ESA Climate Change Initiative (CCI)

Algorithm Selection Report (ASR)

for the Essential Climate Variable (ECV)

Greenhouse Gases (GHG)

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1 Overview

This document is the Algorithm Selection Report (ASR) for the GHG-CCI project (http://www.esa-ghg-cci.org/) of ESA's Climate Change Initiative (CCI). The ASR summarizes the conclusions obtained at the end of the GHG-CCI "Round Robin" (RR) exercise conducted during September 2010 – August 2012 concerning algorithm evaluation and selection.

The main purpose of the RR was to improve existing satellite CO_2 and CH_4 retrieval algorithms in order to meet the challenging GHG-CCI user requirements as specified in the GHG-CCI User Requirements Document (URD) **/URDv1/**, to use these algorithms to generate global multi-year CO_2 and CH_4 time series, to estimate the quality of the satellite retrievals, and to decide which of the (competing and not competing) algorithms to use to generate the Climate Research Data Package (CRDP) to be generated, validated and user assessed in the third year of this project (September 2012 – August 2013).

The GHG-CCI project aims at delivering the Essential Climate Variable (ECV) Greenhouse Gases (GHG) in line with the "Systematic observation requirements for satellite-based products for climate" as defined by GCOS (Global Climate Observing System): "Product A.9: Distribution of greenhouse gases, such as CO_2 and CH_4, of sufficient quality to estimate regional sources and sinks". The CRDP will essentially be the first version of the ECV GHG.

The GHG-CCI evaluation and selection approach is described in the GHG-CCI Round Robin Evaluation Protocol (RREP) **/RREPv2/**.

Within GHG-CCI two types of algorithms are distinguished, ECV Core Algorithms (ECAs) and Additional Constrains Algorithms (ACAs):

- The ECAs 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 (nadir mode) and TANSO/GOSAT (Bands 1-3). For each of these four core products two or more algorithms have been further developed in competition and quality assessed within the GHG-CCI RR. The focus of GHG-CCI are ECAs as near-surface sensitivity of the satellite data is a pre-requisite in order to generate atmospheric GHG data products containing information on regional GHG sources and sinks.
- The ACAs are algorithms for retrieving CO_2 and CH_4 information from satellite data with no or only limited near-surface sensitivity. They have the potential to deliver important additional constraints when used, for example, in an inverse

modeling framework which 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), if they are precise and accurate enough. The ACAs are applied to data from the following instruments: AIRS (mid/upper tropospheric CO_2 columns), IASI (mid/upper tropospheric CO_2 and CH_4 columns), MIPAS/ENVISAT (stratospheric CH_4 profiles), ACE-FTS (stratospheric CO_2 profiles) and SCIAMACHY/ENVISAT in solar occultation mode (stratospheric CH_4 and CO_2 profiles). For each of these products one algorithm has been further developed within GHG-CCI. However, not all ECV relevant aspects have been covered within GHG-CCI (e.g., no dedicated validation) as the focus of GHG-CCI is on the core products generated with ECAs.

An overview about all ECAs and ACAs is given in **Tables 1** and **2**.

In line with the RREP the final GHG-CCI satellite data sets as delivered to the GHG-CCI Round Robin Data Package (RRDP) data base have been independently evaluated by the GHG-CCI Validation Team (VALT) and the satellite retrieval experts of the GHG-CCI Earth Observation Science Team (EOST), in the following simply referred to as EOST:

- The independent validation has been carried out by the independent Validation Team (VALT). The analysis carried out by VALT is described in the "Product Validation and Algorithm Selection Report" (PVASR) **/PVASR/**. It is based on a comparison of the satellite retrievals (ECAs only) with ground-based observations of the Total Carbon Column Observation Network (TCCON) **/Wunch et al., 2010, 2011/**. PVASR also contains the VALT recommendations concerning ECA selection.
- The satellite retrieval experts and data providers of the GHG-CCI EOST have conducted an independent and complementary assessment of the quality of the satellite retrievals as described in the "Algorithm Inter-comparison and Error Characterization & Analysis Report" Version 1 (AIECARv1) **/AIECARv1/**. For ECAs detailed comparisons with TCCON data have been conducted but also an analysis of the global data products by analyzing global and regional maps and time series including comparisons with global models and inter-comparisons of the data sets generated with the competing algorithms. This is important to overcome limitations of the sparse TCCON network. For ACAs AIECARv1 contains a comparison of the achievements with the selection criteria for ACAs as given in the RREP. AIECARv1 also contains the EOST recommendations concerning ECA and ACA selection.

The purpose of this document is to present the final GHG-CCI RR decisions including justification on algorithm selection referring to **/PVASR/** and **/AIECARv1/** for details. The independent and complementary assessments carried out by VALT and EOST essentially resulted in the same conclusions and recommendations. The final GHG-CCI RR decisions as documented in this document have been made by involving the entire GHG-CCI team including the GHG-CCI users represented by the GHG-CCI Climate Research Group (CRG).

Algorithm ID	Algorithm short name	Data product	Institution / algorithm
CO2_SCI_BESD	BESD	XCO_2 from SCIAMACHY	IUP, Univ. Bremen, FP algorithm BESD
CO2_SCI_WFMD	WFMD	XCO_2 from SCIAMACHY	IUP, Univ. Bremen, PR algorithm WFM-DOAS
CO2_GOS_OCFP	OCFP	XCO_2 from GOSAT	Univ.Leicester (ULE), FP algorithm (OCO algorithm)
CO2_GOS_SRFP	SRFP	XCO_2 from GOSAT	SRON, FP algorithm of SRON
CH4_SCI_WFMD	WFMD	XCH_4 from SCIAMACHY	IUP, Univ. Bremen, PR algorithm WFM-DOAS
CH4_SCI_IMAP	IMAP	XCH_4 from SCIAMACHY	SRON, PR algorithm IMAP
CH4_GOS_OCPR	OCPR	XCH_4 from GOSAT	Univ.Leicester (ULE), PR algorithm (adjusted OCO algorithm)
CH4_GOS_OCFP	OCFP	XCH_4 from GOSAT	Univ.Leicester (ULE), FP algorithm (adjusted OCO algorithm)
CH4_GOS_SRPR	SRPR	XCH_4 from GOSAT	SRON, PR algorithm for GOSAT XCH_4
CH4_GOS_SRFP	SRFP	XCH_4 from GOSAT	SRON, FP algorithm for GOSAT XCH_4

Table 1: Overview GHG-CCI ECV Core Algorithms (ECAs). Two types of algorithms are distinguished: “Full Physics” (FP) and “Proxy” (PR). For details see **/ATBDv1/** and **/AIECARv1/**.

Algorithm ID	Algorithm short name	Data product	Institution / algorithm
CO2_AIR_NLIS	NLIS	CO_2 from AIRS	LMD/CNRS neuronal network mid/upper troposphere CO_2 column retrieval algorithm
CO2_IAS_NLIS	NLIS	CO_2 from IASI	LMD/CNRS neuronal network mid/upper troposphere CO_2 column retrieval algorithm
CH4_IAS_NLIS	NLIS	CH_4 from IASI	LMD/CNRS neuronal network mid/upper troposphere CH_4 column retrieval algorithm
CO2_ACE_CLSR	CLSR	CO_2 from ACE-FTS	LMD/CNRS CO_2 profile retrieval algorithm
CH4_MIP_IMK	MIMK	CH_4 from MIPAS	KIT-IMK CH_4 profile retrieval algorithm
CH4_SCI_ONPD	ONPD	CH_4 from SCIAMACHY solar occultation	IUP, Uni. Bremen, Onion Peeling DOAS CH_4 profile retrieval algorithm

Table 2: Overview GHG-CCI Additional Constraints Algorithms (ACAs). For details see **/ATBDv1/** and **/AIECARv1/**.

2 Round Robin Algorithm Selection Decisions

In this section the GHG-CCI RR algorithm selection decisions are reported referring to **/PVASR/** and **/AIECARv1/** for details.

2.1 ECV Core Algorithms (ECAs)

A detailed assessment of the various data products generated with ECAs has been carried out by the GHG-CCI VALT and EOST teams documented in the two reports **/PVASR/** and **/AIECARv1/**, which are the basis for the decisions reported in this document.

Tables 3 and **4** contain an overview about the estimated XCO_2 and XCH_4 data quality as determined by VALT and EOST using different methods (see **/PVASR/** and **/AIECARv1/** for details). As can be seen, the various methods used provide quite similar results. Differences are due to the different methods used but also for other reasons such as different time periods and different locations (e.g., use of different TCCON sites, etc.).

The overall quantitative results listed in **Tables 3** and **4** are largely based on TCCON comparisons. Because the TCCON network is sparse and the accuracy and precision is limited (~0.8 ppm for XCO_2 and ~7 ppb for XCH_4, see **/Wunch et al., 2010, 2011/ /PVASR/ /AIECARv1/**) the final GHG-CCI RR decision is not only based on the results shown in **Tables 3** and **4** but also on an analysis of the global data products as presented in **/AIECARv1/**.

In the following sub-sections, the decisions are reported, including justification, for each of the four core GHG-CCI data products.

GHG-CCI RR: Estimates of achieved data quality: XCO_2 (in ppm)					
Sensor	**Algorithm**	**Precision** **Single observation**	**Precision (*)** **Regional / monthly**	**Relative accuracy**	**Method / comments**
SCIAMACHY	BESD v01.00.01	2.5	2.4	0.7	VALT: PVASR
		2.5	NA	0.8	EOST: DP AIECAR Sect. 7.1
		2.3	1.5	0.9	EOST: EMMA AIECAR Sect. 12.5
SCIAMACHY	WFMD v2.2	4.7	3.2	1.3	VALT: PVASR
		3.8	1.6	0.8	EOST: DP AIECAR Sect. 7.2
		4.4	2.0	1.3	EOST: EMMA AIECAR Sect. 12.5
GOSAT	OCFP v3.0	2.4	2.0	0.6	VALT: PVASR
		2.7	0.2	0.8	EOST: DP AIECAR Sect. 7.3
		2.3	1.6	0.8	EOST: EMMA AIECAR Sect. 12.5
GOSAT	SRFP v1.1	2.6	1.7	1.0	VALT: PVASR
		2.6	NA	1.0	EOST: DP AIECAR Sect. 7.4
		2.5	1.0	0.9	EOST: EMMA AIECAR Sect. 12.5
SCIAMACHY and GOSAT	EMMA v1.3a	3.1	0.8	0.8	EOST: EMMA AIECAR Sect. 12.5
	Required:	< 8 (T) < 3 (B)	< 1.3 (T) < 1.0 (B)	< 0.5 (T) < 0.3 (B)	**/URD GHG-CCI v1/**

Table 3: Overview GHG-CCI estimated data quality for XCO_2. Green indicates that at least the corresponding threshold (T) requirement (see bottom row) has been met (but not necessarily the breakthrough (B) requirement). Note: the numbers largely stem from comparisons at a limited number of ground stations only and may therefore not be fully representative for the global data products. NA means “Not Assessed”. DP means “Data Provider analysis method”, see **/AIECARv1/**. EMMA refers to the “Ensemble Median Algorithm”, see below and **/AIECARv1/.** (*) The monthly regional-scale precision is difficult to estimate. The given values are therefore only very rough estimates and should not be over-interpreted. From: **/PVASR/** and **/AIECARv1/**.

GHG-CCI RR: Estimates of achieved data quality: XCH_4 (in ppb)					
Sensor	**Algorithm**	**Precision** **Single observation**	**Precision (*)** **Regional / monthly**	**Relative accuracy**	**Method / comments**
SCIAMACHY	WFMD v2.3	77 <= 2005: 30 >2005: 70	46 <= 2005: 9 >2005: 13-16	12 All years: 4-12 <= 2005: 3 >2005: 5-12	VALT: PVASR (mainly > 2005) EOST: DP AIECAR Sect. 7.5 **Req. met only for 2003-2005.**
SCIAMACHY	IMAP v6.0	51 <= 2005: 30 >2005: <50	27 <= 2005: 10 >2005: <15	15 All years: 4-13	VALT: PVASR (mainly > 2005) EOST: DP AIECAR Sect. 7.6 **Req. met only for 2003-2005.**
GOSAT	OCPR v3.2	14 14	8 1	3 3	VALT: PVASR EOST: DP AIECAR Sect. 7.7
GOSAT	OCFP v3.2	18 18	12 2	8 8	VALT: PVASR EOST: DP AIECAR Sect. 7.8
GOSAT	SRPR v1.1	15 15	8 NA	4 4	VALT: PVASR EOST: DP AIECAR Sect. 7.9
GOSAT	SRFP v1.1	15 15	9 NA	4 5	VALT: PVASR EOST: DP AIECAR Sect. 7.10
	Required:	< 34 (T) < 17 (B)	< 11 (T) < 5 (B)	< 10 (T) < 5 (B)	**/URD GHG-CCI v1/**

Table 4: Overview GHG-CCI estimated data quality for XCH_4. Green indicates that at least the corresponding threshold (T) requirement (see bottom row) has been met (but not necessarily the breakthrough (B) requirement). Note: the numbers largely stem from comparisons at a limited number of ground stations only and may therefore not be fully representative for the global data products. Note that for SCIAMACHY the comparison has been split into two time periods (2003-2005, no significant detector degradation) and after 2005 (significant detector degradation). (*) The monthly regional-scale precision is difficult to estimate. The given values are therefore only very rough estimates and should not be over-interpreted. From: **/PVASR/** and **/AIECARv1/**.

2.1.1 SCIAMACHY XCH_4

Competing algorithms:

- WFMD **/Schneising et al., 2011, 2012/**
- IMAP **/Frankenberg et al., 2011/**

Selection decision:

- Proceed with both algorithms.

Justification:

Comparison with ground-based TCCON observations revealed that both data products are very similar with respect to biases. This is also true for the estimated single measurement precisions for the time period 2003-2005, where the SCIAMACHY detector in the spectral region needed for methane retrieval did not suffer from major degradation. After 2005, the WFMD methane shows a larger scatter (~80 ppb) compared to IMAP (~50 ppb). Both data products have to be used with care for the time after 2005 due to potential bias issues related to detector degradation. Both data products show a low bias of 20-30 ppb at southern hemisphere TCCON sites which is not yet well understood. Considering only this analysis one could conclude that both data products are essentially equivalent and one may therefore select one of them, e.g., IMAP, because of the lower scatter after 2005 and because IMAP is currently the de-facto standard as IMAP has been extensively used to derive methane emissions (e.g., **/Bergamaschi et al., 2009/**) and because the IMAP product is also the SCIAMACHY methane product used by the European MACC project (http://www.gmes-atmosphere.eu/). Analysis of spatially resolved global methane distributions as generated by the two algorithms however shows significant differences, depending on region and time, which are larger than the required relative accuracy of 10 ppb, i.e., are significant for regional-scale methane surface flux inversions. Due to the lack of appropriate reference data such as TCCON it was not yet possible determine which of the two data products is the most accurate. Therefore, it has been decided to proceed with both algorithms and to contribute with both alternative data products to the CRDP pointing out the strength and weaknesses of the two approaches. Users will be encouraged to use both data sets, to determine to what extent their findings depend on the data product used, and to report these findings to the GHG-CCI retrieval experts, which will continue to further improve the data quality and on obtaining a better understanding of the differences between the two data sets.

2.1.2 GOSAT XCH_4

Competing algorithms:

- OCFP **/Parker et al., 2011/**
- OCPR **/Parker et al., 2011/**
- SRFP **/Butz et al., 2011/ /Schepers et al., 2012/**
- SRPR **/Butz et al., 2011/ /Schepers et al., 2012/**

Selection decision:

- Proceed with OCPR and SRFP.

Justification:

All data products show very similar biases and scatter when compared with ground-based TCCON observations. The number of data points is however significantly higher for the “Proxy” (PR) algorithms compared to the “Full Physics” (FP) algorithms and the agreement between the two PR data products is better than for the FP products indicating a higher level of maturity of the (simpler) PR algorithms. Note that the SCIAMACHY XCH_4 algorithms WFMD and IMAP are also PR algorithms and that the development of the FP algorithms is relatively new and still in its early stage of development. Overall, the OCPR algorithm shown a slightly better performance compared to SRPR (primarily in terms of number of data points at TCCON sites). It has therefore been decided to continue with OCPR within GHG-CCI. The PR XCH_4 algorithms depend on a CO_2 correction using model data. The long-term goal of GHG-CCI is to use a FP algorithm which is independent of a CO_2 model. The SRFP FP algorithm shows a somewhat better performance compared to the OCFP algorithm (lower station-to-station biases at TCCON sites; however also lower number of data points compared to OCFP). It has therefore been decided to continue with the SRFP algorithm.

2.1.3 SCIAMACHY XCO_2

Competing algorithms:

- WFMD **/Heymann et al., 2012/ /Schneising et al., 2011, 2012/**
- BESD **/Reuter et al., 2011/**

Selection decision:

- Proceed with BESD. Consider also proceeding with WFMD, e.g., for EMMA (**/Reuter et al., 2012/**, see below).

Justification:

BESD has higher accuracy and precision compared with WFMD. However, the BESD data set is sparse and WFMD has x3 more data points and better coverage compared to BESD. Therefore, it cannot be excluded that WFMD is better suited for certain applications. WFMD has also been used for the first ensemble product generated with EMMA. It is therefore recommended to also proceed with WFMD, but with lower priority.

2.1.4 GOSAT XCO_2

Competing algorithms:

- OCFP **/Parker et al., 2011/**
- SRFP **/Butz et al., 2011/**

Selection decision:

- Proceed with both algorithms.

Justification:

Using TCCON it was not possible to identify which of the two algorithms is better. Inter-comparison of the global data products shows differences which are larger than the required relative accuracy for XCO_2. The cause or the causes for the observed differences have not yet been identified. It has therefore been decided to continue with both algorithms until the discrepancies between the two data products have been resolved or until a “clear winner” can be identified. It has also been decided to use both data products for the ensemble product generated with EMMA (**/Reuter et al., 2012/**, see below).

2.1.5 XCO_2 ensemble product (EMMA)

As shown in **/AIECARv1/** and in **/Reuter et al., 2012/** none of the existing satellite XCO_2 retrieval algorithms currently meet the challenging relative accuracy requirement of 0.5 ppm (at present approximately 1 ppm has been achieved at TCCON sites as shown in **Table 3**). More work is therefore needed on the individual algorithms.

In order to develop a short/mid term solution GHG-CCI aims at taking advantage of the fact that several state-of-the-art retrieval algorithms and corresponding XCO_2 data products exist, i.e., an ensemble of data products which can be exploited.

All algorithms apparently have different strength and weaknesses. It has been found that all data products appear to suffer from outliers but where they appear and when depends on the algorithm. However, the different algorithms and corresponding data products appear to be sufficiently different such that, for example, the median can be used to identify outliers. This is the underlying idea of the EnseMble Median Algorithm (EMMA). EMMA aims at generating a high quality Level 2 data product based on seven state-of-the-art satellite XCO_2 Level 2 data products (the four XCO_2 algorithms of GHG-CCI (i.e., the two SCIAMACHY algorithms BESD and WFMD and the two GOSAT algorithms OCFP and SRFP) and three non-European algorithms: the two GOSAT NIES algorithms and NASA's ACOS algorithm, see **/AIECARv1/** and **/Reuter et al., 2012/**). Using this approach a first EMMA Level 2 data product has been generated and investigated **/Reuter et al., 2012/** which appears to outperform any of the currently existing individual algorithms, e.g., by elimination of outliers. In addition, EMMA shall be used to document the error estimates from the ensemble scatter. Comparison with the EMMA (median) product also permits to identify potential issues with the individual algorithms and this information can be used to improve the individual algorithms. It therefore has been decided to continue with EMMA within GHG-CCI and to add the EMMA XCO_2 data product to the GHG-CCI product portfolio.

2.2 Additional Constraints Algorithms (ACAs)

All ACAs have been assessed by establishing if the algorithms and corresponding data products and related documentation etc. meet the selection criteria as listed in the RREP. It has been found that all ACAs met these criteria (see **/AIECARv1/**). It has therefore been decided that the latest versions of all ACAs shall be used to generate data products to be added to the CRDP.

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