ESA Climate Change Initiative (CCI)

User Requirements Document (URD)

for the Essential Climate Variable (ECV)

Greenhouse Gases (GHG)

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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.
Version 4.0 – Draft 1	16 Feb. 2024	Draft Author: F. Chevallier; Contributions: M. Buchwitz	Update for Phase 2 of GHG-CCI+ esp. to consider new GCOS requirements (GCOS-245).
Version 4.0	16 May 2024	Final version Author: F. Chevallier; Contributions: M. Buchwitz	Only formal aspects; content identical with Draft 1

Table of Contents

1 Summary

This document states users' requirements for the products of ESA's GHG-CCI project (https://climate.esa.int/en/projects/ghgs/). 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 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+, with a first phase that went from 2019 to 2021 and a second one now from 2022 to 2024. 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-245/**): ECV products "CO2 column average dry air mixing ratio" and "CH4 column average dry air mixing ratio". We specifically address the estimation of regional sources and sinks which was the focus of the previous GCOS requirement formulation: /**GCOS-154**/ stated that the retrievals of CO_2 and CH_4 had to be of sufficient quality to estimate regional sources and sinks. The present user requirements may not apply to other applications or finer spatial scales. An example of requirement changes associated to a change of application is given here when only anthropogenic fluxes are specifically considered.

Ideally, the estimation of surface fluxes 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. So far, seven satellite instruments had or have this capability for the regional scale flux applications:

- 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, International Space Station – ISS, 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.

In addition, new retrieval capabilities are emerging in relation to Copernicus Sentinel-2, Greenhouse Gases Satellite (GHGSat), PRecursore IperSpettrale della Missione Applicativa (PRISMA), Environmental Monitoring and Analysis Program (EnMAP), Landsat or Earth surface Mineral dust source InvesTigation (EMIT) on the ISS.

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, TROPOMI, PRISMA and EnMAP. (OCO-3 data are not included, but also constitute a fundamentally different product lacking global coverage due to its orbit – on the 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. The same is true for the Copernicus Climate Change Service (C3S) as GHG-CCI team members are now also responsible for operationally generating satellite-derived ECV XCO_2 and XCH_4 data products for C3S. Note that the underlying retrieval algorithms have been initially developed in GHG-CCI and are now used in C3S.

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. The IASI products are now also operationally generated via C3S.

2 ECV Greenhouse Gases (GHG)

What is the ECV GHG? Here, the ECV GHG follows the definition of **/GCOS-154/** (see their **Section 1.6**). 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.

Mainly 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, 2015, 2021/ /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, 2020/ /Schneising et al., 2008, 2010, 2011, 2012, 2013, 2014/ /Yokota et al., 2004/ /Yoshida et al., 2010, 2019/ /Palmer et al., 2019/ /Agustí-Panareda et al, 2023/ /Gier et al., 2020/** 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, 2015/ /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, 2020, 2023/ /Yoshida et al., 2010, 2019/ /Islam et al., 2021/ /Lu et al., 2022/ /Lunt et al., 2019, 2021/ /Miller et al., 2019/ /Maasakkers et al., 2019/ /Parker et al., 2020/ /Saunois et al, 2020/ /Hachmeister et al., 2024/.**

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 focuses on XCO_2 from OCO-2, GOSAT-2 and TanSat, and XCH_4 from GOSAT-2 and S5P. XCO_2 and XCH_4 from PRISMA and EnMAP are also considered but with a lower priority. 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/ /GCOS-245/,** the mission requirements of the Copernicus CO2 Monitoring Mission (CO2M) /**ESA, 2020**/ and the requirements formulated by the CCI Climate Modelling User Group (CMUG) **/CMUG, 2022/**.

This URD differs from the above references when needed. For instance, some **/GCOS-245/** requirements partially refer to future missions and cannot be met with the existing satellites used in GHG-CCI. This is the case of their XCO_2 threshold requirements for temporal resolution (72 hours; neither OCO-2 nor GOSAT-2 meet this requirement) and uncertainty (0.8 ppm, 1-sigma) that seem to refer to CO2M (launch 2026). Their threshold stability requirement is 0.03 ppm/year which is according to our experience significantly smaller that the uncertainty of methods used to establish stability (considering "noise" due to sampling aspects, stability of the reference data, etc.). Similarly, for XCH_4, the **/GCOS-245/** threshold uncertainty is 10 ppb (1-sigma), which, for many locations on Earth, cannot be met by S5P. For the breakthrough requirement of 5 ppb, it is argued that this is based on "Expert judgement based on expected improvement of TROPOMI/S5P". Typical TROPOMI/S5P XCH_4 uncertainty is on the order of 15 ppb and this is mainly due to instrument noise and no improvement can change this, except by limiting retrievals to highly reflecting scenes. Furthermore, the arguably most important requirement for users who use our data products for inverse modelling of sources and sinks is related to systematic errors (high accuracy or low biases) but this is not addressed in /**GCOS-245**/ as their uncertainty requirement is essentially a requirement on random error (dispersion, scatter).

This document refers to XCO_2 and XCH_4 as mostly 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 with OCO-2 retrievals have been more robust (e.g. /**Chevallier et al. 2019**/ /**Crowell et al., 2019**/ /**Liu et al., 2017**/ /**Patra et al., 2017**/ /**Peiro et al 2022**/ /**Byrne et al, 2023**/). This is still 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 always 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 (https://climate.esa.int/en/projects/ghgs/. However, other issues like transport model systematic errors and flawed statistical models play a role as well.

Requirements are application-dependent and this URD focusses on the requirements associated with the estimation of regional surface fluxes of CO_2 and CH_4. However, the estimation of anthropogenic emissions is briefly discussed in Section 6.

CCI CMUG compiled a requirement document relevant for this URD **/CMUG, 2022/** derived from GCOS requirements **/GCOS-200/** and other sources. This URD has been written to be as consistent as possible (mostly identical) with the definitions and requirements formulated in **/CMUG, 2022**/ or earlier versions. This also refers to which requirements are covered. Requirements as formulated in **/CMUG, 2022/** are directly included in this URD when we agree with them.

4 Definitions

In this section key definitions are given. They are identical to the definitions given in **/CMUG, 2022/** or earlier versions 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, 2022/** (after **/GCOS-107/,** but contradicted later by **/GCOS-154/ and /GCOS-245/** that acknowledge the international norm) defines it inconsistently with the international standard for metrology, i.e. ISO 5725 **/JCGM, 2012/**. **/CMUG, 2022/** not only breaches the official definition of "accuracy", but also misuses two words ("bias" and "measured") in it. We therefore replace CMUG's "Accuracy" with the expression "Systematic error", following the international norm.

Systematic error: the component of retrieval 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 error ***/JCGM, 2012/***.

Precision is the measure of reproducibility or repeatability of the retrieval 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 retrieval but does not establish the systematic error of the observation. **/CMUG, 2022/**

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, 2022/**

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 the term “**Revisit time**” is also used. The definition is identical with the definition of “Observing cycle”. Both terms refer to the (average) temporal frequency at a given location.*

5 Requirements for regional-scale flux estimation

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 8° × 10° 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^o, 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/).**

/Chevallier et al., 2007/ showed that for CO_2 surface flux inverse modelling "regional biases of a few tenth of a part 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 rather low errors and is therefore 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, at least not at all sites, 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.

5.7 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.

5.8 Requirements for observation operators and other tools

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

5.8.1 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.

5.8.2 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.

5.8.3 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.

5.8.4 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.

5.8.5 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.

5.9 Requirements for data formats and access

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

5.9.1 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.

5.9.2 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.

5.9.3 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.

5.9.4 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.

6 Requirements for the estimation of anthropogenic emissions

Requirements for the estimation of anthropogenic emissions in general differ from those for the estimation of regional fluxes because of the target variables have different temporal and spatial scales. Spatially, a regional flux, whether of anthropogenic origin (e.g., from managed lands or from fossil fuel burning) or not, is usually defined over areas of at least 100×100 km^2 and the uncertainty of the corresponding prior knowledge is correlated over weeks /**Chevallier et al., 2012**/. In contrast, anthropogenic emissions whose plumes are visible from space can reach the scale of an industrial plant and vary from one hour to the next. These specificities have been extensively studied for the preparation of the Copernicus CO_2 Monitoring Mission (CO2M) /**ESA, 2020**/. We follow the CO2M mission requirements here /**ESA, 2020**/, and therefore highlight three main requirement changes compared to those listed above for regional flux estimation:

1. **Horizontal resolution:** the idea here is to image the emission plumes and it is thought that the individual pixels of the images need to reach at least 4 km^2 for that purpose.

2. **Precision:** the precision of the retrievals controls the signal-to-noise of the plume on a given image. It shall be less than 0.7 ppm for XCO_2 (instead of 34 ppm) and less than 10 ppb for XCH_4 (instead of 34 ppb).

3. **Observing cycle:** a weekly coverage over land for latitudes above 40 degrees is deemed important.

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8 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)
CO2M	Copernicus CO2 Monitoring Mission
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
EnMAP	Environmental Monitoring and Analysis Program
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
ISS	International Space Station
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
PRISMA	PRecursore IperSpettrale della Missione Applicativa
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

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