherlands
- P. I. Palmer, Univ. Edinburgh

To be cited as:

GHG-CCI: User Requirements Document for the GHG-CCI+ project of ESA's Climate Change Initiative, pp. 42, version 3.0, 17 February, 2020.

Available from: http://cci.esa.int/ghg/

Change log:

Version Nr.	Date	Status	Reason for change
Version 1 – Final	3 Feb. 2011	Final version Author: M. Buchwitz; Major contributions: F. Chevallier, P. Bergamaschi, I. Aben	New document
Version 2 – Final	28 July 2014	Final version Author: F. Chevallier; Contributions: M. Buchwitz	Full revision for Phase 2 of GHG-CCI. All sections touched.
Version 2.1 – Final	19 Oct. 2016	Final version Contributions: P. Bergamaschi, F. Chevallier, P. Palmer;	- Update of the stability requirement for CH_4, - Clarification in the definition of stability (to cover inter-annual error changes)
Version 3.0 — Final	17 Feb. 2020	Final version Author: J Marshall; Contributions: F. Chevallier	Full revision for GHG-CCI+. All sections changed to reflect current state of both project and available satellites.

Table of Contents

1 Summary

This document states users' requirements for the products of ESA's GHG-CCI project **/Buchwitz et al., 2013/**. The original version of the report was a deliverable of the GHG-CCI project, and is itself a deliverable of this project.

The GHG-CCI project (http://cci.esa.int/ghg/) is one of several projects of ESA's Climate Change Initiative (CCI) **/Hollmann et al., 2013/**. It is led by the Institute of Environmental Physics (IUP), University of Bremen, Germany, (Science Leader: M. Buchwitz) supported by Project Manager M..Reuter and Deputy Project Manager O. Schneising. Following the initial Phase from 2010 to 2013 and the follow-on Phase 2 (2015-2018), the project now continues as GHG-CCI+, from 2019 to 2021. For the sake of simplicity, GHG-CCI is used to describe the project as a whole, and GHG-CCI+ is only used when describing elements specific to the current phase.

The GHG-CCI project aims at delivering the Essential Climate Variable (ECV) for Greenhouse Gases (GHG) from satellite measurements in line with the "Systematic observation requirements for satellite-based products for climate" as defined by GCOS (Global Climate Observing System, **/GCOS-154/**): "Product A.8.1. Retrievals of CO_2 and CH_4 of sufficient quality to estimate regional sources and sinks". The present user requirements exclusively address this application and may not apply to other applications or finer spatial scales.

Ideally, this objective requires satellite observations which are sensitive to near-surface concentration variations of CO_2 and CH_4. Sensitivity close to the surface is critical for accurate surface flux estimation. Currently six satellite instruments have (or have had) this asset:

- SCIAMACHY on ENVISAT (operational from March 2002 to April 2012, measuring XCH_4 and XCO_2)
- TANSO-FTS on board GOSAT (which has been operational since early 2009, observing XCH_4 and XCO_2)
- its follow-on mission GOSAT-2 with instrument TANSO-FTS-2 (launched in October 2018, observing XCH_4 and XCO_2)
- OCO-2 (which was launched in July 2014, observing XCO_2),
- TanSat (launched in December 2016, observing XCO_2),
- TROPOMI on Sentinel-5 Precursor (launched in 2017, observing XCH_4),
- OCO-3 (launched in May 2019, observing XCO_2).

The following five data products can be retrieved from these instruments, which are relevant for GHG-CCI:

- Column-averaged dry air mole fractions of CO_2, i.e., XCO_2 (in ppm), from SCIAMACHY (nadir mode), TANSO-FTS, TANSO-FTS-2, OCO-2, OCO-3, and TanSat.
- Column-averaged dry air mole fractions of CH_4, i.e., XCH_4 (in ppb), from SCIAMACHY (nadir mode), TANSO-FTS, TANSO-FTS-2, and TROPOMI.

While the previous phases of this project focussed primarily on products from SCIAMACHY and GOSAT, the GHG-CCI+ phase is focussed on new and emerging products, namely those from OCO-2, TANSO-FTS-2, TanSat, and TROPOMI. (OCO-3 data are not included, but also constitute a fundamentally different product lacking global coverage due to its orbit – on the International Space Station, ISS – and targeted observation strategy).

The present user requirements are based on peer-reviewed publications, other documents where user requirements have been formulated, and user consultation including users who are (also) involved in the Copernicus Atmosphere Monitoring Service (CAMS, http://www.copernicus-atmosphere.eu/). A close cooperation between GHG-CCI and CAMS has been established and maintained for this purpose.

Previous phases of GHG-CCI also developed algorithms and corresponding data products to obtain information on CO_2 and CH_4 in upper atmospheric layers, including mid/upper tropospheric CO_2 and/or CH_4 from AIRS and IASI, and upper tropospheric and stratospheric CO_2 profiles from ACE-FTS and CH_4 profiles from MIPAS and SCIAMACHY solar occultation. These products are not being considered in GHG-CCI+ and are not included in this URD.

2 ECV Greenhouse Gases (GHG)

What is the ECV GHG? The ECV GHG follows the definition of **/GCOS-154/** (see **Annex A**). The ECV GHG is a publicly-available database and corresponding documentation on satellite-retrieved GHG information for improved quantification of regional surface sources and sinks. This is currently only possible for the two most important anthropogenically-influenced GHGs, carbon dioxide (CO_2) and methane (CH_4). At present other anthropogenically-influenced GHGs are not well monitored from space.

Seven satellite instruments are sensitive to near-surface concentration changes of CO_2 and CH_4 and therefore can best deliver information on regional CO_2 and CH_4 surface fluxes: SCIAMACHY **/Burrows et al., 1995/** /**Bovensmann et al., 1999/** on board ENVISAT, TANSO-FTS on board GOSAT **/Kuze et al., 2010/ /Yokota et al., 2004/**, TANSO-FTS-2 on board GOSAT-2 /**Yoshida et al., 2019**/, OCO-2 **/Boesch et al., 2011/** /**Crisp et al., 2004**/, OCO-3 on the ISS /**Eldering et al., 2018**/, TROPOMI on board S5P /**Hu et al., 2018**/, and TanSat /**Yang et al., 2018**/.

Key input data for (inverse) modelling activities to obtain information on CO_2 and CH_4 regional surface fluxes are column-averaged dry air mole fractions of CO_2 and CH_4, i.e., XCO_2 (in ppm) **/A-Scope, 2008/ /Baker et al., 2010/ /Barkley et al., 2006/ /Boesch et al., 2011/ /Bösch et al., 2006/ /Bréon et al., 2010/ /Bril et al., 2007a, 2007b, 2008, 2009/ /Buchwitz et al., 2000, 2005, 2013/ /Butz et al., 2009/ /Chevallier et al., 2005, 2007, 2009, 2010, 2014/ /Connor et al., 2008/ /Crisp et al., 2004/ /Eldering et al., 2017/ /Feng et al., 2009, 2016/ /Heymann et al., 2012a, 2012b/ /Houweling et al., 2004, 2005/ /Hungershoefer et al., 2010/ /Kaminski et al., 2010/ Miller et al., 2007/ /Nakajima et al., 2010/ /Oshchepkov et al., 2008, 2009/ /O'Dell et al., 2018/ /Rayner and O'Brien, 2001/ /Reuter et al., 2010, 2011, 2013/ /Schneising et al., 2008, 2010, 2011, 2012, 2013, 2014/ /Yokota et al., 2004/ /Yoshida et al., 2010, 2019/** and XCH_4 (in ppb) **/Bergamaschi et al., 2007, 2009/ /Bloom et al., 2010/ /Bousquet et al., 2010/ /Bréon et al., 2010/ /Buchwitz et al., 2000, 2005, 2013/ /Cressot et al., 2014/ /Frankenberg et al., 2005a, 2005b, 2006, 2008, 2011/ /Fraser et al, 2013, 2014/ /Hu et al., 2016, 2018/ /Meirink et al., 2006/ /Nakajima et al., 2010/ /Schneising et al., 2009, 2010, 2011, 2012, 2019/ /Yoshida et al., 2010, 2019/.**

The four data products XCO_2 and XCH_4 from SCIAMACHY and TANSO are the four core products that were generated in the previous phases of this project (using the "ECV Core Algorithms" (ECAs)) and compared with corresponding products generated elsewhere (e.g., at NIES in Japan and NASA/JPL in the US). This phase of the project will focus on XCO_2 from OCO-2, GOSAT-2 and TanSat, and XCH_4 from GOSAT-2 and S5P. Within this document, user requirements for these data products are formulated.

This phase of the project as well as the requirements in this URD are restricted to these core GHG-CCI ECV data products. Other satellite products reporting GHGs exclusively in the upper troposphere/lower stratosphere are not further discussed here

3 URD approach

This document has been written by the GHG-CCI project team, based on inputs from key users who are part of the GHG-CCI Climate User Group (CRG) and other inputs, most notably peer-reviewed publications (e.g., **/Rayner and O'Brien, 2001/ /Bergamaschi et al., 2007/ /Bergamaschi et al., 2009/ /Bloom et al., 2010/ /Bousquet et al., 2010/ /Chevallier et al., 2007/ /Chevallier et al., 2009**/ **/Houweling et al., 2004/ /Hungershoefer et al., 2010/ /Meirink et al., 2006/ /Miller et al., 2007/**) and other publications such as the GCOS requirements /**GCOS-200**/ **/GCOS-107/ /GCOS-154/** and the requirements formulated by the CCI Climate Modelling User Group (CMUG) **/CMUG-RBD, 2015/**.

This document refers to XCO_2 and XCH_4 as retrieved from the TANSO-FTS-2, and the TROPOMI instruments. For the earlier instruments SCIAMACHY and TANSO-FTS, it has already been shown that the XCH_4 retrievals provide strong constraints on regional surface fluxes of CH_4 (e.g., **/Bergamaschi et al., 2009/ /Alexe et al., 2015/ /Turner et al., 2016/**). It has also been shown that these same instruments can deliver important information on CO_2 (e.g., **/Basu et al., 2013/ /Reuter et al., 2014/** /**Reuter et al., 2017**/), although there has been some difficulty in reconciling these flux estimates with those from CO_2 flux estimates based on surface measurements (/**Houweling et al., 2015/ /Chevallier et al., 2014**/). Inverse modelling studies have been performed based on OCO-2 retrievals (e.g. /**Crowell et al., 2019**/ /**Liu et al., 2017**/ /**Patra et al., 2017**/), but the discrepancy with inversions using surface measurements is not fully resolved. This is a topic of active research, in particular within GHG-CCI. One of the reasons is that the requirement on systematic errors, as stated in this URD, is not satisfied with the current generation of products **/Chevallier, 2018**/. This could be seen in the convergence between surface-based and satellite-based CO_2 inversions in the successive Climate Assessment Reports during Phase 2 of GHG-CCI, as the retrieval algorithms improved (http://cci.esa.int/ghg/). However, other issues like transport model systematic errors and flawed statistical models play a role as well.

CCI CMUG compiled a requirements document relevant for this URD **/CMUG-RBD, 2015/** derived from GCOS requirements **/GCOS-107/** and other sources. This URD has been written to be as consistent as possible (mostly identical) with the definitions and requirements formulated in **/CMUG-RBD, 2015/**. This also refers to which requirements are covered. If possible, requirements as formulated in **/CMUG-RBD, 2015/** are directly included in this URD. However, for certain requirements this was not possible as even the CMUG/GCOS threshold (i.e., minimum) requirements are too demanding for the currently available generation of instruments.

4 Definitions

In this section key definitions are given. They are identical to the definitions given in **/CMUG-RBD, 2015/** to ensure consistency with the other CCI projects. However, for the sake of clarity within and outside CCI, we avoid the use of the word "accuracy" in the following (except in verbatim quotations) because **/CMUG-RBD, 2015/** (after **/GCOS-107/,** but contradicted later by **/GCOS-154/** that acknowledges the international norm) defines it inconsistently with the international standard for metrology (i.e. ISO 5725). We replace CMUG's "accuracy" with the expression "Systematic error", following the international norm.

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

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

For GHG-CCI especially the "Relative systematic error" is important. The definition for GHG-CCI is as follows:

Relative systematic error: identical to "Systematic error" but after bias correction.

Bias: estimate of a systematic measurement error ***/JCGM, 2008/***.

Precision is the measure of reproducibility or repeatability of the measurement without reference to an international standard so that precision is a measure of the random and not the systematic error. Suitable averaging of the random error can improve the precision of the measurement but does not establish the systematic error of the observation. **/CMUG-RBD, 2015/**

Note: We quantify precision here as the standard deviation of the error distribution.

Stability is a term often invoked with respect to long-term records when no absolute standard is available to quantitatively establish the systematic error - the bias defining the time-dependent (or instrument-dependent) difference between the observed quantity and the true value. **/CMUG-RBD, 2015/**

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

Representativity is important when comparing with or assimilating in models. Measurements are typically averaged over different horizontal and vertical scales compared to model fields. If the measurements are smaller in scale than the model, the representativity of the measurement can be important. The sampling strategy can also affect this term. **/CMUG-RBD, 2015/**

Threshold requirement: The **threshold** is the limit beyond which the observation is no longer of use for the climate-related application. **/CMUG-RBD, 2015/**

Note 1: 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 while others are not.

Note 2: 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.

Note: This requirement is relative to a given state of the art for the target application. Indeed, the more accurate and precise the satellite XCO_2 and XCH_4 data products are, the larger their information content is. However other errors such as model transport errors do not allow exploitation of the additional information content if they are more accurate than the specified goal requirement.

Breakthrough requirement: The **breakthrough** is an intermediate level between “threshold” and “goal“, 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.

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

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

Observing Cycle is the temporal frequency at which the measurements are obtained. **/CMUG-RBD, 2010/**

*Note: 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.*

5 GHG ECV specific requirements

In this section GHG ECV specific requirements are formulated for the XCO_2 and XCH_4 data products to be retrieved from TANSO-FTS-2, TROPOMI, TanSat, and OCO-2.

5.1 General

The purpose of this URD is to formulate requirements for GHG data products to be generated within the GHG-CCI+ project for regional CO_2 and CH_4 surface flux inverse modelling. There are however also other potentially important applications, e.g., use of the data to improve our understanding of atmospheric transport and mixing or city-scale emission estimation, for which the requirements will most likely be different.

In the following, detailed requirements are given typically by specifying numerical thresholds. Specifying single numbers is difficult and not unproblematic because of the complexity of the process needed to relate satellite observations to surface fluxes. Requirements may depend on time and location (and on each other) and this is likely also true for the quality of the satellite retrievals. It is therefore important not to over-interpret the numerical values given in the requirements. To keep this in mind, a very general "overarching" requirement has been formulated. This overarching general requirement is:

REQ-GHGCCI-GEN-1	The purpose of the GHG-CCI CO_2 and CH_4 ECV data products is to enhance our knowledge about the distribution of atmospheric CO_2 and CH_4, their sources and sinks, and underlying processes. Contributions to such new knowledge obtained from the satellite data products shall be identified and listed. The list shall be made available to the users.

5.2 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 boxes in these studies span a few degrees in latitude and longitude, while the soundings that are being used have a footprint of 10 km or less. Existing studies report a modest impact stemming from this inconsistency (e.g., /**Corbin et al. 2008**/). Therefore no requirements are formulated here.

*Note: Here the requirement might change if a different scale is targeted. As an example, in the development of a mission targeting the quantification of anthropogenic CO_2 emissions from point sources, /**Pinty et al., 2017**/ proposes a spatial resolution of 2x2 km^2 as a minimum requirement. The requirements described in this report are rather in the context of regional scales using global models.*

5.3 Vertical resolution

While vertical resolution would surely provide useful additional information, the utility of column-average retrievals without any vertical resolution has been clearly demonstrated. Therefore no requirements are given here.

5.4 Observing cycle

Based on evidence up to this point, the observing cycle does not seem to be a critical parameter for regional flux inversion, as long as retrievals are assimilated at the time they are made, and not first aggregated into temporal averages. Therefore no requirements are given here.

5.5 Random and systematic errors

In this section requirements for random errors ("precision") and systematic errors for XCO_2 and XCH_4 are given (see Table 1) in the context of regional flux inversion.

Precision requirements are given for single retrievals but also for spatio-temporal averages (1000×1000 km^2, monthly). Requirements for spatio-temporal averages have been formulated to ensure that a significant number of retrievals per month and region are available, at least on average. Alternatively one could formulate a requirement for the number of retrievals 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., it refers to equally sized areas on the Earth's surface.

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

*Note: If the noise is truly random, an instrument with low single retrieval 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 retrieval precision. A stand-alone and instrument-independent single retrieval precision requirement is therefore not very meaningful in and of itself but needs to be combined with (estimates of) the number of (useful) data in a given spatio-temporal interval. However, this URD gives single retrieval precision requirements because they offer the potential advantage of a straight-forward verification based on radiative transfer modelling for single observations and simulated retrievals. Furthermore, poor precision is usually accompanied with state-dependent systematic errors that cannot be damped by averaging over many retrievals. An exception to this might be presented by future active remote sensing missions, such as the planned methane-monitoring MERLIN Mission /**Ehret et al., 2017**/. Integrated-Path Lidar Absorption (IPLA) measurements are characterized by comparatively poor single-shot retrieval precision, but promise significantly lower systematic errors, which are of benefit for inverse modelling /**Bousquet et al., 2018**/.*

Random error (precision) requirements for XCO_2*:*

In **/Rayner and O'Brien, 2001/** it was shown that satellite retrievals of XCO_2 can provide additional information on CO_2 surface fluxes if a precision of 2.5 ppm can be achieved for monthly averages over 8º × 10º large regions. This requirement has been 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 retrieval 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 retrievals 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 retrieval precisions depend on the 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 retrieval precision for TANSO-FTS 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 URD, single retrieval precisions and precisions for spatio-temporal averages (1000×1000 km^2, monthly) have been formulated. The precisions for spatio-temporal averages are (mostly) a factor of 3 better compared to the single retrieval precisions. If the achieved single retrieval precision is identical to the required single retrieval precision and if one assumes that the precision improves with the square root of the number of retrievals added, this implies that at least 10 (uncorrelated) observations are available per month and per 1000×1000 km^2 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 retrieval precision is approximately a factor of 6 relaxed, i.e., 8 ppm (this implies that approx. 36 uncorrelated retrievals per month and region have to be averaged to achieve the 1.3 ppm requirement if the single retrieval precision is (only) 8 ppm). Note that the variability of XCO_2 at the global scale and over 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.

These more demanding goals are pushing the direction of new mission design. **/Pinty et al., 2017**/, when describing the requirements for the planned CO2M mission, refer to a single sounding precision of 1 ppm for a footprint of 1 km^2. GOSAT, launched in 2009, can detect strong sources with a precision of about 2 ppm, while GOSAT-2 aims for a precision of 0.5 ppm. The mission requirements document for CO2M **/Meijer et al., 2019/** specifies a single retrieval precision of 0.7 ppm for a reference scenario with a retrieval footprint not exceeding 2 × 2 km^2, which is considerably stricter than that of current missions.

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.) and in tropical regions with persistent clouds. 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 retrieval precision of 1.5-2% (approx. 25-34 ppb). For the single retrieval 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 of 3 improvement compared to the single retrieval precisions.

The planned CO2M has considerably tighter requirements in its mission requirement document: a single retrieval precision for XCH_4 of 10 ppb for a footprint of 4 km^2 **/Meijer et al., 2019/**. The planned lidar mission MERLIN specifies a retrieval precision (random error) of better than 27 ppb when averaging lidar footprints along a 50-km path **/Ehret et al., 2017/**, but this is balanced by more stringent systematic error requirements.

Systematic error requirements:

The requirements for systematic errors are based on studies using synthetic data (e.g., **/Chevallier et al., 2005a/ /Chevallier et al., 2007/ /Chevallier et al., 2009/ /Meirink et al., 2006/ /Miller et al., 2007/**) and analysis of real data (e.g., **/Bergamaschi et al., 2009/ /Bergamaschi et al., 2007/).**

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 as 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". This is because gradients on this scale are precisely the information content used to deduce fluxes. The GHG-CCI CO_2 threshold requirement for systematic errors is based on an extension of **/Chevallier et al., 2005a/** to TANSO-FTS (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-FTS 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/**, **/Chevallier et al., 2010/** and **/Feng et al., 2016/.**

For XCH_4 the requirements are similar but somewhat more relaxed (as is also the case for TANSO-FTS requirements **/Nakajima et al., 2010/**), because XCH_4 is more variable compared to XCO_2 (in terms of percentage variations compared to its background, 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%" 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., 2009/ /Bergamaschi et al., 2007/**). As a consequence, also the CH_4 bias threshold requirement is challenging.
For systematic errors, missions in the planning phase have even more ambitious requirements, with 5 ppb for CO2M **/Meijer et al., 2019/** and less than 3.7 ppb for MERLIN **/Ehret et al., 2017/**.

The requirements are valid for observations over land, due to two main reasons:

(i) The main application of the GHG-CCI 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.

(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-GHGCCI-ERR-1	The XCO_2 and XCH_4 ECV data products over land shall meet the random error (precision) requirements given in Table 1. *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-GHGCCI-ERR-2	The XCO_2 and XCH_4 ECV data products over land shall meet the systematic error requirements given in Table 1. *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 will improve 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-GHGCCI-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 retrieval 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 is done in e.g. ***/Sheng et al., 2018/****. 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.*

Requirements for regional CO_2 and CH_4 source/sink determination					
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 #)

Table 1: GHG-CCI XCO_2 and XCH_4 random ("precision") and systematic retrieval error requirements for retrievals **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.

5.6 Validation

Validation against high precision / low systematic errors 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. It is being increasingly supplemented by the Collaborative Carbon Column Observing Network (COCCON, **/Frey et al., 2019/**).

According to **/Wunch et al., 2011/**: "Total Carbon Column Observing Network (TCCON) achieves an accuracy and precision in total column retrievals that is unprecedented for remote sensing observations (better than 0.25% for CO_2)." The COCCON retrieval performance approaches the TCCON one (COCCON, **/Frey et al., 2019/**).

According to **/Toon et al., 2009/**: "The precision of the resulting mole fractions retrieved from single spectra is about 0.15% for CO_2, 0.2% for CH_4, 0.3% for N_2O and 0.5% for CO. The absolute accuracy is limited by spectroscopic inadequacies (~1% for CO_2, ~2% for CH_4), but this can be substantially reduced by validation, i.e., airborne profiling using accurate in situ sensors."

This indicates that TCCON has low errors and is therefore well suited for validation of the GHG-CCI XCO_2 and XCH_4 satellite data products. However, we note that TCCON data may not meet the challenging systematic error requirements yet (e.g., https://tccon-wiki.caltech.edu/Network_Policy/Data_Use_Policy/Data_Description#Laser_Sampling_Errors) and therefore may not allow for verification of this requirement in the satellite retrievals.

REQ-GHGCCI-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.*

Note: TCCON will be the basis for validation. Some limitations exist though, mainly due to the sparseness of the TCCON retrieval network. Because of limited TCCON coverage, validation is possible only for a limited range of conditions. Within GHG-CCI the satellite data products will therefore also be compared with other retrievals (e.g., NDACC column-averaged XCH_4 and WMO/AGAGE in-situ observations) and XCO_2 and XCH_4 obtained from state-of-the-art models. However, all these approaches (and appropriate combinations of the available reference data) also have their limitations. How to optimally validate the satellite XCO_2 and XCH_4 data products remains a research topic.

6 Across-ECV requirements

The following shall be considered (from **/CMUG-RBD, 2015/** except *Notes in italic*):

To ensure consistency between ECV datasets, which is important for climate modelling and reanalyses, there are a number of considerations that should be taken into account for the CCI projects.

Firstly, the specification of error characteristics should be provided in a consistent way and, where appropriate, separated into precision, accuracy and stability. The errors should also be specified, where possible, for each single retrieval.

Note: consistency will be facilitated by the adoption of international terminology (ISO 5725), which is not the case at present.

Secondly, the use of common ancillary fields is important. This would ensure a consistent assumption on the atmospheric state for all ECV datasets. For surface fields an agreed SINGLE source for surface albedo, vegetation (LAI, FAPAR), emissivity, ice caps and glacier climatology, sea ice, SST etc. should be defined and agreed by the CCI projects. If this is not done, inevitable inconsistencies will be seen in the products which will be due to different representations of the atmosphere/surface being assumed.

*Note: ERA5 reanalysis fields are a good source of atmospheric fields from 1979 onwards, covering the full satellite record. These were introduced in /**CMUG-RBD, 2010**/, but were not yet available for Phase 2 of GHG-CCI. Given the availability of these products currently (and the phasing out of ERA-Interim), it is foreseen that ERA5 will be used across ECVs going forward.*

Note: It is not clear why this should be the case. The requirements on meteorological data, surface albedo, etc., may differ significantly between the CCI sub-projects. For example, the albedo depends on ground pixel size, wavelength, etc., and the optimal albedo for GHG-CCI and other projects (e.g., GHG-SST) may differ significantly. Similar remarks are also valid for the other parameters. What is essential for GHG-CCI is that those parameters are used which result in the highest quality XCO_2 and XCH_4 retrievals.

Thirdly, horizontal grids should be common to level 3 products to enable easy comparisons and processing of data from different ECV CDRs. Similarly the definition of atmospheric layering should be common across ECVs (e.g. aerosol and clouds) for level 2 and 3 products.

Note: GHG-CCI users require Level 2 for surface flux inverse modelling, not Level 3. For GHG-CCI the atmospheric layering must be such that the quality of the retrieved XCO_2 and XCH_4 is highest (or that at least a good compromise between retrieval error and processing speed can been obtained). For this reason and because XCO_2 and XCH_4 are column-averaged quantities, the use of a common layering is not necessarily appropriate for GHG-CCI.

Fourthly, the CCI should converge on terminology as this can be different for each ECV project and will enhance communication across the project.

Note: This convergence should be consistent with international standards (ISO 5725), which is not the case at present.

Finally, and this is addressed below, the formats and projections of the dataset should be as common as possible and familiar to climate modellers. CCI datasets should be located at a common data centre which can provide a common easy-to-use interface to all the datasets.

7 Requirements for observation operators and other tools

In this section requirements for observation operators and other tools are given.

7.1 Observation operators

In order to construct appropriate observation operators for the GHG-CCI 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-GHGCCI-OO-1	For each ECV data product all information needed to construct the corresponding observation operator such as Averaging Kernels (AK) and the CO_2 and CH_4 a-priori profiles need to be made available.

7.2 Routines and documentation to ingest CDRs

The following shall be considered (from **/CMUG-RBD, 2015/**):

It is vital that climate modellers are able to easily ingest the CCI datasets into their modelling environments. The aim is to make the format as familiar to users as possible (see next section) so they probably have the tools they need already but nevertheless the option of tools to read in the data should be provided. One way to ensure easy to use datasets is to impose a consistent naming convention across the ECV projects and beyond. To make reading the datasets as easy as possible a small software package consisting of source code, documentation, build scripts, and installation tests (sample input data and expected output from test programs in order to verify correct installation) is envisaged as an effective solution by climate modellers.

7.3 Metadata

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

REQ-GHGCCI-META-1	Each GHG ECV data product needs a proper documentation of which metadata have been used. Metadata information shall be given in the Product Specification Document (PSD). This refers to information on the underlying Level 1 data product and the auxiliary data products that were used, such as meteorological data. Additional information shall be given on the GHG-CCI website. This includes, for example, information on satellite or instrument-related anomalies.

7.4 Map projections

Regional surface flux inverse modelling requires XCO_2 and XCH_4 retrievals for the individual ground pixels including exact geolocation (i.e., spatial) and information on the timing. Therefore, Level 2 data products (swath data, not gridded) are the required input data products for inverse modelling and related applications (e.g., CCDAS).

Level 3 data (e.g., gridded weekly or monthly data products) will not be used as input to obtain information on regional GHG surface sources and sinks. Therefore requirements for map projections have not been formulated.

7.5 Colocation software and data

Data products will be made available for the FTS sites used for validation. Requirements for colocation software have not yet been formulated.

8 Requirements for data formats and access

In this section requirements for data formats and data access are given.

8.1 Naming convention and documentation

The Level 2 data products need to be properly documented. A dedicated document, the Product Specification Document (PSD), 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.

The following also needs to be considered:

/CMUG-RBD, 2010/: "To make life simple for users the naming conventions for files, datasets and variables must be commonly agreed between users and data producers. A recommended naming convention for individual variables for the CDRs can be accessed here:
http://cf-pcmdi.llnl.gov/documents/cf-standard-names/standard-name-table/15/cf-standardname-table.html
together with guidance on what the convention is:
http://cf-pcmdi.llnl.gov/documents/cf-standard-names/guidelines".

REQ-GHGCCI-NCD-1	There shall be a Product Specification Document (PSD), 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-GHGCCI-NCD-2	The retrieval algorithms shall be described in sufficient details via an Algorithm Theoretical Basis Document (ATBD) and/or peer-reviewed publications.

8.2 Data formats

The users of the GHG ECV data products, as represented by the GHG-CCI CRG, 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, a-priori profiles, etc.

During Phase 2 of GHG-CCI a standard format was developed within the project, which is expected to continue. This is based on NetCDF with consistent naming of parameters between data products.

The users need Level 2 data products rather than Level 3.

/CMUG-RBD, 2010/: "The use of swath based data (levels 1 and 2) in NetCDF is still under development but remains the preferred option."

Based on this the following requirement has been formulated:

REQ-GHGCCI-DFO-1	The GHG ECV data products shall be in NetCDF format (preferred option) but other data formats are also useful/possible.

8.3 Data access

There shall be a single website where all relevant information about the GHG ECV data products is given including links to documentation and data access information. This website shall be part of the GHG-CCI website. GHG ECV data products shall be made available via the GHG-CCI project website either via web access via a browser or via ftp

REQ-GHGCCI-DA-1	The GHG ECV data products shall be made available via the GHG-CCI project website.

8.4 Level of processing

The data products needed to obtain information on regional CO_2 and CH_4 surface fluxes are the Level 2 data products. Higher level data products will be generated (e.g., Level 3 such as gridded monthly data) but these data products are not required for the main application of the ECV GHG data products.

REQ-GHGCCI-PROC-1	There shall be GHG ECV Level 2 data products appropriate to obtain information on regional CO_2 and CH_4 surface sources and sinks.

9 References

/A-Scope, 2008/ Ingman, P., et al., a-scope – advanced space carbon and climate observation of planet earth, ESA Report for Assessment, Nov 2008, SP1313/1, 2008.

/Alexe et al., 2015/ Alexe, M., Bergamaschi, P., Segers, A., Detmers, R., Butz, A., Hasekamp, O., Guerlet, S., Parker, R., Boesch, H., Frankenberg, C., Scheepmaker, R. A., Dlugokencky, E., Sweeney, C., Wofsy, S. C., and Kort, E. A.: Inverse modelling of CH_4 emissions for 2010–2011 using different satellite retrieval products from GOSAT and SCIAMACHY, Atmos. Chem. Phys., 15, 113–133, 2015.

/Baker et al., 2010/ Baker, D. F., Bösch, H., Doney, S. C., O'Brien, D., and Schimel, D. S.: Carbon source/sink information provided by column CO_2 measurements from the Orbiting Carbon Observatory, Atmos. Chem. Phys., 10, 4145-4165, doi:10.5194/acp-10-4145-2010, 2010.

/Barkley et al., 2006/ Barkley, M. P., Monks, P. S., and Engelen, R. J.: Comparison of SCIAMACHY and AIRS CO_2 measurements over North America during the summer and autumn of 2003, Geophys. Res. Lett., 33, L20805, doi:10.1029/2006GL026807, 2006.

/Basu et al., 2013/ Basu, S., Guerlet, S., Butz, A., Houweling, S., Hasekamp, O., Aben, I., Krummel, P., Steele, P., Langenfelds, R., Torn, M., Biraud, S., Stephens, B., Andrews, A., and Worthy, D.: Global CO_2 fluxes estimated from GOSAT retrievals of total column CO_2, Atmos. Chem. Phys., 13, 8695–8717, 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., 2007/ Bergamaschi, P., Frankenberg, C., Meirink, J.F., Krol, M., Dentener, F., Wagner, T., Platt, U., Kaplan, J.O., Körner, S., Heimann, M., Dlugokencky, E.J., and Goede, A.: Satellite chartography of atmospheric methane from SCIAMACHY onboard ENVISAT: 2. Evaluation based on inverse model simulations, J. Geophys. Res., 112, D02304, doi:10.1029/2006JD007268, 2007.

/Bloom et al., 2010/ Bloom, A. A., Palmer, P. I., Fraser, A., Reay, D. S., and Frankenberg, C.: Large-scale controls of methanogenesis inferred from methane and gravity spaceborne data, Science, 327, 322–325, doi:10.1126/science.1175176, 2010.

/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.

/Bösch et al., 2006/ Bösch, H., Toon, G. C., Sen, B., Washenfelder, R. A., Wennberg, P. O., Buchwitz, M., de Beek, R., Burrows, J. P., Crisp, D., Christi, M., Connor, B. J., Natraj, V., and Yung, Y. L.: Space-based near-infrared CO2 measurements: Testing the Orbiting Carbon Observatory retrieval algorithm and validation concept using SCIAMACHY observations over Park Falls, Wisconsin, J. Geophys. Res., 111, D23302, doi:10.1029/2006JD007080, 2006.

/Bousquet et al., 2010/ Bousquet, P., et al., Source attribution of the changes in atmospheric methane for 2006-2008, Atmos. Chem. Phys. Discuss., 10, 27603-27630, 2010.

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

/**Bousquet et al., 2018**/ Bousquet, P., Pierangelo, C., Bacour, C., Marshall, J., Peylin, P., Ayar, P. V., Ehret, G., Bréon, F.-M., Chevallier, F., Crevoisier, C., Gibert, F., Rairoux, P., Kiemle, C., Armante, R., Bès, C., Cassé, V., Chinaud, J., Chomette, O., Delahaye, T., Edouart, D., Estève, F., Fix, A., Friker, A., Klonecki, A., Wirth, M., Alpers, M., Millet, B. Error budget of the MEthane Remote LIdar missioN (MERLIN) and its impact on the uncertainties of the global methane budget. Journal of Geophysical Research: Atmospheres, 123, 11766-11785, 2018.

/**Bréon et al., 2010/** Bréon, F.-M. and Ciais, P.: Spaceborne remote sensing of greenhouse gas concentrations, C. R. Geosci., 342, 412–424, doi:10.1016/j.crte.2009.09.012, 2010.

/Bril et al., 2007a/ Bril, A., Oshchepkov, S., Yokota, T., and Inoue, G.: Parameterization of aerosol and cirrus cloud effects on reflected sunlight spectra measured from space: application of the equivalence theorem, Applied Optics, Vol.46(13), 2460-2470, 2007.

/Bril et al., 2007b/ Bril A., Oshchepkov S., Yokota T., Carbon dioxide retrieval from reflected sunlight spectra in the presence of cirrus cloud: model studies. Proc.SPIE, 6745 (674502), 1-8, 2007.

/Bril et al., 2008/ Bril A., Oshchepkov S., Yokota T., Correction of atmospheric scattering effects in space-based observations of carbon dioxide: model study of desert dust aerosol. J.Quant.Spectrosc.Radiat.Transfer, 109 (10), 1815-1827, 2008.

/Bril et al., 2009/ Bril A., Oshchepkov S., Yokota T., Retrieval of atmospheric methane from high spectral resolution satellite measurements: a correction for cirrus cloud effects. Appl.Opt., 48 (11), 2139-2148, 2009.

/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, 15231-15246, 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., 2013/ 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. Chedin, 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 Maziere, S. Noel, 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. ODell, 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, pp. 19, in press, 2013.

/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 Astronautica, 35, 445–451, 1995.

/Butz et al., 2009/ Butz, André, Otto P. Hasekamp, Christian Frankenberg, and Ilse Aben, "Retrievals of atmospheric CO2 from simulated space-borne measurements of backscattered near-infrared sunlight: accounting for aerosol effects," Appl. Opt. 48, 3322-3336 (2009)

/Chevallier et al., 2005/ Chevallier, F., R. J. Engelen, and P. Peylin, 2005: The contribution of AIRS data to the estimation of CO_2 sources and sinks. Geophys. Res. Lett., 32, L23801, doi:10.1029/ 2005GL024229.

/Chevallier et al., 2007/ Chevallier, F., F.-M. Bréon, and P. J. Rayner, 2007: 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.

/Chevallier et al., 2009/ Chevallier, F., S. Maksyutov, P. Bousquet, F.-M. Bréon, R. Saito, Y. Yoshida, and T. Yokota, 2009: 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.

/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., P. I. Palmer, L. Feng, H. Boesch, C. O'Dell, and P. Bousquet, Towards robust and consistent regional CO_2 flux estimates from in situ and space-borne measurements of atmospheric CO_2, Geophys. Res. Lett., 41, doi:10.1002/2013GL058772.

/**Chevallier, 2018**/ Chevallier, F.: Comment on “Contrasting carbon cycle responses of the tropical continents to the 2015–2016 El Niño”, Science, 362, eaar5432, doi: 10.1126/science.aar5432, 2018.

/CMUG-RBD, 2015/ Climate Modelling User Group Requirements Baseline Document, CMUG Phase 2 Deliverable 1.1, Number D1.1, Version 0.6, April 2015.

/Connor et al., 2008/ Connor, B. J., H. Boesch, G. Toon, B. Sen, C. Miller, and D. Crisp (2008), Orbiting Carbon Observatory: Inverse method and prospective error analysis, J. Geophys. Res., 113, D05305, doi:10.1029/2006JD008336.

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

/Cressot et al., 2014/ Cressot, C., F. Chevallier, B. Bousquet, C. Crevoisier, E. J. Dlugokencky, A. Fortems-Cheiney, C. Frankenberg, R. Parker, I. Pison, R. A. Scheepmaker, S. A. Montzka, P. B. Krummel, L. P. Steele, and R. L. Langenfelds (2014),: On the consistency between global and regional methane emissions inferred from SCIAMACHY, TANSO-FTS, IASI and surface measurements, Atmos. Chem. Phys., 14, 577-592, doi:10.5194/acp-14-577-2014

/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.

/Crowell et al., 2019/ Crowell, S., Baker, D., Schuh, A., Basu, S., Jacobson, A. R., Chevallier, F., Liu, J., Deng, F., Feng, L., McKain, K., Chatterjee, A., Miller, J. B., Stephens, B. B., Eldering, A., Crisp, D., Schimel, D., Nassar, R., O'Dell, C. W., Oda, T., Sweeney, C., Palmer, P. I., and Jones, D. B. A.: The 2015–2016 carbon cycle as seen from OCO-2 and the global in situ network, Atmos. Chem. Phys., 19, 9797–9831, 2019.

/Ehret et al., 2017/ Ehret, G., Bousquet, P., Pierangelo, C., Alpers, M., Millet, B., Abshire, J. B., Bovensmann, H., Burrows, J. P., Chevallier, F., Ciais, P., Crevoisier, C., Fix, A., Flamant, P., Frankenberg, C., Gibert, F., Heim, B., Heimann, M., Houweling, S., Hubberten, H. W., Jöckel, P., Law, K., Löw, A., Marshall, J., Agusti-Panareda, A., Payan, S., Prigent, C., Rairoux, P., Sachs, T., Scholze, M., Wirth, M. MERLIN: A french-german space lidar mission dedicated to atmospheric methane. Remote Sensing, 9(10):1052, 2017.

/**Eldering et al., 2017/** Eldering, A., O'Dell, C. W., Wennberg, P. O., Crisp, D., Gunson, M. R., Viatte, C., Avis, C., Braverman, A., Castano, R., Chang, A., Chapsky, L., Cheng, C., Connor, B., Dang, L., Doran, G., Fisher, B., Frankenberg, C., Fu, D., Granat, R., Hobbs, J., Lee, R. A. M., Mandrake, L., McDuffie, J., Miller, C. E., Myers, V., Natraj, V., O'Brien, D., Osterman, G. B., Oyafuso, F., Payne, V. H., Pollock, H. R., Polonsky, I., Roehl, C. M., Rosenberg, R., Schwandner, F., Smyth, M., Tang, V., Taylor, T. E., To, C., Wunch, D., and Yoshimizu, J.: The Orbiting Carbon Observatory-2: first 18 months of science data products, Atmos. Meas. Tech., 10, 549–563, 2017.

/**Eldering et al., 2019**/ Eldering, A., Taylor, T. E., O'Dell, C. W., and Pavlick, R.: The OCO-3 mission: measurement objectives and expected performance based on 1 year of simulated data, Atmos. Meas. Tech., 12, 2341–2370, https://doi.org/10.5194/amt-12-2341-2019, 2019.

/**Feng et al., 2009/** Feng L., Palmer P. I., Boesch H., and Dance S., Estimating surface CO_2 fluxes from space-borne CO_2 dry air mole fraction observations using an ensemble Kalman Filter, Atmos. Chem. Phys., 2009.

/Feng et al., 2016/ Feng, L., Palmer, P. I., Parker, R. J., Deutscher, N. M., Feist, D. G., Kivi, R., Morino, I., and Sussmann, R.: Estimates of European uptake of CO_2 inferred from GOSAT X_{CO2} retrievals: sensitivity to measurement bias inside and outside Europe, Atmos. Chem. Phys., 16, 1289–1302, 2016.

/Frankenberg et al., 2005a/ Frankenberg, C., Platt, U., and Wagner, T.: Iterative maximum a posteriori (IMAP-)DOAS for retrieval of strongly absorbing trace gases: Model studies for CH_4 and CO_2 retrieval from near-infrared spectra of SCIAMACHY onboard ENVISAT, Atmos. Chem. Phys., 5, 9-22, 2005.

/Frankenberg et al., 2005b/ Frankenberg, C., Meirink, J. F., van Weele, M., Platt, U., and Wagner, T.: Assessing methane emissions from global spaceborne observations, Science, 308, 1010-1014, 2005.

/Frankenberg et al., 2006/ Frankenberg, C., Meirink, J. F., Bergamaschi, P., Goede, A. P. H., Heimann, M., Körner, S., Platt, U., van Weele, M., and Wagner, T., Satellite chartography of atmospheric methane from SCIAMACHY onboard ENVISAT: Analysis of the years 2003 and 2004, J. Geophys. Res., 111, D07303, 2006.

/Frankenberg et al., 2008/ Frankenberg, C., Bergamaschi, P., Butz, A., Houweling, S., Meirink, J. F., Notholt, J., Petersen, A. K., Schrijver, H., Warneke, T., and Aben, I., Tropical methane emissions: A revised view from SCIAMACHY onboard ENVISAT, Geophys. Res. Lett., 35, L15881, 2008.

/Frankenberg et al., 2011/ Frankenberg, C., Aben, I., Bergamaschi, P., Dlugokencky, E. J., van Hees, R., Houweling, S., van der Meer, P., Snel, R., and Tol, P., Global column-averaged methane mixing ratios from 2003-2009 as derived from SCIAMACHY: Trends and variability, J. Geophys. Res. (in press), 2011.

/**Fraser et al., 2013**/Fraser, A., Palmer, P. I., Feng, L., Boesch, H., Cogan, A., Parker, R., Dlugokencky, E. J., Fraser, P. J., Krummel, P. B., Langenfelds, R. L., O'Doherty, S., Prinn, R. G., Steele, L. P., van der Schoot, M., and Weiss, R. F. Estimating regional methane surface fluxes: the relative importance of surface and GOSAT mole fraction measurements, Atmos. Chem. Phys., 13, 5697-5713, doi:10.5194/acp-13-5697-2013, 2013.

/**Fraser et al., 2014**/ Fraser, A., Palmer, P. I., Feng, L., Bösch, H., Parker, R., Dlugokencky, E. J., Krummel, P. B., and Langenfelds, R. L. Estimating regional fluxes of CO2 and CH4 using space-borne observations of XCH_4 : XCO_2, Atmos. Chem. Phys. Discuss., 14, 15867-15894, doi:10.5194/acpd-14-15867-2014, 2014.

/Frey et al., 2019/ Frey, M., Sha, M. K., Hase, F., Kiel, M., Blumenstock, T., Harig, R., Surawicz, G., Deutscher, N. M., Shiomi, K., Franklin, J. E., Bösch, H., Chen, J., Grutter, M., Ohyama, H., Sun, Y., Butz, A., Mengistu Tsidu, G., Ene, D., Wunch, D., Cao, Z., Garcia, O., Ramonet, M., Vogel, F., and Orphal, J.: Building the COllaborative Carbon Column Observing Network (COCCON): long-term stability and ensemble performance of the EM27/SUN Fourier transform spectrometer, Atmos. Meas. Tech., 12, 1513–1530, https://doi.org/10.5194/amt-12-1513-2019, 2019.

/GCOS-107/ 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”, Prepared by World Meteorological Organization (WMO), Intergovernmental Oceanographic Commission, United Nations Environment Programme (UNEP), International Council for Science, Doc.: GCOS 107 (WMO/TD No. 1338), Sept 2006, 2006.

/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: 2011 update”, Prepared by World Meteorological Organization (WMO), Intergovernmental Oceanographic Commission, United Nations Environment Programme (UNEP), International Council for Science, Doc.: GCOS 154, 2011.

/GCOS-200/ Global Climate Observing System (GCOS), THE GLOBAL OBSERVING SYSTEM FOR CLIMATE: IMPLMENTATION NEEDS, Prepared by World Meteorological Organization (WMO) ; United Nations Educational, Scientific and Cultural

Organization ; Intergovernmental Oceanographic Commission ; United Nations Environment Programme ; International Council of Scientific Unions, Doc.: GCOS 200, 2016.

/Heymann et al., 2012b/ Heymann, J., H. Bovensmann, M. Buchwitz, J. P. Burrows, N. M. Deutscher, J. Notholt, M. Rettinger, M. Reuter, O. Schneising, R. Sussmann, and T. Warneke SCIAMACHY WFM-DOAS XCO_2: reduction of scattering related errors, Atmos. Meas. Tech., 5, 2375-2390, 2012.

/Heymann et al., 2012a/ Heymann, J., O. Schneising, M. Reuter, M. Buchwitz, V. V. Rozanov, V. A. Velazco, H. Bovensmann, and J. P. Burrows, SCIAMACHY WFM-DOAS XCO2: comparison with CarbonTracker XCO_2 focusing on aerosols and thin clouds, Atmos. Meas. Tech., 5, 1935-1952, 2012.

/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., 2015/ Houweling, S., Baker, D., Basu, S., Boesch, H., Butz, A., Chevallier, F., Deng, F., Dlugokencky, E. J., Feng, L., Ganshin, A., Hasekamp, O., Jones, D., Maksyutov, S., Marshall, J., Oda, T., O'Dell, C., Oshchepkov, S., Palmer, P. I., Peylin, P., Poussi, Z., Reum, F., Takagi, H., Yoshida, Y., Zhuravlev, R. An intercomparison of inverse models for estimating sources and sinks of CO_2 using GOSAT measurements. Journal of Geophysical Research-Atmospheres, 120(10), 2015.

/Houweling et al., 2010/ Houweling, S., Aben, I., Bréon, F.-M., Chevallier, F., Deutscher, N., Engelen, R., Gerbig, C., Griffith, D., Hungershoefer, K., Macatangay, R., Marshall, J., Notholt, J., Peters, W., and Serrar, S.: The importance of transport model uncertainties for the estimation of CO_2 sources and sinks using satellite measurements, Atmos. Chem. Phys., 10, 9981–9992, doi:10.5194/acp-10-9981-2010, 2010.

/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., 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.

/Hu et al., 2016/ Hu, H., Hasekamp, O., Butz, A., Galli, A., Landgraf, J., Aan de Brugh, J., Borsdorff, T., Scheepmaker, R., and Aben, I.: The operational methane retrieval algorithm for TROPOMI, Atmos. Meas. Tech., 9, 5423–5440, 2016.

/Hu et al., 2018/ Hu, H., Landgraf, J., Detmers, R., Borsdorff, T., Aan de Brugh, J., Aben, I., et al., Toward global mapping of methane with TROPOMI: First results and intersatellite comparison to GOSAT. *Geophysical Research Letters*, 45, 3682– 3689, 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.

/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., 2010/ Kaminski, T., Scholze, M. and Houweling, S.: Quantifying the benefit of A-SCOPE data for reducing uncertainties in terrestrial carbon fluxes in CCDAS, Tellus, 62B(5), 784–796, 2010.

/Kuze et al., 2010/ Kuze, A., Suto., H., Nakajima, M., and Hamazaki, T., Thermal and near infrared sensor for carbon observation Fourier-transform spectrometer on the Greenhouse Gases Observing Satellite for greenhouse gas monitoring, Applied Optics, Vol. 48, No. 35, 6716-6733, 2010.

/Liu et al., 2017/ Liu, J., Bowman, K. W., Schimel, D. S., Parazoo, N. C., Jiang, Z., Lee, M., Bloom, A. A., Wunch, D., Frankenberg, C., Sun, Y., O'Dell, C. W., Gurney, K. R., Menemenlis, D., Gierach, M., Crisp, D., and Eldering, A.: Contrasting carbon cycle responses of the tropical continents to the 2015–2016 El Niño, Science, 358, 191, 2017.

/Meijer et al., 2019/ Meijer et al., Copernicus CO_2 Monitoring Mission Requirements Document, Issue Date 27/09/2019, EOP-SM/3088/YM-ym, ESA, 2019.

/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.

/Miller et al., 2007/ Miller, C. E., Crisp, D., DeCola, P. L., et al.: Precision requirements for space-based X_{CO2} data, J. Geophys. Res., 112, D10314, doi:10.1029/2006JD007659, 2007.

/Nakajima et al., 2010/ Nakajima, M., A.Kuze, S.Kawakami, K.Shiomi, H.Suto, MONITORING OF THE GREENHOUSE GASES FROM SPACE BY GOSAT, International Archives of the Photogrammetry, Remote Sensing and Spatial Information Science, Volume XXXVIII, Part 8, Kyoto, Japan, 2010.

/O'Dell et al., 2018/ O'Dell, C. W., Eldering, A., Wennberg, P. O., Crisp, D., Gunson, M. R., Fisher, B., Frankenberg, C., Kiel, M., Lindqvist, H., Mandrake, L., Merrelli, A., Natraj, V., Nelson, R. R., Osterman, G. B., Payne, V. H., Taylor, T. E., Wunch, D., Drouin, B. J., Oyafuso, F., Chang, A., McDuffie, J., Smyth, M., Baker, D. F., Basu, S., Chevallier, F., Crowell, S. M. R., Feng, L., Palmer, P. I., Dubey, M., García, O. E., Griffith, D. W. T., Hase, F., Iraci, L. T., Kivi, R., Morino, I., Notholt, J., Ohyama, H., Petri, C., Roehl, C. M., Sha, M. K., Strong, K., Sussmann, R., Te, Y., Uchino, O., and Velazco, V. A.: Improved retrievals of carbon dioxide from Orbiting Carbon Observatory-2 with the version 8 ACOS algorithm, Atmos. Meas. Tech., 11, 6539–6576, 2018.

/Oshchepkov et al., 2008/ Oshchepkov S., Bril A., Yokota T., PPDF-based method to account for atmospheric light scattering in observations of carbon dioxide from space. J.Geophys.Res., 113, D23210, 2008.

/Oshchepkov et al., 2009/ Oshchepkov S., Bril A., Yokota T., An improved photon path length probability density function -based radiative transfer model for space-based observation of greenhouse gases. J.Geophys.Res., 114, D19207, 2009.

/Patra et al./ Patra, P.K., Crisp, D., Kaiser, J.W., Wunch, D., Saeki, T., Ichii, K., Sekiya, T., Wennberg, P. O., Feist, D. G., Pollard, D. F., Griffith, D. W. T., Velazco, V. A., De Maziere, M., Sha, M. K., Roehl, C., Chatterjee, A., and Ishijima, K. The Orbiting Carbon Observatory

(OCO-2) tracks 2–3 peta-gram increase in carbon release to the atmosphere during the 2014–2016 El Niño. *Sci Rep* 7, 13567 (2017).

/Pinty et al., 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: 10.2760/08644, European Commission Joint Research Centre, EUR 28736 EN, 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., et al., Retrieval of atmospheric CO_2 with enhanced accuracy and precision from SCIAMACHY: Validation with FTS measurements and comparison with model results, J. Geophys. Res., 116, D04301, doi:10.1029/2010JD015047, 2011.

/Reuter et al., 2013/ Reuter, M., H. Boesch, 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., 2014/ Reuter, M., Buchwitz, M., Hilker, M., Heymann, J., Schneising, O., Pillai, D., Bovensmann, H., Burrows, J. P., Bösch, H., Parker, R., Butz, A., Hasekamp, O., O'Dell, C. W., Yoshida, Y., Gerbig, C., Nehrkorn, T., Deutscher, N. M., Warneke, T., Notholt, J., Hase, F., Kivi, R., Sussmann, R., Machida, T., Matsueda, H., and Sawa, Y.: Satellite-inferred European carbon sink larger than expected, Atmos. Chem. Phys., 14, 13739–13753, 2014.

/Reuter et al., 2017/ Reuter, M., Buchwitz, M., Hilker, M., Heymann, J., Bovensmann, H., Burrows, J. P., Houweling, S., Liu, Y. Y., Nassar, R., Chevallier, F., Ciais, P., Marshall, J., Reichstein, M. How much CO_2 is taken up by the European terrestrial biosphere? Bulletin of the American Meteoro- logical Society, 98(4), 665-671, 2017.

/**Rodgers, 2000/** Rodgers, C. D., Inverse methods for atmospheric sounding – Theory and practice, World Scientific Series on Atmospheric, Ocean and Planetary Physics Vol. 2, 2000.

/Rodgers and Connor, 2003/ Rodgers, C. D., and B. J. Connor, Intercomparison of remote sounding instruments, J. Geophys. Res., 108(D3), 4116, doi:10.1029/2002JD002299, 2003.

/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, Atm**os. Meas. Tech., 12, 6771–6802**, 2019.

/Schneising et al., 2014/ Schneising, O., M. Reuter, M. Buchwitz, J. Heymann, H. Bovensmann, and J. P. Burrows, 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., 2013/ Schneising, O., J. Heymann, M. Buchwitz, M. Reuter, H. Bovensmann, and J. P. Burrows, Anthropogenic carbon dioxide source areas observed from space: assessment of regional enhancements and trends, Atmos. Chem. Phys., 13, 2445-2454, doi:10.5194/acp-13-2445-2013, 2013.

/Schneising et al., 2012/ Schneising, O., P. Bergamaschi, H. Bovensmann, M. Buchwitz, J. P. Burrows, N. M. Deutscher, D. W. T. Griffith, J. Heymann, R. Macatangay, J. Messerschmidt, J. Notholt, M. Rettinger, M. Reuter, R. Sussmann, V. A. Velazco, T. Warneke, P. O. Wennberg, and D. Wunch, Atmospheric greenhouse gases retrieved from SCIAMACHY: comparison to ground-based FTS measurements and model results, Atmos. Chem. Phys., 12, 1527-1540, 2012.

/Schneising et al., 2011/ Schneising, O., Buchwitz, M., Reuter, M., Heymann, J., Bovensmann, H., Burrows, J. P., 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., 2010/ Schneising, O., Buchwitz, M., Reuter, M., Heymann, J., Bovensmann, H., and Burrows, J. P., Long-term analysis of carbon dioxide and methane column-averaged mole fractions retrieved from SCIAMACHY, Atmos. Chem. Phys. Discuss., 10, 27479-27522, 2010.

/**Schneising et al., 2009/** Schneising, O., Buchwitz, M., Burrows, J. P., Bovensmann, H., Bergamaschi, P., and Peters, W., Three years of greenhouse gas column-averaged dry air mole fractions retrieved from satellite - Part 2: Methane, Atmos. Chem. Phys., 9, 443-465, 2009.

/Schneising et al., 2008/ Schneising, O., Buchwitz, M., Burrows, J. P., Bovensmann, H., Reuter, M., Notholt, J., Macatangay, R., and Warneke, T., Three years of greenhouse gas column-averaged dry air mole fractions retrieved from satellite - Part 1: Carbon dioxide, Atmos. Chem. Phys., 8, 3827-3853, 2008.

/Sheng et al., 2018/ Sheng, J.-X., Jacob, D. J., Maasakkers, J. D., Zhang, Y., and Sulprizio, M. P.: Comparative analysis of low-Earth orbit (TROPOMI) and geostationary (GeoCARB, GEO-CAPE) satellite instruments for constraining methane emissions on fine regional scales: application to the Southeast US, Atmos. Meas. Tech., 11, 6379–6388, 2018.

/Toon et al., 2009/ Toon, Geoffrey, Jean-Francois Blavier, Rebecca Washenfelder, Debra Wunch, Gretchen Keppel-Aleks, Paul Wennberg, Brian Connor, Vanessa Sherlock, David Griffith, Nick Deutscher, Justus Notholt, Total Column Carbon Observing Network (TCCON), publication OSA FTS Meeting, 2009.
Link: http://www.tccon.caltech.edu/publications/OSA_FTS_Meeting_20090323.pdf

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

/Wunch et al., 2011/ Wunch, D, G. C. Toon, J.-F. L. Blavier, R. A. Washenfelder, J. Notholt, B. J. Connor, D. W. T. Griffith, V. Sherlock and P. O. Wennberg. The Total Carbon Column Observing Network. Phil. Trans. R. Soc. A, 369, doi: 10.1098/rsta.2010.0240, 2011.

/**Yang et al., 2018**/ Yang, D., Liu, Y., Cai, Z. *et al.* First Global Carbon Dioxide Maps Produced from TanSat Measurements, *Adv. Atmos. Sci.* **35,** 621–623, 2018.

/Yokota et al., 2004/ Yokota, T., Oguma, H., Morino, I., and Inoue, G.: A nadir looking SWIR sensor to monitor CO_2 column density for Japanese GOSAT project, Proceedings of the twenty-fourth international symposium on space technology and science. Miyazaki: Japan Society for Aeronautical and Space Sciences and ISTS, pp. 887–889, 2004.

/Yoshida et al., 2010/ Yoshida, Y., Ota, Y., Eguchi, N., Kikuchi, N., Nobuta, K., Tran, H., Morino, I., and Yokota, T., Retrieval algorithm for CO_2 and CH_4 column abundances from short-wavelength infrared spectral observations by Greenhouse Gases Observing Satellite, Atmos. Meas, Tech. Discuss., 3, 4791-4833, 2010.

/**Yoshida et al., 2019**/ Yoshida, Y., Oshio, H., Someya, Y., Ohyama, H., Kamei, A., Morino, I., Uchino, O., Saito, M., Noda, M., and Matsunaga, T. "Atmospheric Carbon Dioxide and Methane Observations by GOSAT and GOSAT-2," in *Optical Sensors and Sensing Congress (ES, FTS, HISE, Sensors)*, OSA Technical Digest (Optical Society of America, 2019), paper FTu2B.4, 2019.

10 Acronyms

Abbreviation	Meaning
ACE-FTS	Atmospheric Chemistry Experiment-Fourier Transform Spectrometer
AATSR	Advanced Along Track Scanning Radiometer
ACA	Additional Constraints Algorithm
AIRS	Atmospheric Infrared Sounder
AMSU	Advanced Microwave Sounding Unit
AOD	Aerosol Optical Depth
ATBD	Algorithm Theoretical Basis Document
CCDAS	Carbon Cycle Data Assimilation System
CCI	Climate Change Initiative
CMUG	Climate Modelling User Group (of ESA's CCI)
CRG	Climate Research Group
D/B	Data base
DOAS	Differential Optical Absorption Spectroscopy
DPM	Detailed Processing Model
EC	European Commission
ECA	ECV Core Algorithm
ECMWF	European Centre for Medium Range Weather Forecasting
ECV	Essential Climate Variable
EO	Earth Observation
ESA	European Space Agency
FCDR	Fundamental Climate Data Record
FP	Full Physics
FTIR	Fourier Transform InfraRed
FTS	Fourier Transform Spectrometer
GCOS	Global Climate Observing System

GEO	Group on Earth Observation
GEOSS	Global Earth Observation System of Systems
GHG	GreenHouse Gas
GOME	Global Ozone Monitoring Experiment
GMES	Global Monitoring for Environment and Security
GOSAT	Greenhouse Gases Observing Satellite
GTOS	Global Terrestrial Observing System
IASI	Infrared Atmospheric Sounding Interferometer
IPCC	International Panel in Climate Change
IUP	Institute of Environmental Physics (IUP) of the University of Bremen, Germany
JCGM	Joint Committee for Guides in Metrology
LMD	Laboratoire de Météorologie Dynamique
MACC	Monitoring Atmospheric Composition and Climate, EU GMES project
MERIS	Medium Resolution Imaging Spectrometer
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding
MODIS	Moderate Resolution Imaging Spectrometer
NA	Not applicable
NDACC	Network for the Detection of Atmospheric Composition Change
NASA	National Aeronautics and Space Administration
NIES	National Institute for Environmental Studies
NOAA	National Oceanic and Atmospheric Administration
OCO	Orbiting Carbon Observatory
PBL	Planetary Boundary Layer
RMS	Root-Mean-Square
RTM	Radiative transfer model
SCIAMACHY	SCanning Imaging Absorption spectroMeter for Atmospheric ChartographY
TANSO	Thermal And Near infrared Sensor for carbon Observation
TCCON	Total Carbon Column Observing Network
TES	Tropospheric Emission Spectrometer

11 Annex A: GCOS GHG requirements

The following text is from **/GCOS-154/**, section 3.1.8 "ECV Carbon Dioxide, Methane and other Greenhouse Gases", with some updates based on /**GCOS-200**/ as marked. URDv1 used the previous version of this document, /**GCOS-107**/.

Carbon dioxide is the dominant greenhouse gas emitted by anthropogenic activities. The atmospheric build-up is caused mostly by the combustion of coal, oil, and natural gas and reflects to a significant extent cumulative anthropogenic emissions rather than the current rate of emissions.

Methane (CH_4) is the second most significant anthropogenically emitted greenhouse gas, and its level has also been increasing since preindustrial times.. Other long-lived GHGs include nitrous oxide (N_2O), chlorofluorocarbons (CFCs), hydrochlorofluorocarbons (HCFCs), hydrofluorocarbons (HFCs), sulphur hexafluoride (SF6), and perfluorocarbons (PFCs). The relative radiative forcing of CH_4 in 2008 was about 18 per cent of the total radiative forcing caused by all long-lived greenhouse gases in the atmosphere since the beginning of industrial time. The Kyoto Protocol of the UNFCCC includes future restrictions on the release of GHGs, including CO_2, CH_4, N_2O, HFCs, SF_6, and PFCs. The Montreal Protocol on Substances that Deplete the Ozone Layer includes mandatory restrictions for individual countries on the production and consumption of those CFCs and HCFCs that are also GHGs.

Satellite measurements are emerging as an important component of the overall observing system for CO_2 and CH_4. Methane was first measured in the stratosphere by SAMS in the 1980s and then by HALOE (1991-2005.). The Scanning Imaging Absorption Spectrometer for Atmospheric Cartography (SCIAMACHY) instrument made the first global measurements of tropospheric CH_4, and its data are being used in inverse modelling studies to quantify CH_4 emissions. Methane data are also provided currently by ACE-FTS. The AIRS, TES and IASI high-resolution IR sounders are providing information on both CO_2 and CH_4, although with limited vertical range, and their data also have been used in inverting fluxes via data assimilation. The recently launched Greenhouse Gases Observing Satellite (GOSAT) is starting to provide more complete information. Experience in using the data from GOSAT and the future OCO-2 mission will guide the development of the space-based component of the observing system for these two majors GHGs. The planned Sentinel-5p and Sentinel-5 missions will also measure CH_4. Satellite measurements can potentially provide unique information on global emission source identification, which is not possible with ground-based measurements alone.
In the context of this document, detection of sources and sinks of greenhouse gases is the main focus for space-based measurements. Monitoring of global trends of CO_2 and CH_4 as long-lived gases is adequately covered by surface in situ measurements.

The following is needed for these ECVs:

Product A.8.1 Retrievals of CO_2 and CH_4 of sufficient quality to estimate regional sources and sinks

Benefits

- Improvement in estimates of global means and facilitation of monitoring of the spatial distribution of the key greenhouse gases.
- Satellite-based observations of column values and vertical profiles of the mixing ratio of carbon dioxide, methane and other greenhouse gases, when coupled with reanalysis, providing a tool for assessment of sources and sinks of greenhouse gases, especially CO_2 and CH_4;
- Potential provision of additional background information on the measures on stabilization of the mixing ratios of key greenhouse gases at a level that would prevent dangerous anthropogenic interference with the climate system;
- Provision of estimates of localized surface emissions such as those related to wetlands and rice fields for CH_4 and land-use change for CO_2, where the data products are of sufficient accuracy and resolution.

*Note: This table has been updated to reflect changes the requirements according to the most recent GCOS document, /**GCOS-200**/.*

Target requirements

Variable/ Parameter	Horizontal Resolution	Vertical Resolution	Temporal Resolution	Accuracy	Stability (per decade)
Tropospheric CO_2 column	5-10 km	N/A	4 h	1 ppm	1.5 ppm
Tropospheric CO_2	5-10 km	5 km	4 h	1 ppm	1.5 ppm
Tropospheric CH_4 column	5-10 km	N/A	4 h	10 ppb	7 ppb
Tropospheric CH_4	5-10 km	5 km	4 h	0.5 ppb	0.7 ppb
Stratospheric CH_4	100-200 km	2 km	Daily	5%	0.3%

Rationale: Requirements for tropospheric CO_2 and CH_4 are driven by detection and quantification of the different emission sources via inverse modelling. The primary measurement needed is the tropospheric column, as it provides sensitivity down to the Earth's surface where most of the sinks and sources are located. Research and study of the use of currently available measurements – in situ as well as satellite – in reanalysis is needed to provide a more firmly based statement of essential data requirements, in particular on the extent of detail required in vertical sounding. Initial estimates are based on resolving the values of observed column fluctuations. Time scales that extend from the diurnal to the decadal need to be resolved to allow for a complete description of the processes that determine the distributions of these gases. Spatial variability can be substantial in the planetary boundary layer, reflecting the variability of sources and sinks. Products can, however, be useful for source-sink inversion without resolving the shortest space and time scales.

CH_4 is not well mixed in the stratosphere, where it is the main chemical source of H_2O. The stratospheric product is needed to support the attribution of water-vapour trends and for determining the radiative influences of stratospheric CH_4 and water vapour.

The global trends, seasonal cycle, and latitudinal gradients of the long-lived greenhouse gases N2O, CFCs, HCFCs, HFCs, SF6, and PFCs in the troposphere are well-monitored, using present-day surface networks. Short-term and regional variability of these long-lived gases is mainly in the stratosphere, in relation to their chemical breakdown at these altitudes. Observing the spatio-temporal variability of these gases is important in the stratosphere, where they also provide information on ‘age of air’, but these measurements are largely dependent on the limb/occultation type of satellite observations which are not part of the operational suite of satellite measurements. Some monitoring of the stratospheric distribution changes of long-lived gases is needed for the assessment of radiative and dynamical feedbacks in the stratosphere related to composition changes. Future research studies of these greenhouse gases will, at intervals, require future satellite missions.

Requirements for satellite instruments and satellite datasets
FCDR of appropriate NIR/SWIR/IR radiances, for example through:
• Passive NIR/SWIR operational missions for CO_2 and CH_4, building on the experience with SCIAMACHY and the specialized missions GOSAT and OCO-2 (simultaneous total column CO, such as provided by SCIAMACHY, adds much value for CO_2 source characterization);
• High spectral resolution IR sounding for the upper troposphere and stratosphere, as provided initially by ACE-FTS, AIRS, and IASI;
• Limb-sounding in IR and MW for distributions in the upper troposphere and stratosphere;
• Active NIR/SWIR systems to obtain tropospheric vertical profiles.

Calibration, validation and data archiving needs
• The required comprehensive independent ground-based validation measurements can be provided by the WMO Global Atmosphere Watch (GAW) Global CO_2 and CH_4 Monitoring Networks, including ship and dedicated light aircraft profiles up to 8 km; both these GAW networks are designated by GCOS as comprehensive networks, and subsets are designated as baseline networks;
• A network of surface-based total column CO_2 and CH_4 instruments (TCCON) and continued routine commercial aircraft observations (e.g. CONTRAIL and observations planned by IAGOS-ERI), needed for validation of products;
• Aircraft observations of CO_2 and CH_4, needed to validate the transport in the models that are used in the surface emission inversions using total-column data (part of the total-column variability is related to transport in the upper-troposphere/lower-stratosphere and should not be assigned to the lower troposphere affecting the emission inversion).

Adequacy/inadequacy of current holdings
• Satellite products are still under development, and accuracy requirements have not yet been met (except for CH_4 total column);

• In situ observations of the long-lived gases do not provide a complete 3D distribution in the atmosphere and are rather unevenly distributed in space; most networks are designed for trend detection in the background atmosphere, with minimal sensitivity to (nearby) emissions.

Immediate action, partnerships and international coordination
• Support for the generation of products through retrieval or, in appropriate cases, data assimilation;
• Execution of planned missions and development and implementation of a plan for sustained measurements sufficient to deliver products of the required accuracy;
• Support for the surface and free-tropospheric measurements needed for calibration and validation;
• Derivation of products from AIRS and SCIAMACHY from 2002 onwards, IASI from 2008, GOSAT from 2009 and, in the future, from OCO-2 and from Sentinel-5p/TROPOMI and Sentinel-5 for CH_4;
• Limb-sounding data for retrieval of stratospheric profiles from current instruments, including those from ACE-FTS (CH_4, N_2O), MIPAS (CH_4, N_2O), and MLS (N_2O);
• Additional data provided by TES for the retrieval of tropospheric CH_4;
• Research towards improved future capabilities, including long-term monitoring of CO_2, CH_4 and other GHGs such as N_2O;
• Coordination by WCRP SPARC and IGBP IGAC.

Link to GCOS Implementation Plan (updated to reflect changes in /GCOS-200/, IP-16)
• [IP-16 Action A30] Re-establish sustained limb-scanning satellite measurement of profiles of water vapour, ozone and other important species from UT/LS up to 50 km;
• [IP-16 Action A31] Engage existing networks of ground-based, remote sensing stations (e.g. NDACC, TCCON, GRUAN) to ensure adequate, sustained delivery of data from MAXDOAS, charge coupled device (CCD) spectrometers, lidar, and FTIR instruments for validating satellite remote-sensing of the atmosphere;
• [IP-16 Action A32] Extend and refine the satellite data records (FCDRs and CDRs) for GHG and aerosol ECVs;
• [IP-16 Action A33] Maintain and enhance the WMO GAW Global Atmospheric CO_2 and CH_4 monitoring networks as major contributions to the GCOS Comprehensive Networks for CO_2 and CH_4. Advance the measurement of isotopic forms of CO_2 and CH_4 and of appropriate tracers to separate human from natural influences on the CO_2 and CH_4 budgets;
• [IP-16 Action A34] Define the requirements for providing vertical profiles of CO_2, CH_4 and other GHGs, using recently emerging technology, such as balloon capture technique;
• [IP-16 Action A35] Assess the value of the data provided by current space-based measurements of CO_2 and CH_4, and develop and implement proposals for follow-on missions accordingly.

Other applications
Carbon dioxide and other greenhouse gas distributions may allow improved retrieval of the temperature and water vapour information from IR sounders for NWP and reanalysis; N_2O measurements are needed for constraining the effects of NO_x on ozone.

12 Annex B: CMUG GHG requirements

The following is from **/CMUG-RBD, 2015/** with edits for clarity marked in italics**:**

A comprehensive understanding of greenhouse gases is crucial for informing societal response to climate change. Applications with a need for observations of greenhouse gases such as CO_2 and CH_4 include Model Development, Decadal Forecasting and Regional Source/Sink Determination. As shown in ***Table B.1***, each application has somewhat different observational requirements reflecting the particular aspect of greenhouse gases under consideration.

To elaborate on the GHG observational requirements for Regional Source/Sink Determination, the tabulated values are based on the activities undertaken within the frame of the MACC sub-project on greenhouse gases and on feedbacks from the GHG CMC. The principal products from the MACC sub-project on GHG are:

- 4-dimensional gridded fields of CO_2 and CH_4 produced in near-real-time (based on data assimilation of near-real-time data products, typically from operational satellites),
- 4-dimensional gridded fields of CO_2 and CH_4 produced in "delayed mode" (6 months delay, to allow data assimilation of research-mode satellite data products),
- 3-dimensional gridded fluxes of CO_2 and CH_4 produced in "delayed mode",
- Re-analysed concentration and flux fields of CO_2 and CH_4 for the period 2003-2010.

Flux fields are an important factor for decision-makers at several levels, and need to be estimated with confidence. The fidelity of flux estimates is strongly influenced by accuracy and stability of the observations that are used as input to the data assimilation and re-analysis systems. This drives the requirements given in ***Table B.1*** for some of the required parameters.

The requirements for full GHG concentration profiles are given in *the data sheet of the GHG-CCI*. In general, differences were found in the user requirements even when the same application was considered. An important element to consider in this regard is the actual target each user focuses on (e.g. cities rather than countries).

Horizontal Resolution and Observing Cycle requirements have become more stringent than what *is* suggested by GCOS and by the CMUG Phase 1 URD. This is because if on one hand they reflect the spatial and temporal variability of important classes of regional sources and sinks on the other they also reflect improvements in the models, especially in terms of increased horizontal resolution. The need for good flux estimates makes the current requirements for accuracy and stability generally more demanding than previous GCOS and the CMUG Phase 1 user requirements.

Parameter	Application	Horizontal Resolution	Vertical Resolution	Observing Cycle	Precision	Accuracy	Stability	Types of error
Trace gas profile CH_4 - Troposphere column	Regional source/sink determination	5/20/50 km	N/A	3/4/6 h	0.1/0.5/1% 2/10/20 ppb	0.1/0.5/2.0% 2/10/20 ppb	0.5/0.7/2.0 %/dec 2/7/35 ppb/dec	SSEOB
Trace gas profile CH_4 - Total column	model development	25km	N/A	6 h	1%	1%	10ppb/dec	SSEOB
	decadal f/c	20km	N/A	Daily	<<10 ppb	<<10 ppb	2%/dec 35 ppb/dec	SSAOB
	Regional source/sink determination	10/50/100 km	N/A	3/4/6 h	0.25/0.5/1% 5/10/20 ppb	0.1/0.5/2.0% 2/10/40 ppb	0.1/0.5/2.0 %/dec 2/10/35 ppb/dec	SSEOB
Trace gas profile CO_2 - Total column	model development	25km		6h	0.5/1ppm	0.5/1ppm	0.1/0.5ppm/dec	SSEOB
	decadal f/c	2/5/20km	N/A	Daily	0.3/0.5/1% 1/1.5/3 ppm	0.3/0.5/1% 1/1.5/3.0 ppm	0.5/1.5/2 %/dec 2/5/8 ppm/dec	SSAOB
	Regional source/sink determination	5/20/50 km	N/A	3/6/24 h	0.25/0.5/0.75% 1/2/3 ppm	0.25/0.5/1% 1/2/4.0 ppm	0.5/1.5/2 %/dec 2/5/8 ppm/dec	SSEOB
Trace gas profile CO_2 - Troposphere column	Regional source/sink determination	5/20/50 km	N/A	3/4/6 h	0.15/0.4/0.5% 0.5/1.5/2 ppm	0.15/0.5/1% 0.5/1.5/4.0 ppm	0.15/0.5/2 %/dec 0.5/1.5/7.5 ppm/dec	SSEOB

Table B.1: Requirements for satellite observations of greenhouse gases (from **/CMUG-RBD, 2015/**). *Error type "SSEOB" refers to Single sensor uncertainty estimates for every observation. "SSAOB" refers to Single sensor accuracy estimates for every observation. These can be thought of as random and systematic errors respectively.*

The requirements are given for tropospheric and total column only, in recognition that requirements for profile data would be very demanding for existing satellite data. In the event that data providers consider it feasible to provide profile data approaching GCOS requirements, then more refined user requirements could be given in a future update of this document. The user community increasingly asks for horizontal and vertical resolution in the Lower Stratosphere to be the same as that for the Higher Troposphere, in contrast to previous GCOS requirements. As mentioned above, other applications of greenhouse gas observations may have different sets of requirements. For example, the detection of CH_4 emissions from pipelines or similar small sources would require higher horizontal resolution and vertical resolution in the lower troposphere.

Turning now to the GHG observation requirements for decadal forecasting, it is principally the distribution of the trace gases at the start of the forecast that can be important to help define the atmospheric fields. This consideration was translated in the Phase 1 URD in a requirement of long period averages as sufficient for decadal forecasts. The latest consultation seems to indicate that a much higher observing cycle would be useful. Additionally, more stringent requirements have been made for the horizontal resolution that is now comparable with that needed in other applications. Similar to the ozone section above, it would be important to provide not only merged GHG products but also products from single sensors as separate datasets. Users also pointed out that the harmonisation between the various datasets is a key aspect to efficiently using the data.

End of document