ESA Climate Change Initiative (CCI)

Round Robin Evaluation Protocol (RREP)

for the Essential Climate Variable (ECV)

Greenhouse Gases (GHG)

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Change log:

Version Nr.	Date	Status	Reason for change
Draft 1	16. Dec. 2010	Initial Draft for GHG-CCI project team & ESA	New document. Main purpose: Input for discussion with GHG-CCI team
Draft 2	27. Jan. 2011	Improved Draft	To consider comments from GHG-CCI team
Draft 3	3. Mar. 2011	Improved Draft	Several minor editorial corrections; “ensemble option” added
Version 1	8. Mar. 2011	Approved by CRG	To compile final version 1
Version 2	17. Aug. 2011	Approved by GHG-CCI team incl. CRG	Selection criteria for ACAs added

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1 Overview

The GHG-CCI project aims at generating global satellite derived data sets of atmospheric CO_2 and CH_4 information useful for constraining regional surface fluxes (emission and uptake) via inverse modeling of these two important anthropogenic greenhouse gases (GHG) (see GHG-CCI User Requirements Document **/URD GHG-CCI v1/**).

The four core GHG-CCI ECV data products generated with the GHG-CCI "ECV Core Algorithms" (ECAs) are XCO_2 (in ppm) and XCH_4 (in ppb) from SCIAMACHY/ENVISAT and TANSO-FTS/GOSAT. Within GHG-CCI several ECAs are being further improved and the corresponding data products evaluated. Several algorithms are being further developed within this project – at least two for each of the four core products. It is planned to select the best algorithm for each of the four core products (i.e., four algorithms or less).

Within the GHG-CCI project two types of algorithms to retrieve CO_2 and CH_4 information from satellite data are distinguished:

- **"ECV Core Algorithms" (ECAs):**
    - These are algorithms for retrieving near-surface sensitive column-averaged mixing ratios of CO_2 and CH_4, denoted XCO_2 and XCH_4, from SCIAMACHY/ENVISAT and TANSO/GOSAT.
- **"Additional Constraints Algorithms" (ACAs):**
    - These are algorithms for retrieving CO_2 and CH_4 information from satellite data with no or limited near-surface sensitivity. They have the potential to deliver important additional constraints when used in a (inverse modelling) framework that exploits satellite data to infer information on surface fluxes. This is because they can constrain CO_2 and CH_4 in upper layers, i.e., layers above the Planetary Boundary Layer (PBL).

This document describes how the algorithm selection will be done at the end of the 2 year "Round Robin" (RR) phase of the GHG-CCI project.

The selection of ECAs will be based on (but not limited to) comparisons with the highly precise and accurate ground-based TCCON FTS XCO_2 and XCH_4 retrievals. For each product and each FTS site several of Figures of Merit (FoM) - bias, standard deviation, etc. - will be computed to characterize the quality of a given data product. In addition, minimum requirements for each FoM have been defined. The FoMs will be computed by the independent GHG-CCI VALidation Team (VALT). In addition, the FoMs will also be determined by the retrieval team to cross-check and to find out to what extent the results depend of the details of the analysis method chosen.

This information will be evaluated by the independent GHG-CCI Climate Research Group (CRG). Due to limitations of this approach (e.g., spatial sparseness of the FTS reference data), the GHG-CCI CRG also needs to base the selection on their experts knowledge /

judgment. For this purpose, additional information will be made available. This comprises global and regional maps and time series of the satellite data products including comparisons with model data and comparisons with the data products generated with the competing ECAs and other satellite derived data products of the same quantity (if available) generated elsewhere (e.g., at NIES and NASA). Last but not least, the CRG will to some extent also use and analyze the GHG-CCI data products. It is expected that for each product a clear “winner” can be identified. In case several ECAs have an identical performance, the CRG will decide together with the retrieval team, which algorithm will be used to generate the corresponding ECV. In case several ECAs have a different performance and if it cannot be decided unambiguously which ECA is the best an option is to use a similar approach as also used for climate models, namely an “ensemble approach”, i.e., to use several retrievals when confronting the satellite retrievals with models e.g. via direct comparison or inverse modeling. This is expected to provide important additional error information, namely an estimate of algorithm dependent errors (taking this into account the ensemble approach is likely superior compared to using a single data product for reliably estimating surface fluxes and their uncertainties).

Within GHG-CCI several ACAs will also be further improved and their quality will be assessed. ACAs are not in competition within GHG-CCI. They deliver sub-columns and vertical profiles of CO_2 and CH_4. Instruments used are AIRS, IASI, MIPAS, SCIAMACHY in solar occultation mode, and ACE-FTS.

The approach proposed in this document is the baseline defined at project start. If it turns out that refinements are needed or that even an entirely different approach is required, this baseline may change.

2 EVC Core Algorithms (ECAs)

2.1 Spatio-temporal requirements for TCCON comparisons

Within the comparison period FTS, GOSAT, and SCIAMACHY data should all be available. This is important to assess the consistency of the SCIAMACHY and GOSAT time series which requires overlap in time.

Additionally, the period should cover at least one year in order to draw conclusions on, e.g., the seasonal cycle representation (in case a seasonal cycle is expected). Ideally, the period should cover full years only, so that no seasons are over-weighted within the comparison statistics.

SCIAMACHY is operational since 2002 and is, therefore, not limiting the selection. GOSAT was launched in January 2009 and calibrated Level 1 data are available since April 2009. Many FTS sites are operational longer than GOSAT data are available; however, there are some sites which got operational not before August 2009 (see **Table 1**).

Resulting from the limitations of data availability, 01.01.2010 – 31.12.2010 (baseline, to be confirmed) has been chosen as the minimum comparison time period of the Round-Robin (RR) exercise for SCIAMACHY and GOSAT. This is however not sufficient.

Especially for SCIAMACHY, but also for GOSAT, it is important to also analyze longer time periods. For example, 2010 is not a representative year for the quality of the SCIAMACHY methane retrievals due to severe detector degradation after October 2005. It is therefore important to also include the years before 2010, i.e., ideally 2003-2010 for SCIAMACHY and 2009 (partially) to (at least) 2010 for GOSAT.

2010 is therefore the mandatory year which needs to be analyzed for both SCIAMACHY and GOSAT. This is also important in order to assess the consistency of the data products of the two sensors. In addition, all the other years where data of the corresponding satellite are available shall also if possible be analyzed (per year, i.e., independently for each year, and for those FTS sites where data are available).

Table 1 lists all TCCON sites (https://tccon-wiki.caltech.edu/) which have been chosen for the RR comparison with TCCON. This means nearly all TCCON sites which fully cover the comparison period are used. Only the sites Eureka (Canada), Ny Alesund (Spitsbergen), and Izana (Tenerife) have been excluded because of orography, jagged coastline, ocean, and/or persistently snow/ice covered surfaces.

Note that due to detector degradation issues, the quality of the SCIAMACHY methane retrievals is highest before November 2005. Comparison of data products with TCCON for 2003-2005 is limited to a few stations only and only after mid 2004. Therefore the list of FTS sites to be used for comparison may have to be extended, e.g., using also NDACC FTS

sites/retrievals. This will be decided later in the project, when the quality of the NDACC retrievals for this purpose has been assessed in (more) detail.

For all chosen TCCON sites all “good” satellite retrievals shall be used for the comparison (note that either the data product contains only “good” data as determined by the retrieval team or the data product contains a corresponding quality flag).

For the comparison, all satellite retrievals within a given distance (radius or latitude/longitude range) around the FTS sites shall be used. The optimal distance still needs to be defined. A smaller distance (e.g., 100 km) is preferred for better representativeness but may result in too few data points for comparison (at present 500 km is typically used for GOSAT). It is therefore suggested to deliver all retrievals within a 500 km radius around the FTS sites and to perform comparisons using 3 radii: 100 km, 350 km and 500 km.

In addition, the comparison shall be limited to satellite retrievals over land.

The temporal co-registration criterion is 2 hours, i.e., only FTS data shall be used for comparison, which have been obtained within +/- 2 hours compared to the time of the satellite retrievals.

Site	Established	Lat	Lon	Alt. [km]	PI
Bialystok, Poland	03/2009	53.23N	23.025E	0.18	Notholt, Warnecke
Bremen, Germany	07/2004	53.10N	8.85E	0.04	Notholt, Warnecke
Darwin, Australia	08/2005	12.424S	130.892E	0.03	Griffith
Garmisch, Germany	07/2007	47.476N	11.063E	0.74	Sussman
Karlsruhe, Germany	09/2009	49.100N	8.438E	0.11	Blumenstock, Hase
Lamont, USA	07/2008	36.604N	97.486W	0.32	Wennberg
Lauder, New Zealand	06/2004	45.038S	169.684E	0.37	Sherlock, Connor
Orleans, France	08/2009	47.97N	2.113E	0.13	Notholt, Warnecke
Park Falls, USA	05/2004	45.945N	90.273W	0.44	Wennberg
Sodankyla, Finland *)	01/2009	67.368N	26.633E	0.18	Kyro
Tsukuba, Japan *)	12/2008	36.0513N	140.1215E	0.03	Morino
Wollongong, Australia	05/2008	34.406S	150.879E	0.03	Griffith

*) If available

Table 1: Overview TCCON sites as planned to be used for RR (baseline, to be confirmed).

2.2 Spatio-temporal requirements for other comparisons

As explained above, the selection will likely not only been based on comparisons with TCCON but also on comparisons with other remote sensing data sets (e.g., NADCC), with models and by comparisons with the corresponding data products generated elsewhere (especially at NIES and NASA-ACOS). The spatio-temporal interval covered by this activity shall be as large as possible for this purpose (ideally global, all years) but depending on processing speed and other factors there may be limitations.

In any case, the retrieval teams shall aim at providing as much as possible information to the CRG to allow CRG to make a good decision. The larger the data set, the better. The main document for documenting the achievements in terms of data coverage and estimated quality is the “Algorithm Inter-comparison and Error Characterization & Analysis Report” (AIECAR), a key deliverable of the GHG-CCI project (version 0, i.e., AIECARv0, is due in August 2011).

In the following, a more detailed specification of “other comparisons” is not given (see AIECARv0 for details; available on the GHG-CCI website in Sept. 2011). Focus of the following is to describe in more detail the comparison with TCCON.

2.3 Figures of Merit for TCCON comparisons

Each individual satellite retrieval fulfilling the spatial and temporal collocation criteria for the TCCON comparisons shall be used for the comparison as long as it is flagged “good” (as indicated by the quality flag of the individual data product or by using pre-filtered data products delivered by the retrieval team).

The RR exercise aims at identifying the best SCIAMACHY XCO_2, SCIAMACHY XCH_4, GOSAT XCO_2, and GOSAT XCH_4 algorithm.

Several different important selection criteria (“Figures of Merit”) have been defined to characterize the performance of a given algorithm, as will be discussed below.

One can expect that different algorithms will have different strengths and weaknesses. Therefore, ideally a procedure (“benchmark formula”) would be good which combines all criteria into one single score value. This aspect has been extensively discussed within GHG-CCI. There is however consensus that at present no reliable procedure exists which guarantees the selection of the best algorithm. In addition, there are issues related to the FTS data to be used for comparisons, in particular the potentially severe limitations due to the spatial sparseness of the TCCON network. Therefore it has been decided not to define a benchmark formula now. Furthermore it has been decided to also provide the users with additional information such as maps and time series and comparisons with models and other (corresponding) data products. The GHG-CCI CRG is confident that using this information and their expert knowledge (as well as additional analysis carried out by the CRG) it is

possible to make a well justified objective decision on which algorithm to use for the ECV generation (in year 3 of the GHG-CCI project).

In **Table 2** the Figures of Merit (FoM), which have been identified, are presented.

For each FoM a threshold value is given indicating the minimum required performance (by defining a potential “rejection interval”). An algorithm and its corresponding data product is considered to be of very low quality (e.g., large bias relative to FTS) and/or hard or not to be evaluated (e.g., too few retrievals) if one or more of the FoM do not meet the corresponding minimum requirement.

In addition, auxiliary criteria (“Aux”) have been defined to provide potentially important additional information.

For each (algorithm and its corresponding) data product and for each FTS site (and for each of the 3 spatial co-location radii) and each year, a table has to be generated to provide the information described in **Table 2**.

To enable a quantitative analysis of the results, files in a to be specified format have to be generated and used (baseline: ASCII tables).

The FoM and auxiliary information will be computed by the retrieval team and by the validation team to double check the correctness of the computation and/or to check the sensitivity of the numerical values on the details of the computational method.

Note: The FoM may be computed after bias correction. If a bias correction has been applied this needs to be properly documented and this information has to be made publicly available.

GHG-CCI Round Robin Figures of Merit (FoM) for satellite – TCCON comparisons				
FoM ID	FoM	Unit	Threshold (rejection range; baseline; all numbers are to be confirmed)	Explanation
FoM_B	Bias [1)]	XCO_2: ppm XCH_4: ppb	XCO_2: > 4 XCH_4: > 40	Annual bias = Average difference Sat-FTS for entire year
FoM_B1	Bias JFM	"	"	Seasonal bias
FoM_B2	Bias AMJ	"	"	Seasonal bias
FoM_B3	Bias JAS	"	"	Seasonal bias
FoM_B4	Bias OND	"	"	Seasonal bias
FoM_SD	StdDev	"	XCO2: > 12 XCH4: > 90	Standard deviation Sat-FTS
FoM_R	Linear correlation coefficient	dimensionless	> -0.2 and < 0.2	Pearson's R (Sat., FTS)
FoM_NR	Number of sat. retrievals	dimensionless	< 10	Entire year
Aux_FA	Fraction of a-priori information	dimensionless	> 0.05	Range: 0-1. 1: data product fully determined by a-priori; 0: no influence of a-priori; Mathematical definition: TBD
Aux_PS	Processing speed (to process 1 year of data)	dimensionless (time in units of realtime)	< 1	Time needed to process 1 year of global data on the existing infrastructure; 2 means that 1 year of data requires 2 years of processing time
Aux_ND	Number of days processed	dimensionless	< 10	Number of days used for comparison for entire year

Table 2: Figures of Merit and additional auxiliary information to be used to characterize a given data product at a certain FTS site (for a certain spatial co-location radius) during a certain year.

3 Additional Constraints Algorithms (ACAs)

In this section selection criteria are presented. Within GHG-CCI several ACAs are being further developed to retrieve CO_2 and CH_4 information from AIRS, IASI, MIPAS, ACE-FTS and SCIAMACHY solar occultation measurements. The focus of GHG-CCI is on ECAs but ACAs are also being considered although with lower priority. To consider this, the ACAs are not in competition. There is no dedicated validation effort and the requirements on documentation are less demanding. Nevertheless, depending on the achieved data quality and other criteria, the GHG-CCI ECV data base, which will be established in the 3rd year of this project, may contain data products generated with ACAs in addition to the products generated with ECAs. Initial selection criteria are formulated in the following.

3.1 Overview ACAs

The following table gives a short overview about the GHG-CCI ACAs:

ACA identifier	Description
CO2_AIR_NLIS	LMD's CO_2 retrieval algorithm for AIRS delivering mid/upper tropospheric columns
CO2_IAS_NLIS	LMD's CO_2 retrieval algorithm for IASI delivering mid/upper tropospheric columns
CH4_IAS_NLIS	LMD's CH_4 retrieval algorithm for IASI delivering mid/upper tropospheric columns
CO2_ACE_CLSR	LMD's CO_2 retrieval algorithm for ACE-FTS delivering vertical profiles
CH4_MIP_IMK	KIT IMK's CH_4 retrieval algorithm for MIPAS FTS delivering vertical profiles
CH4_SCI_ONPD	IUP-Bremen's CH_4 retrieval algorithm for SCIAMACHY solar occultation FTS delivering vertical profiles

3.2 Selection criteria for ACAs

In this section the criteria are defined which need to be fulfilled if a data product generated with a certain ACA shall be part of the GHG-CCI ECV data base, which will be generated in the 3rd year of the GHG-CCI project.

The following 11 criteria need to be fulfilled for an ACA data product to become part of the GHG-CCI ECV data base:

1. The algorithm needs to be properly documented. This needs to be achieved by providing the relevant input for the different versions of the GHG-CCI Algorithm Theoretical Basis Document (ATBD, v0 (due in month 12), v1 (due in month 24) and v2 (due in month 30)).
2. The data product quality needs to be properly documented including error analysis / error characterization and (at least to some extent) validation by comparison with independent measurements. This needs to be achieved by providing the relevant input for the different versions of the GHG-CCI Algorithm Inter-comparison and Error Characterization & Analysis Report (AIECAR, v0 (due in month 12), v1 (due in month 24)).
3. The data product needs to be appropriately characterized in particular w.r.t. to altitude sensitivity and *a priori* information. Ideally, averaging kernel and *a priori* profiles shall be delivered for each individual sounding. As a minimum, this information shall be made available using a look-up-table (or equivalent), if appropriate (e.g., if variability is sufficiently small). The accompanying documentation shall be detailed enough for the data users (e.g., GHG-CCI CRG, see below) to understand how the data set has been generated and what the underlying assumptions and limitations (if any) are.
4. The data product format and content shall be described within (the current or a future version of) the GHG-CCI "Product Specification Document" (PSD) **/PSD GHG-CCI v3/** or via a stand-alone document which shall be publicly available from the GHG-CCI website.
5. The data product shall cover at least one entire year (ideally, if possible (e.g., no sensor limitations), in the time period 2009-2010 as this is the time period where also SCIAMACHY and GOSAT ECA products will be available).
6. The data product shall be delivered to the GHG-CCI Round Robin Data Package (RRDP) data base.
7. The data product needs to be under version control, i.e., a unique version number needs to be assigned to each data set delivered which uniquely defines how the data product has been generated (including all relevant input data).
8. The information made available via the documents listed above shall be detailed enough to allow traceable statements on the data quality (accuracy and precision) and the amount of data processed as well as the algorithm used to generate the data product.
9. The institution which aims at delivering its data product to the GHG-CCI ECV data base agrees to nominate a contact person who will serve as contact point for data users.
10. The institution which aims at delivering its data product to the GHG-CCI ECV data base agrees to consider (existing and possible new future) requirements related to the data product formulated by the CCI Climate Modelling User Group (CMUG), e.g., related to data formats, naming conventions, etc.
11. The GHG-CCI Climate Research Group (CRG) has no objection to add the data product to the GHG-CCI ECV data base.

4 References

/PSD GHG-CCI v1/ Product Specification Document (PSP), ESA Climate Change Initiative (CCI) GHG-CCI project, Version1/Draft3, 14 Feb 2011, available from: , http://www.esa-ghg-cci.org/sites/default/files/documents/public/documents/PSDv1_GHG-CCI_final.pdf, 2011.

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