GHG-CCI Mid-Term Progress Report

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1. Overall Project Status

1.1 Summary of Overall Progress to date

The GHG-CCI project has significantly advanced the European capabilities in the important and relatively new area of "Greenhouse Gas" (GHG) observations from space. Major achievements are, for example, first promising GOSAT GHG retrievals including first peer-reviewed publications and extended SCIAMACHY GHG time series and improved data quality and error characterization. The GHG-CCI project is on schedule and the Round Robin (RR) exercise will be finished as initially planned end of August 2012. No major problems have been encountered.

1.2 Basic Project Data:

1.2.1 Tasks Status

Task#	Task	Start MM/YY#)	End MM/YY#)
Task 1	Requirements Analysis and Product Specification	*09/10*	*02/11*)*
Task 2	Algorithm development, inter-comparison, selection	*09/10*	*08/12*
Task 3	System proto-typing, ECV Production	*03/11*	*02/13*
Task 4	Final Product Validation & User Assessment	*03/13*	*08/13*
Task 5	System Specification	*§)*	*§)*

#) Including listed month

*) Listed is the initial time period. Task extended to 02/13 to consider future updates

§) Formally, GHG-CCI has no Task 5 to compensate for the extended (2 year) RR. Nevertheless, GHG-CCI has carried out Task 5 related activities (e.g., SRDv1.0 has been delivered on 1 Dec. 2011)

1.2.2 Deliverables status

Deliv.#	Deliverable	Date Accepted
D1.1	URD	*02/11*
D1.2	PSD	*03/12*
D1.3	DARD	*02/11*
	Uncertainty Characterization Document	*08/11*
D2.4	Round Robin Data Package	*02/12*
D2.5	Algorithm Selection Report	*08/12*
D2.6	ATBD V.1	*03/12*
D5.1	SRD	*12/11*
D5.3	SSD V1	*§)*
D3.5	Climate Research Data Package	*02/13*
D4.1	Validation Report	*05/13*
D4.2	Climate Assessment Report	*08/13*

§) GHG-CCI has no Task 5 to compensate for the extended (2 year) RR. Therefore, SSD is not a GHG-CCI deliverable.

1.2.3 Team Composition

Science Leader: M. Buchwitz, Institute of Environmental Physics (IUP), Univ. Bremen (UB), Germany
Project Manager: H. Boesch, Univ. Leicester, UK
Deputy Project Manager: M. Reuter, IUP-UB
EO Science Team (EOST): M. Buchwitz (lead), involved institutions: IUP-UB, Univ. Leicester, SRON, LMD, KIT, BIRA, Empa
Climate Research Group (CRG): F. Chevallier (lead), involved institutions: LSCE, JRC, FastOpt
System Engineering Team (SET): G. Lichtenberg (lead), involved institutions: DLR

2. Requirements Analysis and Product Specification

2.1 User Consultation

The GHG-CCI user requirements are based on GHG-CCI CRG user expertise including MACC, peer-reviewed publications and other documents, which have been generated primarily in the context of the GHG satellite missions SCIAMACHY, GOSAT, OCO and CarbonSat. They are based on dedicated Observing System Simulation Experiments (OSSE) and experience with real data (primarily SCIAMACHY). The GHG-CCI URD was favorably reviewed by the CCI CMUG. CMUG highlighted that the GHG-CCI URD could serve as a template for the other ECV projects. The most important requirements are single measurement precision, regional scale monthly precision (corresponding to a sufficiently large number of "good" observations) and relative accuracy. Whereas the precision requirements have typically been met, achieving the demanding relative accuracy requirement of better than 0.5 ppm for XCO_2 is currently the greatest remaining challenge (~1 ppm at validation sites has been achieved).

2.2 International Scientific coordination

The GHG-CCI team members are closely cooperating with many national and international institutions (e.g., NASA, NOAA, JRC, ECMWF, NIES, WMO), programmes/projects (e.g., ICOS, TRANSCOM, MACC, GCP, IGAC, iCACGP), networks (e.g., TCCON, GAW, AGAGE) and committees (e.g., COSPAR and ESA Mission Advisory Groups (MAG) such as the Sentinel 5/5-P and CarbonSat MAGs). GHG-CCI is working in close cooperation with the European GMES Atmospheric Core Service MACC (currently MACC-II). GHG-CCI is delivering data to MACC (for delayed mode assimilation) and MACC provides feedback on the data quality. GHG-CCI is also working in close cooperation with the GOSAT teams at JAXA and NIES and the NASA-ACOS team which is currently preparing for the launch of OCO-2. GHG-CCI team members are participating as session chairs and co-organizer in various international conferences (e.g., EGU, IWGGMS, COSPAR). The GHG-CCI project achievements have been presented at several major conferences such as EGU 2011 and 2012, Vienna, Planet under Pressure, London, IWGGMS-7 and 8, Edinburgh and Pasadena, and ESA ATMOS 2012, Bruges, Belgium.

2.3 ECV products description

An overview about the GHG-CCI core EVC products is given in the two tables below. These products are generated using so-called ECV Core Algorithms (ECAs). The main application is to use these products in combination with global models within an inverse modeling framework in order to obtain information on regional CO_2 and CH_4 surface fluxes (sources and sinks). During the on-going RR phase, several ECAs per product are being further developed and assessed in competition. In addition, algorithms to retrieve CO_2 and CH_4 in upper atmospheric layers, e.g., from IASI and MIPAS, are also being further developed. These algorithms are called Additional Constraints Algorithms (ACAs). The focus of the current Phase 1 of CCI are ECAs. Therefore, ACA generated products are not listed here.

ECV Product Name: XCO_2 from SCIAMACHY/ENVISAT and TANSO/GOSAT						
Parameter	**Sensors**	**Spatial coverage**	**Spatial grid**	**Temporal coverage**	**Temporal resolution**	**Total Data Volume *)**
XCO_2 in ppm	SCIAMACHY	Global (cloud free land)	Sensor pixel (typic. 30x60km²)	2003-2010	Sensor resolution (cloud free land)	~50 MB/month
XCO_2 in ppm	TANSO	Global (cloud free)	Sensor pixel (10 km pixel size, non-contiguous)	Mid 2009 - 2010	Sensor resolution (cloud free)	~20 MB/month
Explanatory text: Product: XCO_2 is the column-averaged dry air mole fraction of CO_2 Product level: Level 2 (mole fraction in ppm) Main application: Regional-scale CO_2 surface flux inverse modeling Remarks: An ensemble product using several algorithms with SCIAMACHY & GOSAT combined and/or GOSAT individually is also in preparation to be generated using the EnseMble Median Algorithm (EMMA) *) Rough estimate (depends on to be selected algorithm(s))						

ECV Product Name: XCH_4 from SCIAMACHY/ENVISAT and TANSO/GOSAT						
Parameter	**Sensors**	**Spatial coverage**	**Spatial grid**	**Temporal coverage**	**Temporal resolution**	**Total Data Volume*)**
XCH_4 in ppb	SCIAMACHY	Global (cloud free)	Sensor pixel (typic. 30x60km²)	2003-2010	Sensor resolution (cloud free)	~80 MB/month
XCH_4 in ppb	TANSO	Global (cloud free)	Sensor pixel (10 km pixel size, non-contiguous)	Mid 2009 - 2010	Sensor resolution (cloud free)	~20 MB/month
Explanatory text: Product: XCH_4 is the column-averaged dry air mole fraction of CH_4 Product level: Level 2 (mole fraction in ppb) Main application: Regional-scale CH_4 surface flux inverse modeling *) Rough estimate (depends on to be selected algorithm(s))						

3. Algorithm Development, Intercomparison and Selection

3.1 Results of Round Robin inter-comparison

The GHG-CCI Round Robin (RR) exercise is ongoing until end of August 2012. Detailed preliminary comparison results are shown in the GHG-CCI Algorithm Intercomparison and Error Characterization Report (AIECAR) available on the GHG-CCI website. The final selection will be made following the criteria as given in the GHG-CCI RR Evaluation Protocol (RREP, also available on the GHG-CCI website). Several Figures of Merit (FoM) have been defined to guide the selection. They are largely based on differences to Total Carbon Column Observing Network (TCCON) reference data. Because TCCON is sparse other information will also be used such as user expertise and additional information such as global and regional maps and time series and satellite – model comparison results. For each of the ECV Core Algorithms (ECAs) two or more competing algorithms have been further developed and used to generate the RRDP which is currently being analyzed. For the ACAs, which are not in competition, a number of criteria have been defined in the RREP which need to be fulfilled for an algorithm to be selected. The main goal of the GHG-CCI RR is to decide which algorithms to use to generate the CRDP. The final decision and its justification will be reported in a dedicated document, the Algorithm Selection Report (ASR), available beginning of September 2012.

3.2 Expected Product Improvements

The core GHG-CCI data products are near surface sensitive satellite retrievals of XCO_2 and XCH_4 from SCIAMACHY (launch 2002) and GOSAT (launch 2009). The only GHG-CCI pre-cursor products are the scientific SCIAMACHY data products which covered approximately the first 3 years of the ENVISAT mission. Within GHG-CCI these data sets have been extended (now covering more than 7 years) and improved with respect to quality (higher accuracy) and better error characterization. Within the initial phase of the GHG-CCI project the first good quality GOSAT retrievals have been generated by GHG-CCI team members as well as by non-European institutions (NIES and NASA). Although not all problems have been solved yet for all data products, this is of high benefit for the climate / inverse modeling community as these are important input data needed to better constrain GHG surface fluxes (emissions and sinks).

4. System Proto-typing and ECV Production

4.1 Data Gathering and Data Quality

Core input data are SCIAMACHY and GOSAT Level 1 files. In addition, a number of other input data sets are used such as other satellite data (e.g., IASI, MIPAS, MERIS, ACE-FTS), global model data (e.g., ECMWF, TM5, CarbonTracker). Due to problems with the initial version 7 of the SCIAMACHY Level 1 data the RR suffers to some extent from calibration issues but this problem has been reported and resolved and the already existing improved Level 1 data will be used when generating the CRDP. GHG-CCI is working in close cooperation with the SCIAMACHY Quality Working Group (team members are in both groups) and with the GOSAT calibration experts at JAXA.

4.2 Product Generation

Depending on algorithm, virtually all existing data (at least until end of 2010) have been processed or will be processed soon. The GHG-CCI CRDP will include SCIAMACHY derived products for 2003-2010 and GOSAT data for mid 2009 to 2010. The CRDP will be available in March 2013. Quality control is implemented by various measures but primarily by detailed comparisons with ground-based TCCON retrievals. During GHG-CCI the quality and amount of the data products has been significantly improved. Much longer time series exist now and they have higher accuracy as documented in several peer-reviewed publications. Despite these improvements not all requirements have been met yet. More work is needed to meet the demanding relative accuracy requirement for XCO_2. Therefore all algorithms are still being improved. Measures have been implemented towards a promising short-/mid-term solution ("EMMA", see below).

5. Product Validation and User Assessment

5.1 Product Validation (plans)

Key validation network for the validation of the GHG-CCI core data products XCO_2 and XCH_4 is the Total Carbon Column Observing Network (TCCON) as this network has been designed and developed for this purpose (initially for NASA's OCO mission). The quantities measured by TCCON can essentially be directly compared with the satellite retrievals. Unfortunately, the TCCON network is quite sparse. Therefore it is planned to also use other data (NDACC XCO_2 and XCH_4, in-situ GAW and AGAGE combined with models) for the final validation of the CRDP.

5.2 Uncertainty Characterization

Uncertainties are quantified using different complementary methods: Simulations are primarily used to quantify various sources of systematic errors and comparisons with highly accurate and precise reference data (primarily TCCON) are used to assess the quality of the real data in terms of random and systematic errors. Reliable uncertainty estimates are very important for the GHG-CCI users as they are key input parameters for assimilation and inverse modeling systems. Currently provided to the users are uncertainty estimates for each single observation quantifying primarily the random component of the total uncertainty. Users would like to get also a reliable estimate of the systematic error for each observation but this is hardly possible. The main challenge is to reliably detect and quantify systematic errors remote from TCCON validation sites, especially for XCO_2 but also for XCH_4. To deal with this GHG-CCI is currently developing the EnseMble Median Algorithm (EMMA). EMMA uses an ensemble of satellite XCO_2 retrievals. The goals of EMMA are: (i) to obtain realistic uncertainties from the ensemble scatter, (ii) to identify outliers by comparison with the ensemble median (to be used to improve the individual algorithms), and (iii) to generate a new Level 2 product based on the ensemble. Preliminary analysis indicates that EMMA outperforms each of the individual data products.

5.3 ECV Data Access and exploitation

The products are made available via the GHG-CCI website but also via dedicated websites of the participating institutions. A key exploitation issue in the context of determining the quality of the data products is the limited number of appropriate validation sites (TCCON network). A number of measures are being implemented to mitigate the impact of this (EMMA (see above), use of models, other networks). GHG-CCI closely cooperates with MACC

primarily by delivering data products to MACC and by obtaining feedback from MACC on the usefulness of the data. For example, the SCIAMACHY XCH_4 product is one of the core GHG satellite data sets currently used within MACC. In addition a large number of other (mainly scientific) users are using the GHG-CCI data products for various applications. The GHG-CCI CRG will perform a final evaluation of the CRDP in June-August 2013 after the CRDP has been validated (March-July 3013).

6. System Specification

The GHG-CCI RR phase is ongoing until end of August 2012, i.e., the final algorithm selection has not yet been made. Within GHG-CCI existing scientific processing systems have been further developed. The H/W configuration depends largely on the algorithm. For example the fast Look-up-table (LUT) based WFMD algorithm only requires a single workstation to process an entire orbit of SCIAMACHY data in a few minutes but the GOSAT XCO_2 OCFP algorithm uses a super computer with more than 1000 CPUs. Also the S/W components differ significantly (e.g., different programming languages/compiler) but essentially all teams are using UNIX systems. Input data volumes are large (official SCIAMACHY and GOSAT Level 1 products; ~400 MB/orbit) but the output volumes are quite small (Level 2, typically 20 MB/month). The priority requirements for a sustainable GHG-CCI processing system are:

1. Continuous improvements of the existing system with the goal to further enhance the accuracy of the data products and to extend the time series (a re-implementation of the complex retrieval systems is not recommended).
2. The data products need frequent re-processing also during the development phase, e.g., to determine how to optimally minimize biases caused by instrument degradation; this requires high processing power.
3. Availability of all required input data as soon as available (there is however no near-real-time need as quality has priority over speed for GHG-CCI).

7. Plan to complete Phase 1

GHG-CCI is in the final stage of the RR phase which will finish end of August 2012. The RR results and final selection will be documented in three major documents: PVASR written by the independent validation team, AIECARv1 written by the retrieval team and ASR (Algorithm Selection Report, written be the entire team but led and approved by the CRG). ASR will summarize the detailed results given in PCASR and AIECARv1 focusing on the decision results and decision justification. From September 2012 to February 2013 the CRDP will be generated using the selected algorithms. From March-Mai 2013 the CRDP will be validated (PVIR) and finally evaluated by the users (CAR).

8. General comments/feedback to ESA

GHG-CCI acknowledges the flexibility of ESA during Phase 1 especially with respect to "scientific needs" in contrast to "system specification / engineering needs". Some comments are repeated here which have been made by GHG-CCI and other ECV projects during various meetings:

- CCI Phase 1 suffers scientifically from the large number of deliverables. This significantly limits the time available for scientific exploitation of the generated data products and other important scientific activities. All ECV projects expressed their hope that this will improve in Phase 2.
- It is considered mandatory that the CCI also in future phases not only focusses on system engineering / system development aspects but on science aspects with the primary goal to

generate useful high-quality data sets as required by the climate / inverse modeling user community ("as accurate and long as possible"). The data sets must reflect the state of the art as otherwise they will not be used. This requires that CCI has to be a science driven programme also in future phases. It is important that CCI includes ECV projects which are in "science mode" rather than in "operational mode". This is particularly relevant for projects such as GHG-CCI which are generating important challenging new key ECVs from single non-operational sensors such as SCIAMACHY/ENVISAT and TANSO/GOSAT.

9. List of Relevant Scientific Publications

Butz, A., S. Guerlet, O. Hasekamp, D. Schepers, A. Galli, I. Aben, C. Frankenberg, J.-M. Hartmann, H. Tran, A. Kuze, G. Keppel-Aleks, G. Toon, D. Wunch, P. Wennberg, N. Deutscher, D. Griffith, R. Macatangay, J. Messerschmidt, J. Notholt, T. Warneke, Toward accurate CO_2 and CH_4 observations from GOSAT, *Geophys. Res. Lett.*, 38, L14812, doi:10.1029/2011GL047888. 2011.

Frankenberg, C., I. Aben, P. Bergamaschi, E. J. Dlugokencky, R. van Hees, S. Houweling, P. van der Meer, R. Snel, and P. Tol, Global column-averaged methane mixing ratios from 2003-2009 as derived from SCIAMACHY: Trends and variability, *J. Geophys. Res.*, doi:10.1029/2010JD014849, 2011.

Parker, R., H. Boesch, A. Cogan, et al., Methane Observations from the Greenhouse gases Observing SATellite: Comparison to Ground-based TCCON data and Model Calculations, *Geophys. Res. Lett.*, 38, L15807, doi:10.1029/2011GL047871, 2011.

Reuter, M., H. Bovensmann, M. Buchwitz, J. P. Burrows, B. J. Connor, N. M. Deutscher, D. W. T. Griffith, J. Heymann, G. Keppel-Aleks, J. Messerschmidt, J. Notholt, C. Petri, J. Robinson, O. Schneising, V. Sherlock, V. Velazco, T. Warneke, P. O. Wennberg, and D. Wunch, Retrieval of atmospheric CO_2 with enhanced accuracy and precision from SCIAMACHY: Validation with FTS measurements and comparison with model results, *J. Geophys. Res.*, doi:10.1029/2010JD015047, 2011.

Schneising, O., M. Buchwitz, M. Reuter, J. Heymann, H. Bovensmann, and J. P. Burrows, Long-term analysis of carbon dioxide and methane column-averaged mole fractions retrieved from SCIAMACHY, *Atmos. Chem. Phys.*, 11, 2863-2880, doi:10.5194/acp-11-2863-2011, 2011.