



**HAL**  
open science

## The Greenhouse Gas Climate Change Initiative (GHG-CCI): Comparison and quality assessment of near-surface-sensitive satellite-derived CO<sub>2</sub> and CH<sub>4</sub> global data sets

M. Buchwitz, M. Reuter, O. Schneising, H. Boesch, S. Guerlet, B. Dils, I. Aben, Raymond Armante, P. Bergamaschi, T. Blumenstock, et al.

### ► To cite this version:

M. Buchwitz, M. Reuter, O. Schneising, H. Boesch, S. Guerlet, et al.. The Greenhouse Gas Climate Change Initiative (GHG-CCI): Comparison and quality assessment of near-surface-sensitive satellite-derived CO<sub>2</sub> and CH<sub>4</sub> global data sets. *Remote Sensing of Environment*, 2015, 162, pp.344 - 362. 10.1016/j.rse.2013.04.024 . hal-01806208

**HAL Id: hal-01806208**

**<https://hal.science/hal-01806208v1>**

Submitted on 3 Nov 2020

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

1     **The Greenhouse Gas Climate Change Initiative (GHG-CCI): comparison and quality**  
2     **assessment of near-surface-sensitive satellite-derived CO<sub>2</sub> and CH<sub>4</sub> global data sets**

3  
4     *M. Buchwitz*<sup>1,\*</sup>, *M. Reuter*<sup>1</sup>, *O. Schneising*<sup>1</sup>, *H. Boesch*<sup>2</sup>, *S. Guerlet*<sup>3, #</sup>, *B. Dils*<sup>4</sup>, *I. Aben*<sup>3</sup>, *R. Armante*<sup>6</sup>, *P.*  
5     *Bergamaschi*<sup>10</sup>, *T. Blumenstock*<sup>7</sup>, *H. Bovensmann*<sup>1</sup>, *D. Brunner*<sup>8</sup>, *B. Buchmann*<sup>8</sup>, *J. P. Burrows*<sup>1</sup>, *A. Butz*<sup>7</sup>, *A.*  
6     *Chédin*<sup>6</sup>, *F. Chevallier*<sup>9</sup>, *C. D. Crevoisier*<sup>6</sup>, *N. M. Deutscher*<sup>1, 16</sup>, *C. Frankenberg*<sup>11, 20</sup>, *F. Hase*<sup>7</sup>, *O. P. Hasekamp*<sup>3</sup>,  
7     *J. Heymann*<sup>1</sup>, *T. Kaminski*<sup>12</sup>, *A. Laeng*<sup>7</sup>, *G. Lichtenberg*<sup>5</sup>, *M. De Mazière*<sup>4</sup>, *S. Noël*<sup>1</sup>, *J. Notholt*<sup>1</sup>, *J. Orphal*<sup>7</sup>, *C.*  
8     *Popp*<sup>8, §</sup>, *R. Parker*<sup>2</sup>, *M. Scholze*<sup>12, 13</sup>, *R. Sussmann*<sup>7</sup>, *G. P. Stiller*<sup>7</sup>, *T. Warneke*<sup>1</sup>, *C. Zehner*<sup>14</sup>, *A. Bril*<sup>15</sup>, *D. Crisp*<sup>11</sup>,  
9     *D. W. T. Griffith*<sup>16</sup>, *A. Kuze*<sup>17</sup>, *C. O'Dell*<sup>18</sup>, *S. Oshchepkov*<sup>15</sup>, *V. Sherlock*<sup>19</sup>, *H. Suto*<sup>17</sup>, *P. Wennberg*<sup>20</sup>, *D. Wunch*<sup>20</sup>,  
10    *T. Yokota*<sup>15</sup>, *Y. Yoshida*<sup>15</sup>

- 11  
12    1. *Institute of Environmental Physics (IUP), University of Bremen, Bremen, Germany*  
13    2. *University of Leicester, Leicester, United Kingdom.*  
14    3. *SRON Netherlands Institute for Space Research, Utrecht, Netherlands.*  
15    4. *Belgian Institute for Space Aeronomy (BIRA), Brussels, Belgium.*  
16    5. *Deutsches Zentrum für Luft- und Raumfahrt (DLR), Oberpfaffenhofen, Germany.*  
17    6. *Laboratoire de Météorologie Dynamique (LMD), Palaiseau, France.*  
18    7. *Karlsruhe Institute of Technology (KIT), Karlsruhe and Garmisch-Partenkirchen, Germany.*  
19    8. *Swiss Federal Laboratories for Materials Science and Technology (Empa), Dübendorf, Switzerland.*  
20    9. *Laboratoire des Sciences du Climate et de l'Environnement (LSCE), Gif-sur-Yvette, France.*  
21    10. *European Commission Joint Research Centre (EC-JRC), Institute for Environment and Sustainability (IES),*  
22    *Air and Climate Unit, Ispra, Italy.*  
23    11. *Jet Propulsion Laboratory (JPL), Pasadena, California, United States of America.*  
24    12. *FastOpt GmbH, Hamburg, Germany.*  
25    13. *University of Bristol, Bristol, United Kingdom.*  
26    14. *European Space Agency (ESA), ESRI, Frascati, Italy.*  
27    15. *National Institute for Environmental Studies (NIES), Tsukuba, Japan.*  
28    16. *University of Wollongong, Wollongong, Australia.*  
29    17. *Japan Aerospace Exploration Agency (JAXA), Tsukuba, Japan.*  
30    18. *Colorado State University (CSU), Fort Collins, Colorado, United States of America.*

31 *19. National Institute of Water and Atmospheric Research (NIWA), Lauder, New Zealand.*  
32 *20. California Institute of Technology, Pasadena, California, United States of America.*  
33 *#) Now at: Laboratoire de Météorologie Dynamique (LMD), Institut Pierre-Simon Laplace, Paris, France.*  
34 *§) Now at: National Museum of Natural History, Smithsonian Institution, Washington, DC, USA, and Harvard-*  
35 *Smithsonian Center for Astrophysics, Cambridge, Massachusetts, USA.*  
36  
37 *\*) Corresponding author: Michael Buchwitz, Institute of Environmental Physics (IUP), University of Bremen,*  
38 *FBI, Otto Hahn Allee 1, 28334 Bremen, Germany, Phone: +49-(0)421-218-62086, Fax: +49-(0)421-218-62070,*  
39 *E-mail: [Michael.Buchwitz@iup.physik.uni-bremen.de](mailto:Michael.Buchwitz@iup.physik.uni-bremen.de).*

## 41 **Abstract**

42 The GHG-CCI project is one of several projects of the European Space Agency's (ESA) Climate Change  
43 Initiative (CCI). The goal of the CCI is to generate and deliver data sets of various satellite-derived Essential  
44 Climate Variables (ECVs) in line with GCOS (Global Climate Observing System) requirements. The "ECV  
45 Greenhouse Gases" (ECV GHG) is the global distribution of important climate relevant gases – atmospheric CO<sub>2</sub>  
46 and CH<sub>4</sub> - with a quality sufficient to obtain information on regional CO<sub>2</sub> and CH<sub>4</sub> sources and sinks. Two  
47 satellite instruments deliver the main input data for GHG-CCI: SCIAMACHY/ENVISAT and TANSO-  
48 FTS/GOSAT. The first order priority goal of GHG-CCI is the further development of retrieval algorithms for  
49 near-surface-sensitive column-averaged dry air mole fractions of CO<sub>2</sub> and CH<sub>4</sub>, denoted XCO<sub>2</sub> and XCH<sub>4</sub>, to  
50 meet the demanding user requirements. GHG-CCI focusses on four core data products: XCO<sub>2</sub> from  
51 SCIAMACHY and TANSO and XCH<sub>4</sub> from the same two sensors. For each of the four core data products at  
52 least two candidate retrieval algorithms have been independently further developed and the corresponding data  
53 products have been quality-assessed and inter-compared. This activity is referred to as "Round Robin" (RR)  
54 activity within the CCI. The main goal of the RR was to identify for each of the four core products which  
55 algorithms should be used to generate the Climate Research Data Package (CRDP). The CRDP will essentially  
56 be the first version of the ECV GHG. This manuscript gives an overview of the GHG-CCI RR and related  
57 activities. This comprises the establishment of the user requirements, the improvement of the candidate retrieval  
58 algorithms and comparisons with ground-based observations and models. The manuscript summarizes the final  
59 RR algorithm selection decision and its justification. Comparison with ground-based Total Carbon Column

60 Observing Network (TCCON) data indicates that the “breakthrough” single measurement precision requirement  
61 has been met for SCIAMACHY and TANSO XCO<sub>2</sub> (< 3 ppm) and TANSO XCH<sub>4</sub> (< 17 ppb). The achieved  
62 relative accuracy for XCH<sub>4</sub> is 3-15 ppb for SCIAMACHY and 2-8 ppb for TANSO depending on algorithm and  
63 time period. Meeting the 0.5 ppm systematic error requirement for XCO<sub>2</sub> remains a challenge: approximately 1  
64 ppm has been achieved at the validation sites but also larger differences have been found in regions remote from  
65 TCCON. More research is needed to identify the causes for the observed differences. In this context GHG-CCI  
66 suggests taking advantage of the ensemble of existing data products, for example, via the EnseMble Median  
67 Algorithm (EMMA).

68

69 *Keywords: SCIAMACHY, GOSAT, Greenhouse gases, Carbon dioxide, Methane, Climate Change*

70

## 71 **1. Introduction**

72 Carbon dioxide (CO<sub>2</sub>) is the most important anthropogenic greenhouse gas (GHG) contributing to  
73 global warming (Solomon et al., 2007). Despite its importance, our knowledge of the CO<sub>2</sub> sources and  
74 sinks has significant gaps (e.g., Stephens et al., 2007, Canadell et al., 2010) and despite efforts to  
75 reduce CO<sub>2</sub> emissions, atmospheric CO<sub>2</sub> continues to increase at a rate of approximately 2 ppm/year  
76 (Figure 1 top panel; see also Schneising et al., 2011, and references given therein; for a detailed  
77 discussion of Fig. 1 see Sect. 4). An improved understanding of the CO<sub>2</sub> sources and sinks is needed  
78 for reliable prediction of the future climate of our planet (Solomon et al., 2007). This is also true for  
79 methane (CH<sub>4</sub>, Figure 1 bottom panel). Atmospheric methane levels increased until about the year  
80 2000, were rather stable during ~2000-2006, but started to increase again in recent years (Rigby et al.,  
81 2008, Dlugokencky et al., 2009, Schneising et al., 2011, Frankenberg et al., 2011). Unfortunately, it is  
82 not well understood why methane was stable in the years before 2007 (e.g., Simpson et al., 2012) nor  
83 why it started to increase again at a rate of approximately 7-8 ppb/year (Schneising et al., 2011).

84 Global satellite observations sensitive to near-surface CO<sub>2</sub> and CH<sub>4</sub> variations can contribute to a  
85 better understanding of the regional sources and sinks of these important greenhouse gases.

86 Information on GHG surface fluxes (emissions and uptake) can be obtained by inverse modeling of

87 surface fluxes (e.g., Chevallier et al., 2007, Bergamaschi et al., 2009), where satellite observations are  
88 compared with predictions of a (chemistry) transport model (e.g., Figure 2) and satellite minus model  
89 mismatches are minimized by modifying the surface fluxes used by the model. This requires satellite  
90 retrievals to meet challenging requirements, as small errors of the satellite-retrieved atmospheric GHG  
91 distributions may result in large errors of the inferred GHG surface fluxes (e.g., Meirink et al., 2006,  
92 Chevallier et al., 2005). Instead of direct optimization of surface fluxes it is also possible to optimize  
93 (other) model parameters used to model the fluxes, as done in Carbon Cycle Data Assimilation  
94 Systems (CCDAS) (e.g., Kaminski et al., 2010, 2012) or other approaches (e.g., Bloom et al., 2010).  
95 The goal of the GHG-CCI project is to generate the Essential Climate Variable (ECV) Greenhouse  
96 Gases (GHG) as defined by GCOS (Global Climate Observing System): “Distribution of greenhouse  
97 gases, such as CO<sub>2</sub> and CH<sub>4</sub>, of sufficient quality to estimate regional sources and sinks” (GCOS,  
98 2006). In order to get information on regional GHG sources and sinks, satellite measurements must be  
99 sensitive to near-surface GHG concentration variations. Currently only two satellite instruments  
100 deliver (or have delivered until recently) measurements which fulfill this requirement: SCIAMACHY  
101 on ENVISAT (March 2002 – April 2012) (Bovensmann et al., 1999) and TANSO-FTS on-board  
102 GOSAT (launched in January 2009) (Kuze et al., 2009). Both instruments perform (or have  
103 performed) nadir observations of reflected solar radiation in the near-infrared/short-wave-infrared  
104 (NIR/SWIR) spectral region, covering the relevant absorption bands of CO<sub>2</sub> and CH<sub>4</sub>. They also cover  
105 the O<sub>2</sub> A-band spectral region to obtain “dry-air columns” needed for computing GHG dry-air column  
106 averaged mole fractions and/or to obtain information on clouds and aerosols. These two instruments  
107 are therefore the two core sensors used by GHG-CCI and the near-surface-sensitive column-averaged  
108 dry air mole fractions of atmospheric CO<sub>2</sub> and CH<sub>4</sub>, denoted XCO<sub>2</sub> (in ppm) and XCH<sub>4</sub> (in ppb), are  
109 the core data products of GHG CCI. In addition, other sensors or viewing modes are also used (e.g.,  
110 MIPAS/ENVISAT and SCIAMACHY solar occultation mode for stratospheric CH<sub>4</sub> profiles and  
111 IASI/METOP for mid/upper tropospheric CO<sub>2</sub> and CH<sub>4</sub> columns) as they provide additional  
112 constraints for atmospheric layers above the planetary boundary layer. The focus of the first two years

113 of the GHG-CCI project (September 2010 – August 2012) was to develop existing retrieval algorithms  
114 further, in order to improve the accuracy of the retrieved GHG data products.

115 The focus of GHG-CCI lies on ECV Core Algorithms (ECAs) and their core data products XCO<sub>2</sub> and  
116 XCH<sub>4</sub>, which is also the focus of this manuscript. Other algorithms, referred to as Additional  
117 Constraints Algorithms (ACAs), are algorithms to retrieve CO<sub>2</sub> and/or CH<sub>4</sub> information from satellite  
118 data which have no or only little near surface sensitivity but are sensitive to GHG variations in upper  
119 layers (the ACAs are listed in Table 3 and further discussed in Section 6).

120 Several existing candidate ECAs were selected at the outset of the project for ongoing development,  
121 and have been iteratively improved upon through the course of the algorithm inter-comparison and  
122 validation activity. This activity is referred to as “Round Robin” (RR) exercise within the CCI.

123 The goal of the RR was to determine which ECA performs best to generate a given GHG-CCI core  
124 data product. The selected ECAs will be used in the third year of this project to generate the Climate  
125 Research Data Package (CRDP), which will essentially be the first version of the ECV GHG. The  
126 description of the RR approach and its results is the focus of this manuscript. Note that previous  
127 publications focused on individual algorithms and their data product. Only recently have results  
128 obtained using different algorithms been compared, most notably by Oshchepkov et al., 2012, for  
129 TANSO/GOSAT XCO<sub>2</sub>. This manuscript is therefore one of the first focusing on inter-comparisons.

130 This manuscript is structured as follows: Section 2 presents an overview of the GHG-CCI project  
131 followed by a description of the user requirements in Section 3. In Section 4 the retrieval algorithms  
132 are briefly described. The main part of this manuscript is Section 5 where the RR approach and its  
133 main results are presented and discussed. Section 6 provides a short overview of the Additional  
134 Constraints Algorithms (ACAs) also used within GHG-CCI but not the focus of this manuscript.  
135 Section 7 gives a short overview of the Climate Research Data Package (CRDP) to be generated using  
136 the selected algorithms. A summary and conclusions are given in Section 8.

## 137 **2. GHG-CCI project overview**

138 The GHG-CCI project covers all aspects needed to generate the ECV GHG and to assess its quality  
139 and usefulness. This includes the use of appropriate satellite instruments (primarily  
140 SCIAMACHY/ENVISAT and TANSO/GOSAT to generate global XCO<sub>2</sub> and XCH<sub>4</sub> time series),  
141 calibration aspects (related to "Level 0-1 processing", primarily for SCIAMACHY), and development  
142 and application of retrieval algorithms to convert the satellite-measured spectra into atmospheric CO<sub>2</sub>  
143 and CH<sub>4</sub> information ("Level 1-2 processing"). Also included is the analysis of the resulting global  
144 data sets, including validation and user assessments, focusing on inverse modeling of regional surface  
145 fluxes (i.e., "Level 2-4 processing"). Note that the fluxes (Level 4 products) will most likely be  
146 derived from Level 2 data rather than from (spatio-temporally averaged and potentially gap-filled)  
147 Level 3 data products, as Level 2 data contain more information than those at Level 3 and usually  
148 benefit from better error characterization.

149 Level 1 data (i.e., geolocated and calibrated radiances) are input data for CCI (i.e., Level 0-1  
150 processing is covered by other projects). SCIAMACHY Level 0-1 processing experts are part of the  
151 GHG-CCI team in order to provide expertise and to ensure that the findings of the study feed back to  
152 improve future Level 1 data products if necessary. Close links have been established with the GOSAT  
153 team at JAXA for GOSAT Level 1 data access, expertise and feedback.

154 The SCIAMACHY and TANSO Level 1 data products are de-facto used as Fundamental Climate Data  
155 Records (FCDRs, see GCOS, 2006) despite the fact that no dedicated inter-calibration or merging  
156 efforts are currently foreseen. Consistency between the time series of the two GHG-CCI core satellites  
157 is addressed at the level of the Level 2 data products. Ideally, an ECV data product or Thematic  
158 Climate Data Record (TCDR) of a given quantity should be a single merged data record obtained from  
159 all available appropriate sensors such as SCIAMACHY and TANSO for satellite-derived XCO<sub>2</sub>.  
160 However, within the present initial stage of this project only first steps in this direction have been  
161 carried out (see Section 5).

162 The ground-based validation of the "satellite-derived" XCO<sub>2</sub> and XCH<sub>4</sub> data products largely relies on  
163 the Total Carbon Column Observing Network (TCCON) (Wunch et al., 2010, 2011a) as this network

164 has been designed and developed for this purpose. Methods to also use data from other sources in the  
165 future (e.g., NDACC (see Sussmann et al., 2013), GAW) are being developed in parallel. Aircraft  
166 observations, e.g., HIPPO (e.g., Wofsy, 2011, Wecht et al., 2012), are also interesting, but have not yet  
167 been used directly (indirectly some of these data have been used via the calibration of TCCON, see  
168 Sect. 5.2.1).

169 A dedicated GHG-CCI Climate Research Group (CRG) has been set up to represent the users of the  
170 satellite-derived CO<sub>2</sub> and CH<sub>4</sub> data products and to provide expertise on inverse modeling of surface  
171 fluxes, CCDAS and other user related aspects. A strong link exists between GHG-CCI and the EU FP7  
172 GMES project MACC-II (Monitoring of Atmospheric Composition and Climate - Interim  
173 Implementation, <http://www.gmes-atmosphere.eu/>) that provides feedback on the data quality.

174 Key activities carried out in the first two years of this project were the establishment of the user  
175 requirements (Section 3), the further development of retrieval algorithms (described briefly in Section  
176 4) and data processing and data analysis with the goal of identifying which algorithms perform best  
177 (“Round Robin” (RR)). The description of these RR activities and their results is the focus of this  
178 manuscript (Section 5). In the third year of this project the selected algorithms will be used to generate  
179 the CRDP (see Section 7), which will subsequently be validated and assessed by users.

### 180 **3. User requirements**

181 An important initial activity carried out in this project was the establishment of the user requirements.  
182 They have been formulated in detail in the GHG-CCI User Requirements Document (URD) (Buchwitz  
183 et al., 2011a). The requirements are based on peer-reviewed publications primarily prepared in the  
184 context of existing or planned satellite missions and GHG-CCI CRG user expertise and experience  
185 with existing satellite data.

186 Most critical are the requirements on random and systematic errors listed in Table 1. The most  
187 challenging requirement is the one on biases for XCO<sub>2</sub>. The threshold requirement is 0.5 ppm because  
188 even errors of a few tenths of a ppm can result in large errors of the inferred CO<sub>2</sub> surface fluxes when  
189 used as input data for inverse modeling schemes (e.g., Chevallier et al., 2005). However, to what



190 extent systematic errors result in biases of the inferred fluxes depends on the spatio-temporal pattern  
191 of the systematic errors. A global bias, even if considerably larger than the required 0.5 ppm, would  
192 not be critical because it can easily be detected and corrected *ad hoc*. Most critical are state-dependent  
193 systematic errors, which result in regional-scale (~1000 km) biases on medium time scales (~  
194 monthly), because they will likely be missed by bias-correction schemes. As the overall impact of the  
195 atmospheric concentration error on the surface flux error depends on the spatio-temporal pattern of the  
196 concentration error, the values listed in Table 1 have to be interpreted with care. The requirements  
197 reflect what the GHG-CCI users would like to see achieved. The utility of the data can ultimately only  
198 be determined by careful analysis. The numbers listed in Table 1 serve to give a rough indication of the  
199 required uncertainties but should not be over-interpreted.

200 The requirements for XCH<sub>4</sub> are also challenging but somewhat less demanding than those for XCO<sub>2</sub>.  
201 The main reason is that XCH<sub>4</sub> is more variable compared to XCO<sub>2</sub> relative to its background value on  
202 the spatio-temporal scales relevant for the satellite retrievals (e.g, Frankenberg et al., 2005, 2011,  
203 Meirink et al., 2006, Bergamaschi et al., 2009, Schneising et al., 2011, 2012).

#### 204 **4. Retrieval algorithms**

205 In this section, a brief overview of each retrieval algorithm used for the GHG-CCI RR is given. The  
206 reader is referred to peer-reviewed publications for details. All algorithms used within the GHG-CCI  
207 RR are also described in the GHG-CCI Algorithm Theoretical Basis Document (ATBD) (Reuter et al.,  
208 2012a).

209 The ECV Core Algorithms (ECAs) generate one or more of the four GHG-CCI core data products,  
210 XCO<sub>2</sub> (in ppm) and XCH<sub>4</sub> (in ppb) from SCIAMACHY and TANSO (each of the four combinations is  
211 a separate product). An overview of these algorithms is given in Table 2 and briefly described in the  
212 following sub-sections. Results obtained with all ECAs are shown in Fig. 1: the top panel shows  
213 northern hemispheric (NH) time series of XCO<sub>2</sub> and the bottom panel XCH<sub>4</sub> time series. As can be  
214 seen, the various XCO<sub>2</sub> time series (generated with the various algorithms described in the following  
215 sub-sections) are similar but not exactly identical. There are clear differences, e.g., a difference of the  
216 seasonal cycle amplitude, between the two SCIAMACHY algorithms WFMD (Schneising et al., 2011,

217 Heymann et al., 2012b) and BESD (Reuter et al., 2011) likely due to sub-visual cirrus clouds not  
218 explicitly considered by WFMD. Differences are also due to the different spatial sampling of the  
219 various data products. From Figure 1 it can therefore typically not be concluded which data product is  
220 the most accurate. This requires, for example, a careful comparison with independent accurate ground-  
221 based observations (see Section 5.2). However, one obvious problem can be identified: the  
222 SCIAMACHY XCH<sub>4</sub> product generated with the IMAP algorithm (Frankenberg et al., 2011) suffers  
223 from a significant high bias (relative to several other TANSO/GOSAT XCH<sub>4</sub> data products) during the  
224 year 2010 (highlighted by the dotted line). This problem is related to SCIAMACHY detector  
225 degradation issues which are not yet properly dealt with by the SCIAMACHY radiometric calibration  
226 nor compensated by the IMAP algorithm (note that the second SCIAMACHY XCH<sub>4</sub> algorithm  
227 WFMD (Schneising et al., 2011) has not yet been applied to 2010 data; the WFMD time series covers  
228 only the years 2003-2009). As will be discussed in more detail below, the most challenging problems  
229 addressed within GHG-CCI are related to achieving the required accuracy: for XCO<sub>2</sub> this is a  
230 challenge because of demanding user requirements and for XCH<sub>4</sub> the most important challenge was to  
231 deal with the progressive SCIAMACHY detector degradation in the spectral region needed for  
232 methane retrieval which started in October 2005 (see Schneising et al., 2011, and Frankenberg et al.,  
233 2011, for a detailed discussion).

#### 234 **4.1 Full Physics (FP) and Proxy (PR) algorithms**

235 Within GHG-CCI, two types of ECAs can be distinguished: The “Full Physics” (FP) algorithms and  
236 the light path “Proxy” (PR) algorithms (see also Schepers et al., 2012).

237 FP algorithms model all relevant physical effects such as scattering by aerosols and clouds and have  
238 corresponding elements as part of the state vector, which contains all parameters which are to be  
239 retrieved. The FP algorithms obtain the dry air column-averaged mole fraction (needed to compute the  
240 dry air column-averaged mole fractions of the GHG, i.e., XCO<sub>2</sub> and/or XCH<sub>4</sub>) either from the  
241 retrieved surface pressure or using meteorological information.

242 The PR algorithms are based on computing the dry air column-averaged mole fraction using a  
243 “reference gas”, which has to be much less variable than the gas of interest on the relevant spatio-  
244 temporal scales. The PR method is used for XCH<sub>4</sub> retrieval using CO<sub>2</sub> as a reference gas. The XCH<sub>4</sub> is  
245 essentially obtained from computing the ratio of the retrieved CH<sub>4</sub> column and the retrieved CO<sub>2</sub>  
246 column. The advantage of this method is that it is potentially very fast, accurate and robust (as several  
247 systematic errors cancel in the CH<sub>4</sub>/CO<sub>2</sub> column ratio). The disadvantage is that a correction is needed  
248 for CO<sub>2</sub> variability, typically based on a global model (see, e.g., Frankenberg et al., 2005, 2011, Parker  
249 et al., 2011, Schneising et al., 2009, 2011, Schepers et al., 2012).

## 250 **4.2 SCIAMACHY XCO<sub>2</sub> algorithms**

251 The Weighting Function Modified (WFM) Differential Optical Absorption Spectroscopy (DOAS)  
252 algorithm (WFM-DOAS or WFMD) has been developed to retrieve vertical columns of several  
253 atmospheric gases including the GHGs discussed in this manuscript (Buchwitz et al., 2000). During  
254 the last decade, this algorithm has been significantly improved and used to generate global multi-year  
255 XCO<sub>2</sub> and XCH<sub>4</sub> data sets from SCIAMACHY (Buchwitz et al., 2005, 2007; Schneising et al., 2008,  
256 2009). Within GHG-CCI, WFMD has been further improved and used to generate long-term  
257 consistent time series (Schneising et al., 2011, 2012, Heymann et al., 2012a, 2012b). WFMD has been  
258 implemented as a fast look-up table (LUT) based retrieval scheme to avoid time consuming radiative  
259 transfer (RT) simulations. WFMD is a least-squares method using a single constant atmospheric prior  
260 (e.g., single constant CO<sub>2</sub> and CH<sub>4</sub> mixing ratio profiles, a single aerosol scenario, no clouds). WFMD  
261 can process one orbit of SCIAMACHY observations in a few minutes on a single workstation.  
262 Aerosols and cirrus clouds are only treated approximately by considering spectrally broad band effects  
263 by a low-order polynomial and by post-processing filtering. Overall, this results in small but  
264 significant biases, especially for XCO<sub>2</sub> (Heymann et al., 2012a). Recently, an improved version of  
265 WFMD has been developed for SCIAMACHY XCO<sub>2</sub> retrieval (Heymann et al., 2012b, see also  
266 Figure 2) and the XCO<sub>2</sub> data set generated with this latest version has been used for the GHG-CCI RR.  
267 For SCIAMACHY XCH<sub>4</sub> retrieval, the WFMD version described in Schneising et al., 2011, 2012, has  
268 been used (see below).

269 The Bremen Optimal Estimation DOAS (BESD) FP algorithm was specifically developed for accurate  
270 and precise SCIAMACHY XCO<sub>2</sub> retrieval considering aerosols and clouds thereby overcoming  
271 limitations of the WFMD algorithm (Reuter et al., 2010, 2011). In contrast to WFMD, BESD is not  
272 based on a LUT scheme but uses on-line RT model simulations. BESD is therefore computationally  
273 much more demanding. Also, unlike WFMD, BESD is based on Optimal Estimation (OE, Rodgers,  
274 2000) and aerosol and cirrus parameters are state vector elements and retrieved in addition to XCO<sub>2</sub>.

### 275 **4.3 TANSO XCO<sub>2</sub> algorithms**

276 Both GHG-CCI TANSO XCO<sub>2</sub> retrieval algorithms are FP algorithms: the University of Leicester's  
277 (UoL) OCO (Orbiting Carbon Observatory, Crisp et al., 2004) FP ("UoL-FP" or OCFP) algorithm  
278 (Cogan et al., 2012, Parker et al., 2011) and the RemoteC (or SRON Full Physics (SRFP)) algorithm  
279 (Butz et al., 2011). Both algorithms are based on adjusting parameters of a surface-atmosphere state  
280 vector and other parameters to the satellite observations, but differ in many details (different RT  
281 models, different inversion schemes (OE or Tikhonov-Phillips), different schemes for aerosol  
282 modeling and inversion, use of different pre-processing and post-processing steps, etc.) as discussed in  
283 Cogan et al., 2012, Parker et al., 2011, and Butz et al., 2011.

### 284 **4.4 SCIAMACHY XCH<sub>4</sub> algorithms**

285 For SCIAMACHY XCH<sub>4</sub> retrievals, PR algorithms are used: WFMD (Schneising et al., 2011, see  
286 above) and IMAP (Iterative Maximum A Posteriori) DOAS (Frankenberg et al., 2011). These  
287 algorithms were already well developed when GHG-CCI started but had essentially only been applied  
288 to retrieve XCH<sub>4</sub> from the first three years of the ENVISAT mission (e.g., Schneising et al., 2008).  
289 Within GHG-CCI, this time series has been significantly extended. The key challenge was (and partly  
290 still is, see Figure 1) to deal with the significant detector degradation in the spectral region needed for  
291 methane retrievals after 2005 (see Frankenberg et al., 2011, and Schneising et al., 2011, for details).

## 292 **4.5 TANSO XCH<sub>4</sub> algorithms**

293 To overcome the key limitation of the XCH<sub>4</sub> PR algorithms, namely the need to correct the retrieved  
294 XCH<sub>4</sub> for CO<sub>2</sub> variations using a model, FP algorithms are also used within GHG-CCI, but only for  
295 TANSO. TANSO has higher spectral resolution than SCIAMACHY which is exploited to also retrieve  
296 scattering parameters in addition to CH<sub>4</sub>. Two TANSO XCH<sub>4</sub> FP retrieval algorithms are being used  
297 within GHG-CCI, which are also used for TANSO XCO<sub>2</sub> retrieval (see above), OCFP (Parker et al.,  
298 2011) and SRFP (Butz et al., 2011), in addition to the two PR algorithms OCPR (Parker et al., 2011)  
299 and SRPR (Schepers et al., 2012).

## 300 **5. Round Robin approach and results**

301 In this section an overview of the GHG-CCI Round Robin (RR) activities is given which have been  
302 carried out in the first two years of this project.

### 303 **5.1 Round Robin approach**

304 The ultimate goal of the GHG-CCI RR was to identify which algorithms and corresponding data  
305 products to use for generating the CRDP. This comprised the further development of existing retrieval  
306 algorithms with the goal of meeting the challenging user requirements, the application of these  
307 algorithms to generate global multi-year XCO<sub>2</sub> and XCH<sub>4</sub> sets, the comparison with ground-based  
308 reference data and inter-comparisons of the data products generated with the competing ECAs.

309 The selection procedure for ECAs and ACAs is described in the GHG-CCI Round Robin Evaluation  
310 Protocol (RREP, Buchwitz et al., 2011b). Initially the plan was to develop a score-based selection  
311 scheme, i.e., to compute a single number for each algorithm / data product (the higher the number, the  
312 better the algorithm), mainly based on satellite – ground-based observation differences. However, this  
313 was not pursued because a scientifically sound basis for the classification could not be established.  
314 Instead a set of Figures of Merit (FoM), mostly based on differences between satellite and ground-  
315 based observations, have been defined (see RREP, Buchwitz et al., 2011b) and evaluated. However, as  
316 explained in the RREP and also shown in this manuscript, the comparison with the ground-based  
317 observations is only one component for the final selection primarily because of the sparseness of the

318 ground-based network (see Section 5.2). Another major component of the selection procedure was the  
319 analysis of (global and regional) maps and time series, including comparisons with global state-of-the-  
320 art models, and inter-comparisons of the data products generated with the different candidate  
321 algorithms. Note that “blind testing” has not been used as it would have been possible to identify the  
322 algorithms/products by using some of their characteristics such as averaging kernels and spatial  
323 coverage. Some key results of this RR activity are presented here including a summary of the main RR  
324 decision results given in Section 5.6 for ECAs and Section 6 for ACAs.

325 According to the initial ESA specification of the CCI RR exercise it was required to evaluate  
326 “algorithms”. However, complex algorithms such as the ones used within GHG-CCI can hardly be  
327 evaluated, especially not in terms of identifying “the best one” in terms of smallest biases when  
328 applied to real data. Simulated retrievals have been performed (see, e.g., Buchwitz et al., 2011c,  
329 2012a, and references given therein) but only for the individual algorithms and not in a consistent  
330 manner. This would have been a major activity incompatible with the CCI schedule especially if the  
331 goal would have been to obtain a better understanding of the differences between the data products  
332 obtained from the real observations. In this context it has not been identified that any of the algorithms  
333 suffer from obvious shortcomings. All XCO<sub>2</sub> algorithms, for example, use different approaches to  
334 mitigate biases due to scattering by aerosols and (thin) clouds, but it is virtually impossible to identify  
335 *a priori*, e.g., based on a description of the algorithms and the simulation results, which of the  
336 approaches will result in the smallest XCO<sub>2</sub> or XCH<sub>4</sub> biases when applied to real data.

337 What has been evaluated in detail are the end products, i.e., the quality of the XCO<sub>2</sub> and XCH<sub>4</sub> data  
338 products. This means that primarily data products have been evaluated during RR but not algorithms.  
339 As shown in this manuscript, this is not a trivial task, e.g., due to the sparseness of the TCCON  
340 reference data. Therefore, as shown in this manuscript, the RR decisions are not only based on  
341 comparisons with TCCON. The satellite retrieval team focused on producing the best possible end  
342 products. Which input data to use and how to treat them, e.g., in a dedicated pre-processing step, has  
343 not been prescribed. Pre-processing steps may be critical for the quality of the end product. This is  
344 particularly true if the instrument shows significant degradation as is the case for SCIAMACHY after

345 2005 especially in the spectral region needed for methane retrieval. To deal with this, quite different  
346 approaches have been used by the two algorithms IMAP (Frankenberg et al., 2011) and WFMD  
347 (Schneising et al., 2011, 2012). For example, IMAP uses as input data spectra that have been  
348 specifically calibrated at SRON and IMAP also uses a single so-called “Dead and Bad detector Pixel  
349 Mask” (DBPM), needed to reject detector pixels which are not useful. In contrast, WFMD uses the  
350 official standard SCIAMACHY Level 1 data product with standard calibration and several DBPMs,  
351 each optimized for a certain time period, typically covering one or more years (see Schneising et al.,  
352 2011, for details).

353 Finally, it is important to highlight the preliminary nature of the RR. This is due to the fact that all  
354 Level 1 input data and retrieval algorithms are continuously being improved. An algorithm / data  
355 product currently identified to be the best one will not necessarily be the best one in the future. GHG-  
356 CCI therefore needs to be flexible and will aim to consider this in future phases of the CCI.

## 357 **5.2 Comparison with ground-based (TCCON) observations**

### 358 **5.2.1 TCCON data and error characteristics**

359 The most relevant ground-based observations for the validation of the satellite-derived XCO<sub>2</sub> and  
360 XCH<sub>4</sub> data products are the corresponding data products of the TCCON. The TCCON data products  
361 have been obtained from the TCCON website ([www.tcon.caltech.edu/](http://www.tcon.caltech.edu/); latest access Feb. 2012 using  
362 version GGG2009, i.e., not the latest version GGG2012, which was not available for the GHG-CCI  
363 Round Robin comparison) or have been provided by the TCCON PIs. The TCCON products have  
364 been calibrated to WMO/GAW in situ trace gas measurement scales using aircraft observations  
365 (Wunch et al., 2010, Deutscher et al., 2010, Geibel et al., 2012, Messerschmidt et al., 2012). The best  
366 independent estimates of the TCCON inter-site comparability to date are provided by these  
367 independent aircraft calibration data. While not exhaustive, these demonstrate consistency at the 0.1%  
368 level (1-sigma) for XCO<sub>2</sub> (~0.4 ppm) and 0.2% for XCH<sub>4</sub> (~4 ppb), with no obvious inter-hemispheric  
369 differences (Wunch et al., 2010). Nevertheless, the TCCON team recognizes that inter-site  
370 comparability needs to be better characterized, especially for methane (e.g., at Darwin and  
371 Wollongong, not discussed in the references cited above), and work is in progress to achieve this. The

372 systematic and random errors of single TCCON data are therefore typically 0.4 ppm for XCO<sub>2</sub> (1-  
373 sigma) and 4 ppb (1-sigma) for XCH<sub>4</sub> (Notholt et al., 2012, based on Wunch et al., 2010). Due to these  
374 errors of the TCCON data (but also for other reasons, e.g., non-perfect spatio-temporal co-location)  
375 the estimated systematic and random errors of the satellite retrievals as reported here have to be  
376 interpreted as upper limit estimates, i.e., the satellite data errors are likely smaller than reported here.

### 377 **5.2.2 Inter-comparison method**

378 Different inter-comparison methods have been used, e.g., to ensure robustness of the findings. In  
379 addition to the method used and results obtained by the validation team (Notholt et al., 2012), which  
380 are summarized in this manuscript, independent inter-comparisons of the satellite data products with  
381 TCCON have also been carried out by the satellite data product provider (Buchwitz et al., 2012a). The  
382 methods differ by various aspects such as investigated time period and direct comparison or  
383 comparison after transformation to common *a priori* profiles and application of averaging kernels.  
384 Each satellite data product provider performed an independent validation of his data product  
385 (considering averaging kernels or not) covering the entire time series (to the extent possible given the  
386 limitations of the TCCON data, see Tab. 4). In contrast, the validation team has applied the same  
387 method to all satellite data products and has, for a given product, only used a time period where data  
388 from all competing algorithms were available (SCIAMACHY: XCO<sub>2</sub>: 2006-2009; XCH<sub>4</sub>: 2003-2009,  
389 TANSO: mid 2009-2010).

390 The method used by the validation team is based on a direct comparison of the co-located satellite and  
391 TCCON data products. No correction for different *a priori* profiles and averaging kernels has been  
392 applied. Note that it is not trivial to consider averaging kernels for the XCO<sub>2</sub> and XCH<sub>4</sub> satellite and  
393 TCCON retrievals as strictly speaking this requires a reliable estimate of the real atmospheric  
394 variability, which is unknown. This aspect is discussed in detail in Wunch et al., 2011b, where the  
395 impact of this correction for TANSO XCO<sub>2</sub> is discussed at Lamont, USA, where the real variability of  
396 the CO<sub>2</sub> profiles is obtained using regular aircraft and other observations. For the global data sets this  
397 is not possible. Nevertheless, for some of the satellite products, averaging kernels have been applied  
398 by the satellite data provider. For example, Reuter et al., 2013, has applied individual averaging



399 kernels for all XCO<sub>2</sub> products from SCIAMACHY and TANSO by adjusting all retrievals to a  
400 common *a priori* using the Simple Empirical CO<sub>2</sub> Model (SECM) described in Reuter et al., 2012b.  
401 They found that the adjustments are typically a few tenth of a ppm. Reuter et al., 2012b, estimated the  
402 smoothing errors and found that it is typically 0.17 ppm for SCIAMACHY XCO<sub>2</sub> and 0.05 ppm for  
403 TCCON XCO<sub>2</sub>. These results indicate that the impact of applying or not applying the averaging  
404 kernels for satellite – TCCON comparisons is small. The reason is that the averaging kernels of the  
405 TCCON and the satellite data are close to unity and the resulting smoothing error is therefore typically  
406 quite small, especially for XCO<sub>2</sub>. For methane the (relative) smoothing errors are somewhat larger, as  
407 methane is more variable. For example, Parker et al., 2011, found that “the mean smoothing error  
408 difference included in the GOSAT to TCCON comparisons can account for 15.7 to 17.4 ppb for the  
409 northerly sites and for 1.1 ppb at the lowest latitude site”. For the SCIAMACHY XCH<sub>4</sub> validation  
410 results presented in Schneising et al., 2012, it has been found that applying averaging kernels (by  
411 using TM5 model profiles as a common *a priori*) leads to adjustments of 0.4% (approx. 7 ppb).  
412 Overall it has been found that the validation results obtained by the validation team (Notholt et al.,  
413 2012) and the satellite data provider (Buchwitz et al., 2012a), where averaging kernels have been  
414 applied for at least some of the products, agree well, especially for XCO<sub>2</sub> (Buchwitz et al., 2012b).  
415 The comparison of the various methods used to quantify random and systematic errors of the satellite  
416 products (Buchwitz et al., 2012b) indicates that the RR validation results are robust.

417 In the following, the results obtained by the validation team are presented. Detailed results will be  
418 reported elsewhere (Dils et al., manuscript in preparation, preliminary title: “The Greenhouse Gas  
419 Climate Change Initiative (GHG-CCI): Comparative validation of SCIAMACHY and TANSO-FTS  
420 CO<sub>2</sub> and CH<sub>4</sub> retrieval algorithm products with measurements from the TCCON network”). Therefore  
421 we here give only a short overview highlighting major findings.

422 For each product and each TCCON site a number of Figures of Merit (FoMs) have been computed by  
423 the validation team. Key results are shown in Fig. 3 for XCO<sub>2</sub> and Fig. 4 for XCH<sub>4</sub>., discussed in detail  
424 in dedicated sub-sections below. Shown are comparisons of the four GHG-CCI core data products  
425 generated with two or more of the candidate algorithms at the 10 TCCON sites listed in Table 4. The

426 results shown in Figs. 3 and 4 have been generated using a spatio-temporal co-location criterion of 2  
427 hours and 500 km (for alternative co-location criteria see Notholt et al., 2012). Several numerical  
428 values are given, which are also listed in Table 5, computed from satellite minus TCCON differences  
429 for each single satellite retrieval and the corresponding TCCON mean value. On the left hand side of  
430 Figs. 3 and 4 the mean satellite-TCCON differences are shown for each of the 10 TCCON sites and all  
431 four core data products and their corresponding ECAs. For each ECA the standard deviation of the  
432 station-to-station bias has been computed (“StdDev”) and the total number of co-located satellite  
433 retrievals used for comparison (“N”). The standard deviation of the station-to-station bias is  
434 interpreted as a relevant measure of the systematic error (“relative accuracy” or “relative bias”). The  
435 standard deviation is more relevant to characterize systematic errors compared to, for example, the  
436 mean difference. Most critical is to achieve high “relative accuracy” (or low “relative bias”) not  
437 necessarily high “absolute accuracy” (although this would of course be better). For example, a  
438 constant offset of the satellite data would not be critical if the data are being used for surface flux  
439 inverse modeling (see Section 3) and this is considered by computing the standard deviation. On the  
440 right hand side of Figs. 3 and 4 the standard deviations of the satellite-TCCON differences are shown  
441 for each TCCON site. They are a measure of the random error (scatter) of the satellite retrievals. The  
442 corresponding mean value over all TCCON sites is used to characterize the mean random error (or  
443 “precision”) of the corresponding satellite data product. In the following, Figs. 3 and 4 are discussed in  
444 more detail for each of the products.

### 445 **5.2.3 Satellite XCO<sub>2</sub> comparisons with TCCON**

446 The comparison of the two SCIAMACHY XCO<sub>2</sub> retrieval algorithms WFMD and BESD with  
447 TCCON shows the following (Figure 3, top half): BESD has typically lower systematic errors (0.7  
448 ppm) compared to WFMD (1.3 ppm) and also a higher precision (2.3 ppm compared to 5.1 ppm).  
449 Ultimately it can be expected that the biases of BESD will be even lower as it has been identified (not  
450 shown) that the BESD RR data set suffers from problems related to the SCIAMACHY Level 1 data  
451 product used (version 7 consolidation level u, “L1v7u”). This data product was used because it was the  
452 latest version available when the final RR data set had to be generated and because it also covers the

453 time period after 2009. The previous Level 1 version 6 (L1v6), used by WFMD, does not suffer from  
454 these problems but is only available until the end of 2009, where the WFMD data set ends. It has been  
455 found that BESD retrievals for selected months using the improved new version L1v7w have much  
456 lower biases especially because the many outliers caused by the L1v7u spectra are not present any  
457 more (not shown). It is therefore necessary and planned to reprocess the entire SCIAMACHY data set  
458 with BESD using L1v7w, e.g., for the generation of the CRDP. A potentially important pro for  
459 WFMD for certain applications is the much larger number of data points.

460 The comparison of the two TANSO XCO<sub>2</sub> retrieval algorithms OCFP and SRFP with TCCON shows  
461 the following (Figure 3, bottom half): The biases depend on site and are typically in the range +/- 1  
462 ppm. They are very similar for both algorithms. This is also true for the standard deviation of the  
463 difference between the TANSO and TCCON estimates, which is typically in the range 2-3 ppm. The  
464 number of co-locations is also nearly identical for both algorithms but varies significantly from site to  
465 site, which is true for all comparisons shown in Figs. 3 and 4.

466 As shown in Table 5, the precision requirement for XCO<sub>2</sub> is met by all algorithms. WFMD meets the  
467 threshold requirement and the other algorithms including BESD even meet the breakthrough  
468 requirement. The challenging 0.5 ppm bias requirement has however not yet been met but several  
469 algorithms achieve a performance close to the threshold requirement (0.6-0.9 ppm, depending on  
470 algorithm).

#### 471 **5.2.4 Satellite XCH<sub>4</sub> comparisons with TCCON**

472 The comparison of the two SCIAMACHY XCH<sub>4</sub> retrieval algorithms WFMD and IMAP with  
473 TCCON shows the following (Figure 4, top half): Overall, the systematic differences with respect to  
474 TCCON vary from site to site from nearly 0 ppb at Lamont to 20-30 ppb at the southern hemisphere  
475 (SH) sites Darwin, Wollongong, and Lauder, but are very similar for WFMD and IMAP. The reason  
476 for the large differences at these SH sites have not yet been identified. This is probably not due to the  
477 TCCON reference data as these differences are larger than the estimated TCCON inter-site  
478 comparability (see Sect. 5.2.1) and also the comparison with TANSO XCH<sub>4</sub> (see below) does not  
479 show this type of systematic deviation (the OCFP results however also show a low bias at the SH sites

480 compared to the northern sites esp. at Darwin). Agreement is within +/- 10 ppb if these SH sites are  
481 excluded. In order to obtain an estimate of the relative biases (i.e., considering that an overall offset is  
482 not critical), the standard deviation of the station-to-station biases has been computed: it amounts to 11  
483 ppb for WFMD and 15 ppb for IMAP. The standard deviation of the satellite-TCCON differences,  
484 which is a measure of the single measurement precision (1-sigma), is on average 82 ppb for WFMD  
485 and 50 ppb for IMAP. Because nearly all TCCON sites started operation after 2005 (see Table 4), i.e.,  
486 after the loss of important SCIAMACHY methane detector pixels due to detector degradation, the  
487 values listed for SCIAMACHY in Figure 4 are not representative for the years 2003-2005. Until the  
488 end of 2005 the performance was much better and the corresponding values are listed in curved  
489 brackets in Table 5. A possible explanation for the larger scatter (worse precision) of WFMD after  
490 2005 is that WFMD is an unconstrained least-squares algorithm whereas IMAP is based on Optimal  
491 Estimation and uses detailed CH<sub>4</sub> information (as a function of latitude, altitude and time but not  
492 longitude) from a global model as *a priori* information. This raises the question why the precision of  
493 the two data products is similar for 2003-2005. This could be related to the fact that only a single  
494 DBPM is used by IMAP whereas WFMD has used a DBPM optimized for 2003-2005. Another  
495 possible explanation could be the use of differently calibrated input data. As shown in Fig. 4, the  
496 number of satellite soundings used varies significantly from site to site, but overall is very similar for  
497 WFMD (N=37628) and IMAP (39489) (at least at TCCON sites, for other locations this may not be  
498 true, see Figures 9 and 10).

499 The comparison of the four TANSO XCH<sub>4</sub> retrieval algorithms (OCPR, OCFP, SRPR, SRFP) with  
500 TCCON shows the following (Figure 4, bottom half): The biases depend on the TCCON site but are in  
501 the range +/- 15 ppb. The estimated relative bias is best for OCPR (2 ppb) and worst for OCFP (8  
502 ppb). OCPR has the largest number of data points (followed by SRPR). The number of data points is  
503 higher for the PR algorithms (OCPR and SRPR) compared to the FP algorithms (OCFP and SRFP).  
504 The FP algorithm with the lowest relative bias is SRFP (3 ppb). The PR algorithm with the lowest  
505 relative bias is OCPR (2 ppb). The standard deviation of the satellite – TCCON differences are nearly  
506 identical for all four algorithms.

507 As shown in Table 5, the SCIAMACHY XCH<sub>4</sub> product for 2003-2005 meets the threshold precision  
508 requirement (but not for 2006 and later years due to the detector degradation). In contrast, the TANSO  
509 XCH<sub>4</sub> has a much higher precision and even the breakthrough precision requirement is met by all  
510 algorithms. All TANSO XCH<sub>4</sub> algorithms meet the relative accuracy (relative bias) user requirement -  
511 some are close to or even better than the goal requirement. For SCIAMACHY this is only true for  
512 2003-2005.

513 Concerning the final RR algorithm selection decision, it is important not to over-interpret the  
514 numerical values listed in Table 5 due to the sparseness of the TCCON sites. For this and other  
515 reasons, the TCCON comparisons presented and discussed in this section are only one key component  
516 of the GHG-CCI RR activities. Therefore, more comparisons have been conducted, for XCO<sub>2</sub> and  
517 XCH<sub>4</sub>, as described in the following.

### 518 **5.3 Inter-comparison of XCO<sub>2</sub> data products**

519 Within GHG-CCI two algorithms have been further developed to retrieve XCO<sub>2</sub> from SCIAMACHY,  
520 namely WFMD and BESD, and two algorithms to retrieve XCO<sub>2</sub> from TANSO, namely OCFP and  
521 SRFP. In addition, there are three non-European TANSO algorithms presented and discussed in the  
522 peer-reviewed literature whose data products have also been used for comparison: (i) the official  
523 operational TANSO algorithm (v02.xx) developed at the National Institute for Environmental Studies  
524 (NIES) in Japan (Yoshida et al., 2011; in the following referred to as “NIES” algorithm), (ii) a  
525 scientific algorithm called PPDF (Pathlength Probability Density Function) also developed at NIES  
526 (Bril et al., 2007, Oshchepkov et al., 2008, 2009, 2011, 2012), and (iii) NASA/JPL’s ACOS  
527 (Atmospheric CO<sub>2</sub> Observations from Space) v2.9 algorithm (O’Dell et al., 2012, Crisp et al., 2012).

528 The global XCO<sub>2</sub> data products from all 7 algorithms have been inter-compared within GHG-CCI  
529 (Reuter et al. 2013, Buchwitz et al., 2012a). The analysis revealed the following: The various satellite  
530 XCO<sub>2</sub> data products all capture the expected large scale variations of atmospheric CO<sub>2</sub> such as the  
531 time dependent north-south gradient (Figures 5 and 6, discussed below) and the CO<sub>2</sub> increase and  
532 seasonal cycle (Figure 1) but exhibit differences in the spatio-temporal pattern which – depending on  
533 region and time – may exceed the relative bias user requirement of 0.5 ppm.

534 Typical examples are shown in Figures 5 and 6. Figure 5 shows comparisons of the four GHG-CCI  
535 XCO<sub>2</sub> algorithms (BESD, WFMD, SRFP, OCFP). Figure 6 shows the GHG-CCI algorithms as well as  
536 the three non-European algorithms mentioned above (ACOS (v2.9), PPDF (NIES PPDF-D), and NIES  
537 (v02.xx)) for the two months September 2009 and May 2010. Also shown is the ensemble data  
538 product generated with the Ensemble Median Algorithm (EMMA) algorithm, discussed below,  
539 TCCON XCO<sub>2</sub>, and XCO<sub>2</sub> from NOAA's CO<sub>2</sub> assimilation system CarbonTracker (CT) (Peters et al.,  
540 2007). As can be seen, all satellite retrieval algorithms capture the north-south XCO<sub>2</sub> gradient, which  
541 is significantly different for the two months shown, in good to reasonable agreement with TCCON and  
542 CarbonTracker (Figure 6). As can also be seen, differences between the data products often exceed 0.5  
543 ppm, particularly at locations remote from TCCON sites (e.g., Sahara, South America, Africa). As  
544 discussed in Section 5.2, it appears virtually impossible to use TCCON to determine which algorithm  
545 performs best, at least for TANSO. For SCIAMACHY it has been shown that BESD outperforms  
546 WFMD in terms of single measurement precision and bias not however in terms of number of  
547 observations, which is significantly higher for WFMD. It is also likely that a "best data product" for  
548 all conditions does not exist at present as each retrieval algorithm is expected to have its strengths and  
549 weaknesses. Therefore, which algorithm performs best may depend on the spatio-temporal interval of  
550 interest. Clearly, more research is needed to understand the differences between the various XCO<sub>2</sub> data  
551 sets shown in Figures 5 and 6. One approach to further assess the relative quality of the various  
552 satellite-derived global XCO<sub>2</sub> data sets is to compare them with their median. This approach is  
553 presented in the following section.

### 554 **5.3.1 Comparison with ensemble median (EMMA)**

555 In this section we aim at answering two related questions: (i) How to determine which data product is  
556 likely "the best", if the largest differences are at locations remote from validation sites? (ii) Which data  
557 product should be used for inverse modeling of surface fluxes if all products differ and if it is not clear  
558 which product would give the most reliable results? To answer these questions we use the median of  
559 the various XCO<sub>2</sub> products. The situation appears to be similar to that for climate modeling: it is not  
560 clear which "model" is the best and (remote from validation sites) there is no truth to compare with. A

561 promising approach to deal with this is to make use of the fact that several state-of-the-art algorithms  
562 and corresponding XCO<sub>2</sub> data products are available, i.e., an ensemble of data products, which can be  
563 exploited. This is the underlying idea of the Ensemble Median Algorithm (EMMA, Reuter et al.,  
564 2013). As described in more detail below and in Reuter et al., 2013, EMMA computes the median of  
565 an ensemble of individual XCO<sub>2</sub> data products, which can be used for comparison with the individual  
566 data products, e.g., to identify outliers. However, the EMMA XCO<sub>2</sub> product has also been generated to  
567 be useful as a stand-alone XCO<sub>2</sub> data product for inverse modeling and other applications.

568 The strength of using an ensemble of satellite data products was highlighted at the end of the first year  
569 of the GHG-CCI project (Buchwitz et al., 2011c), when biases (0.5%) between Bialystok TCCON  
570 XCO<sub>2</sub> and co-incident satellite data were identified in the majority of algorithms participating in the  
571 GHG-CCI. This bias occurred due to an empirical correction of known magnitude, to account for a  
572 laser-sampling bias in the FTS data before September 21, 2009, inadvertently being applied in the  
573 wrong direction. A bias in XCH<sub>4</sub> in the early part of the Bialystok time series that occurred due to  
574 missing fits in one of the CH<sub>4</sub> micro-windows was also brought to light by comparisons to the  
575 ensemble of satellite retrievals. The identification and quantification of these biases would most likely  
576 not have been possible with a single algorithm / data product, due to difficulty in proving that such  
577 relatively small differences are not due to possible retrieval algorithm issues.

578 A detailed description of EMMA is presented in Reuter et al., 2013. Therefore here only a short  
579 overview is given. The presented version of EMMA (v1.3a) uses the 7 individual satellite XCO<sub>2</sub>  
580 products shown in Figs. 6 and 7 and generates a Level 2 product (i.e., a product containing the XCO<sub>2</sub>  
581 of the individual satellite soundings including uncertainty estimate and other information such as  
582 averaging kernels) using the median in each 10°x10° monthly grid cell (“voxel”). In short, EMMA  
583 works as follows: For each voxel, the mean XCO<sub>2</sub> value is computed for each of the 7 individual data  
584 products. The median of the 7 mean values determines which of the individual satellite Level 2 data  
585 products is used for the EMMA data product for that voxel (if a certain voxel is not covered by all 7  
586 data products, a smaller number of data products is used). Using the median has several advantages  
587 compared to, for example, using the mean value. A key aspect is that the median is robust with respect

588 to outliers. Using the median essentially removes outliers. This is of critical importance as each of the  
589 individual data products appears to suffer from outliers but where they appear and when is not known  
590 *a priori* and depends on the algorithm. Of at least equal importance is that the GHG-CCI users need a  
591 Level 2 data product (individual soundings) and not a Level 3 data product (e.g., gridded monthly  
592 averages). Furthermore, the use of an ensemble of data products possibly permits the generation of  
593 more reliable uncertainty estimates, obtained from a combination of the ensemble scatter and the  
594 reported uncertainties of the individual algorithms (which are primarily estimates of the random  
595 uncertainty). This would in particular be important to get a handle on the systematic error component  
596 of the uncertainty, which is very difficult (if not impossible) to reliably quantify for each algorithm  
597 individually. For an ensemble, this would strictly speaking require that the median is bias free which is  
598 unlikely to be the case. Nevertheless, the spatio-temporal intervals where the various data products  
599 disagree are very likely intervals where the data products need to be used with care. In any case,  
600 reliable XCO<sub>2</sub> error estimates of the satellite retrievals are of critical importance for the user of the  
601 GHG-CCI atmospheric data products.

602 Figures such as Figure 6 also permits the determination of which of the data sets agree and which  
603 disagree. For example, the EMMA product, but also most of the individual TANSO products and  
604 SCIAMACHY/BESD, agree well or at least reasonably with each other as well as with TCCON and  
605 CarbonTracker (see green and yellow smileys), whereas this is not always true for the two very fast  
606 algorithms WFMD and PPDF (see red smileys). Figure 7 shows pie charts indicating the overall  
607 agreement and disagreement of each of the individual algorithms with the median. The results are  
608 consistent with the already reported findings, e.g., better performance of BESD compared to WFMD  
609 and similar performance of the TANSO XCO<sub>2</sub> algorithms.

610 A large number of other comparisons of the individual data products and the EMMA product with  
611 TCCON but also with CarbonTracker have been carried out. Figure 8 shows, as an example, a  
612 comparison of the amplitude of the XCO<sub>2</sub> seasonal cycle. As can be seen, all satellite data shown  
613 suggest that the seasonal cycle is underestimated by CarbonTracker by ~1.5 +/- 0.5 ppm peak-to-peak.  
614 Using only a single data product it would be difficult to “prove” that such a relatively small difference



615 (~0.3% of the total column) is significant and not caused by or at least significantly influenced by  
616 retrieval issues (see, e.g., the discussion given in Schneising et al., 2011, on this topic). Using an  
617 ensemble of data products based on more than one satellite and using several essentially independent  
618 algorithms allows one to draw more confident conclusions with respect to the interpretation of satellite  
619 – model XCO<sub>2</sub> differences than would be possible using a single data product only. Within GHG-CCI  
620 it is therefore planned to continue the efforts on EMMA in addition to further developing the  
621 individual algorithms.

#### 622 **5.4 Inter-comparison of SCIAMACHY XCH<sub>4</sub> data products**

623 The multi-year global retrievals obtained from the two SCIAMACHY XCH<sub>4</sub> algorithms, WFMD and  
624 IMAP, have been compared with one another. Figure 9 shows, as a typical example, a comparison of  
625 one month (August 2005) of the global WFMD and IMAP data products (Figure 10 shows the  
626 corresponding results for July 2009; results for other months are shown in Buchwitz et al., 2012a). As  
627 can be seen, the monthly XCH<sub>4</sub> maps generated with the two algorithms show – depending on region -  
628 similar but also significantly different patterns. Both maps show higher methane concentrations over  
629 the Northern Hemisphere (NH), where most of the methane sources are located, compared to the  
630 Southern Hemisphere (SH). Both data sets agree reasonably well (within typically +/- 10 ppb) over  
631 most parts of the SH land areas but over some areas WFMD XCH<sub>4</sub> can be up to approximately 20 ppb  
632 higher. Over the NH the situation appears to be more complex. Both data sets show elevated methane  
633 over large parts of China, south-east Asia and India, but the patterns are not identical, with WFMD  
634 being higher over south-east Asia and lower over parts of India compared to IMAP. WFMD and  
635 IMAP not only use differently calibrated input data (standard versus non-standard calibration) and  
636 different retrieval methods (least squares versus OE), but also different post-processing quality  
637 filtering schemes. The latter is reflected by differences in spatial coverage (e.g., WFMD methane is  
638 not restricted to land observations only) and number of retrievals over a given region (see right hand  
639 side panels of Figure 9). The data density differs significantly depending on region. Typically WFMD  
640 has many more data points over the Sahara and other areas in the ~10°-40°N latitude range but also  
641 over mid/northern Australia and the mid/western part of the US, whereas IMAP has higher data

642 density over South America and mid/high northern latitudes. Large differences between the two data  
643 sets are also visible over large parts of northern Africa, where IMAP methane is higher (by approx. 40  
644 ppb) and Greenland, where WFMD methane is higher (by approx. 40 ppb). The reasons for the  
645 differences have not yet been identified. It has also not yet been assessed to what extent inferred  
646 regional methane fluxes would differ depending on which data set is used as input data for inverse  
647 modeling of regional methane fluxes. Significant differences can be expected as the regional  
648 differences exceed the bias threshold requirement of less than 10 ppb. The discussion also shows that  
649 depending on region the differences can be significantly larger than the estimated biases listed in Table  
650 5, which are based on the analysis of the satellite data at TCCON sites only. Clearly, more research is  
651 needed to understand the differences between the two SCIAMACHY methane data sets discussed in  
652 this section.

### 653 **5.5 Inter-comparison of TANSO XCH<sub>4</sub> data products**

654 Within GHG-CCI, four TANSO XCH<sub>4</sub> retrieval algorithms have been further developed and used to  
655 generate global data sets which have been inter-compared and compared with TCCON retrievals and  
656 global model data (Buchwitz et al., 2012a). The four retrieval algorithms are the FP and PR algorithms  
657 developed by SRON (SRFP, SRPR) and Univ. Leicester (UoL; OCFP and OCPR algorithms).

658 For the PR algorithms, which are based on the retrieval of ratios of the CH<sub>4</sub> to CO<sub>2</sub> columns, followed  
659 by a model-based CO<sub>2</sub> correction to compute XCH<sub>4</sub>, the column ratios have been compared as well as  
660 the final XCH<sub>4</sub> product. As expected, it has been found that the agreement between the ratios is  
661 typically somewhat better compared to the XCH<sub>4</sub> products due to differences between the model-based  
662 CO<sub>2</sub> correction as used by SRON and UoL (see Buchwitz et al., 2012a, for details). Overall and in line  
663 with the discussion presented in Section 5.2, it has been found that the two PR products agree nearly  
664 equally well with the TCCON ground-based observations. A direct comparison of the two data  
665 products at TCCON sites is also shown in Figure 11 indicating agreement within typically 10 ppb (1-  
666 sigma). Nevertheless, inspection of global maps also reveals significant differences, depending on  
667 region and time. Qualitatively, this is similar to the results found for the SCIAMACHY data sets  
668 discussed in the previous section, but the differences shown in Figure 11 for TANSO are significantly

669 smaller compared to the differences for SCIAMACHY shown in Figures 9 and 10. Figure 11 shows a  
670 global OCFP-SRFP methane difference map for July 2009. As can be seen, the differences may  
671 exceed 5 ppb (breakthrough requirement) or even 10 ppb (threshold requirement) over certain  
672 extended regions such as India. Comparisons between the two FP TANSO XCH<sub>4</sub> data products OCFP  
673 and SRFP have also been carried out. Using SRFP, two years of global TANSO data have been  
674 retrieved but the comparison had to be limited to TCCON sites only because of limitations of the  
675 OCFP data set which is not yet available globally. It has been found that the inter-station bias is  
676 smaller for SRFP (~4 ppb) compared to OCFP (~8 ppb) and that the scatter of the SRFP data is  
677 somewhat smaller compared to the OCFP (14 ppb versus 16 ppb). These findings are consistent with  
678 the results presented in Table 5 but have been derived independently (see Buchwitz et al., 2012a). It  
679 has also been found that the agreement between the two PR algorithms is significantly better than the  
680 agreement between the two FP algorithms. This may be due to the fact that PR algorithms are simpler  
681 but may also indicate that at the current stage of development the PR algorithms are more mature (note  
682 that they also deliver much more data points, see Section 5.2).

## 683 **5.6 Algorithm selection results**

684 The main goal of the RR exercise was to determine which satellite retrieval algorithms to use to  
685 generate the CRDP. Based on the results presented and discussed in the previous sections, algorithms  
686 have been selected. The selection results are presented in the following sub-sections.

### 687 **5.6.1 Selection results: SCIAMACHY and GOSAT XCO<sub>2</sub>**

688 Within GHG-CCI, two SCIAMACHY and two TANSO XCO<sub>2</sub> algorithms have been further  
689 developed and the corresponding data products have been inter-compared. They have also been  
690 compared with three other TANSO XCO<sub>2</sub> data products generated outside of this project: with the two  
691 TANSO XCO<sub>2</sub> products generated at NIES, Japan, (i.e., the operational TANSO product (Yoshida et  
692 al., 2011) and the scientific PPDF product (Oshchepkov et al., 2011)) and with the NASA ACOS team  
693 product (O'Dell et al., 2012, Crisp et al., 2012). Analysis of all seven products indicates that the  
694 precision requirement has been met, but not the very demanding bias requirement of less than 0.5 ppm

695 (approximately 1 ppm has been achieved at TCCON sites). Clearly, more work on the individual  
696 retrieval algorithms is required to achieve this goal and it has been decided to continue with all  
697 algorithms. A possible exception is the fast SCIAMACHY XCO<sub>2</sub> WFMD algorithm, which shows a  
698 reduced data quality in terms of precision and biases compared to the computationally much more  
699 demanding BESD algorithm. On the other hand the WFMD product has significantly (3-4 times) more  
700 data points compared to BESD and therefore much better coverage compared to any of the other data  
701 products including BESD. GHG-CCI aims at taking advantage of the fact that an ensemble of state-of-  
702 the-art data products exists which can be exploited. To this end, the EnSEmble Median Algorithm  
703 (EMMA) has been developed (Reuter et al., 2013). EMMA generates a Level 2 XCO<sub>2</sub> product using  
704 the median of the individual data products thereby largely eliminating outliers of the data products  
705 generated with the individual algorithms. EMMA may also improve the error characterization using  
706 the ensemble scatter. Preliminary analysis indicates that EMMA outperforms each of the individual  
707 algorithms. EMMA also permits the identification of potential weaknesses of the individual  
708 algorithms, which can be used to improve the individual algorithms. Taking this into account, it has  
709 been decided to proceed with all satellite XCO<sub>2</sub> algorithms and to add the EMMA data product to the  
710 GHG-CCI product portfolio.

#### 711 **5.6.2 Selection results: SCIAMACHY XCH<sub>4</sub>**

712 Data products generated with two algorithms have been assessed: WFMD (Schneising et al., 2011,  
713 2012) and IMAP (Frankenberg et al., 2011). Comparison with ground-based TCCON observations  
714 revealed that both data products are very similar with respect to biases. This is also true for the  
715 estimated single measurement precisions for the time period 2003-2005, when the SCIAMACHY  
716 detector did not yet suffer from major degradation in the spectral region needed for methane retrieval.  
717 After 2005, the WFMD methane shows a larger scatter (~80 ppb) compared to IMAP (~50 ppb). Both  
718 data products have to be used with care for the time after 2005 due to potential bias issues related to  
719 detector degradation as indicated by the TCCON comparison at southern hemisphere TCCON sites,  
720 where both data products show a low bias of 20-30 ppb depending on FTS site. Considering only this

721 analysis, one would conclude that both data products are essentially equivalent and one may therefore  
722 select one of them. Analysis of spatially resolved global methane distributions as generated by the two  
723 algorithms however shows significant differences, depending on region and time, which are larger  
724 than the required maximum bias of 10 ppb, i.e., are significant for regional-scale methane surface flux  
725 inversions. Due to the lack of appropriate reference data such as TCCON, it was not yet possible to  
726 determine which of the two data products is the most accurate. Therefore, it has been decided to  
727 proceed with both algorithms and to contribute with both alternative data products to the CRDP  
728 pointing out the strength and weaknesses of the two approaches. Users will be encouraged to use both  
729 data sets, to determine to what extent their findings depend on the data product used, and to report  
730 these findings to the GHG-CCI retrieval experts.

### 731 **5.6.3 Selection results: TANSO XCH<sub>4</sub>**

732 Four algorithms and their corresponding data products have been evaluated: OCFP and OCPR (Parker  
733 et al., 2011) and SRFP and SRPR (Butz et al., 2011). All data products show very similar biases and  
734 scatter when compared with ground-based TCCON observations. The number of data points is  
735 however significantly higher for the “Proxy” (PR) algorithms compared to the “Full Physics” (FP)  
736 algorithms and the agreement between the two PR data products is better than for the FP products,  
737 indicating a higher level of maturity of the (simpler) PR algorithms. Note that the SCIAMACHY  
738 XCH<sub>4</sub> algorithms, WFMD and IMAP, are also PR algorithms and that the FP algorithms are relatively  
739 new and currently in their early stages of development. Overall, the OCPR algorithm shows a slightly  
740 better performance compared to SRPR (primarily in terms of number of data points at TCCON sites).  
741 It has therefore been decided to continue with OCPR within GHG-CCI. The PR XCH<sub>4</sub> algorithms  
742 depend on a CO<sub>2</sub> correction using model data. The long-term goal of GHG-CCI is to use a FP  
743 algorithm that is independent of a CO<sub>2</sub> model. Because the SRFP algorithm shows a somewhat better  
744 performance compared to the OCFP algorithm (e.g., lower station-to-station biases at TCCON  
745 sites), it has been decided to continue with the SRFP algorithm, despite the lower number of data  
746 points compared to OCFP. In summary, four TANSO XCH<sub>4</sub> algorithms have been evaluated as part of

747 the GHG-CCI RR and two of these algorithms have been selected for further use within GHG-CCI:  
748 OCPR and SRFP.

## 749 **6. Additional Constraints Algorithms (ACAs)**

750 The Additional Constraints Algorithms (ACAs) are algorithms to retrieve CO<sub>2</sub> and/or CH<sub>4</sub> information  
751 for layers above the planetary boundary layer. ACAs are applied to several satellite instruments. An  
752 overview of the ACAs used within GHG-CCI is given in Table 3. As the ACAs are not the focus of  
753 this manuscript the reader is referred to the references listed in Table 3 (including caption) for details  
754 on each of these algorithms and corresponding data products.

755 For ACAs only one algorithm per data product has been considered within GHG-CCI, i.e., ACAs are  
756 also being further developed but not in competition and not by covering all aspects (e.g., no dedicated  
757 validation). For ACAs a number of criteria have been defined which need to be fulfilled to contribute  
758 to the CRDP but detailed user requirements have not been formulated.

759 Only a limited assessment of the data products generated with ACAs has been conducted during the  
760 initial phase of GHG-CCI described in this manuscript because the focus was on ECAs. However, for  
761 each of the ACAs listed in Table 3 it has been determined if the selection criteria specified in the  
762 Round Robin Evaluation Procedure (RREP, Buchwitz et al., 2011b) have been met. The RREP defines  
763 11 criteria for ACAs which need to be fulfilled for a given ACA to contribute to the CRDP. The  
764 criteria are mostly qualitative and refer to a required minimum level of documentation, error analysis  
765 and related auxiliary information. All ACA products are potentially useful for GHG-CCI climate  
766 applications as they deliver additional information on CO<sub>2</sub> and/or CH<sub>4</sub> thereby providing potentially  
767 important constraints when used, for example, within an appropriate inverse modeling framework to  
768 derive regional surface fluxes from the satellite observations. However, no detailed user requirements  
769 are currently available, no dedicated validation has been performed within GHG-CCI and it has also  
770 not been assessed to what extent the existing products are useful or not useful for GHG surface flux  
771 inverse modeling. More research is needed to assess the usefulness of these data products for climate

772 relevant applications. It has been identified that all ACAs fulfill the requirements listed in the RREP  
773 and that all ACA products can therefore be included in the CRDP.

## 774 **7. Climate Research Data Package (CRDP)**

775 The goal of the GHG-CCI RR was to decide which algorithms to use to generate the CRDP. It is  
776 planned to generate the CRDP during September 2012 to March 2013. Table 6 presents an overview  
777 of the planned content of the CRDP in terms of data products and their spatio-temporal coverage. The  
778 CRDP will contain all relevant information needed for inverse modeling such as single observation  
779 uncertainties, *a priori* profiles and averaging kernels. The CRDP will be validated during March-May  
780 2013 and subsequently evaluated by the GHG-CCI users (June-August 2013). By the end of August,  
781 the CRDP along with the corresponding documentation will be made publicly available via the GHG-  
782 CCI website.

## 783 **8. Summary and conclusions**

784 An overview of the main activities and results achieved during the first two years of the GHG-CCI  
785 project of ESA's Climate Change Initiative (CCI) has been presented, focusing on the CCI "Round  
786 Robin" (RR) exercise. The goal of CCI is to generate a number of Essential Climate Variables (ECVs)  
787 in-line with GCOS (Global Climate Observing System) requirements and guidelines using European  
788 Earth observation data and data from ESA Third Party Missions (TPM) such as GOSAT. To achieve  
789 this, several existing state-of-the-art retrieval algorithms for retrieving XCO<sub>2</sub> and XCH<sub>4</sub> from  
790 SCIAMACHY/ENVISAT and TANSO/GOSAT nadir radiance spectra have been further improved in  
791 order to meet challenging requirements for the targeted regional CO<sub>2</sub> and CH<sub>4</sub> surface flux  
792 (source/sink) application as defined by the GHG-CCI Climate Research Group (CRG). The ultimate  
793 goal of the RR was to identify and select the best algorithms to be used for generating the Climate  
794 Research Data Package (CRDP), which will essentially be the first version of the CCI ECV GHG data  
795 base. In addition, retrieval algorithms for a number of other satellite instruments such as IASI and  
796 MIPAS have also been further developed, but not in competition.

797 Substantial progress has been made during the first two years (September 2010 – August 2012) of the  
798 GHG-CCI project. For example, longer XCO<sub>2</sub> and XCH<sub>4</sub> time series have been generated from  
799 SCIAMACHY with improved data quality and better error characterization (Reuter et al., 2011,  
800 Frankenberg et al., 2011, Schneising et al., 2011, 2012, Heymann et al., 2012a, 2012b). The same is  
801 true for TANSO (Butz et al., 2011, Parker et al., 2011, Schepers et al., 2012, Cogan et al., 2012).

802 Several retrieval algorithms have been further developed in competition during the GHG-CCI RR and  
803 used to generate global multi-year data sets of XCO<sub>2</sub> and XCH<sub>4</sub> from SCIAMACHY and TANSO.  
804 The data products have been evaluated by comparison with ground-based TCCON observations, by  
805 inter-comparisons of the data products generated with the different candidate algorithms, and by  
806 comparisons with other data sets including global models. Due to the sparseness of the TCCON  
807 network it was not planned to base the algorithm selection decision only on satellite – TCCON  
808 comparisons. It has been found that nearly all candidate algorithms produce data with very similar  
809 quality at TCCON sites, i.e., show similar satellite – TCCON differences. Significant differences have  
810 however been found remote from TCCON when comparing the global data sets, e.g., when comparing  
811 global maps. Depending on region and time, it has been found that the differences may exceed the  
812 systematic error requirements of less than 0.5 ppm for XCO<sub>2</sub> and 10 ppb for XCH<sub>4</sub>. It has been  
813 identified that more research is needed in order to understand the differences between the various data  
814 sets. It was therefore not possible for all products to clearly identify which of the candidate algorithms  
815 performs best. The goal of the RR was to identify which of the competing algorithms to use for the  
816 CRDP. The selected algorithms are listed in Table 6. A summary of the RR algorithm selection  
817 decision and justification is given in Section 5.6 for the GHG-CCI ECV core data products and in  
818 Section 6 for additional products generated with algorithms not in competition during the RR phase.

819 The climate and inverse modeling community requires long-term datasets of near-surface-sensitive  
820 CO<sub>2</sub> and CH<sub>4</sub> observations that are as accurate and precise as possible. The goal of GHG-CCI is to  
821 build up such a time series starting with SCIAMACHY/ENVISAT (March 2002 – April 2012) and  
822 being continued with GOSAT (launch 2009) and future GHG satellite missions such as OCO-2  
823 (Boesch et al., 2011), Sentinel-5-Precursor (Butz et al., 2012) and potentially CarbonSat



824 (Bovensmann et al., 2010). As shown in this manuscript, significant progress has been made to  
825 achieve this goal, but more work is needed in order to meet the demanding user requirements for as  
826 many conditions as possible.

## 827 **9. Acknowledgements**

828 This work was primarily funded by ESA/ESRIN (GHG-CCI) but also received funding from EU FP7  
829 (grant agreement No. 283576, MACC-II), DLR (SADOS), and the State and the University of  
830 Bremen. We thank the members of the GOSAT Project (JAXA, NIES, and Ministry of the  
831 Environment (MoE), Japan) for providing GOSAT Level 1B and Level 2 data products (GOSAT RA1  
832 PI project CONSCIGO). The ACOS v2.9 data were produced by the ACOS/OCO-2 project at the Jet  
833 Propulsion Laboratory, California Institute of Technology, and obtained from the ACOS/OCO-2 data  
834 archive maintained at the NASA Goddard Earth Science Data and Information Services Center. We  
835 thank NOAA for making available the CarbonTracker CO<sub>2</sub> fields. We also thank TCCON and related  
836 funding organizations (NASA grants NNX11AG01G, NAG5-12247, NNG05-GD07G, NASA  
837 Orbiting Carbon Observatory Program, DOE ARM program, the Australian Research Council,  
838 DP0879468 and LP0562346, the EU projects IMECC and GEOmon, the Senate of Bremen). Last but  
839 not least we would like to thank the two referees for helpful comments.

840

841

842 **10. References**

843 Bergamaschi, P., Frankenberg, C., Meirink, J.F., Krol, M., Dentener, F., Wagner, T., Platt, U., Kaplan,  
844 J.O., Körner, S., Heimann, M., Dlugokencky, E.J., Goede, A. (2007), Satellite cartography of  
845 atmospheric methane from SCIAMACHY onboard ENVISAT: 2. Evaluation based on inverse  
846 model simulations, *J. Geophys. Res.*, 112, D02304, doi:10.1029/2006JD007268.

847 Bergamaschi, P., Frankenberg, C., Meirink, J. F., Krol, M., Villani, M. G., Houweling, S., Dentener,  
848 F., Dlugokencky, E. J., Miller, J. B., Gatti, L. V., Engel, A., Levin, I. (2009), Inverse modeling  
849 of global and regional CH<sub>4</sub> emissions using SCIAMACHY satellite retrievals, *J. Geophys.*  
850 *Res.*, 114, D22301, doi:10.1029/2009JD01228.

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

854 Boesch, H., Baker, D., Connor, B., Crisp, D., Miller, C. (2011): Global Characterization of CO<sub>2</sub>  
855 Column Retrievals from Shortwave-Infrared Satellite Observations of the Orbiting Carbon  
856 Observatory-2 Mission, *Remote Sens.*, 3, 270–304, doi:10.3390/rs3020270,  
857 <http://www.mdpi.com/2072-4292/3/2/270/> .

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

861 Bovensmann, H., Buchwitz, M., Burrows, J. P., Reuter, M., Krings, T., Gerilowski, K., Schneising, O.,  
862 Heymann, J., Tretner, A., Erzinger, J. (2010), A remote sensing technique for global  
863 monitoring of power plant CO<sub>2</sub> emissions from space and related applications, *Atmos. Meas.*  
864 *Tech.*, 3, 781-811.

865 Bril, A., Oshchepkov, S., Yokota, T., Inoue, G. (2007): Parameterization of aerosol and cirrus cloud  
866 effects on reflected sunlight spectra measured from space: application of the equivalence  
867 theorem, *Appl. Opt.*, Vol.46(13), 2460-2470.

868 Buchwitz, M., Rozanov, V. V., Burrows, J. P. (2000), A near-infrared optimized DOAS method for  
869 the fast global retrieval of atmospheric CH<sub>4</sub>, CO, CO<sub>2</sub>, H<sub>2</sub>O, and N<sub>2</sub>O total column amounts  
870 from SCIAMACHY Envisat-1 nadir radiances, *J. Geophys. Res.*, 105, 15,231-15,245.

871 Buchwitz, M., de Beek, R., Burrows, J. P., Bovensmann, H., Warneke, T., Notholt, J., Meirink, J. F.,  
872 Goede, A. P. H., Bergamaschi, P., Körner, S., Heimann, M., Schulz, A. (2005), Atmospheric  
873 methane and carbon dioxide from SCIAMACHY satellite data: Initial comparison with  
874 chemistry and transport models, *Atmos. Chem. Phys.*, 5, 941-962.

875 Buchwitz, M., Schneising, O., Burrows, J. P., Bovensmann, H., Reuter, M., Notholt, J. (2007), First  
876 direct observation of the atmospheric CO<sub>2</sub> year-to-year increase from space, *Atmos. Chem.*  
877 *Phys.*, 7, 4249-4256.

878 Buchwitz, M., Chevallier, F., Bergamaschi, P. (2011a), User Requirements Document (URD) for the  
879 GHG-CCI project of ESA's Climate Change Initiative, Technical Report, pp. 45, version 1  
880 (URDv1), 3. February 2011, available from <http://www.esa-ghg-cci.org>.

881 Buchwitz, M., Reuter, M., Chevallier, F., Bergamaschi, P. (2011b), Round Robin Evaluation Protocol  
882 (RREP) for the GHG-CCI project of ESA's Climate Change Initiative, Technical Report, pp.  
883 15, version 2 (RREPV2), 17. August 2011, available from <http://www.esa-ghg-cci.org>.

884 Buchwitz, M., Reuter, M., Schneising, O., Parker, R., Guerlet, Noël, S., S. Crevoisier, C., Laeng, A.  
885 (2011c), Algorithm Inter-comparison and Error Characterization & Analysis Report  
886 (AIECAR) of the GHG-CCI project of ESA's Climate Change Initiative, Technical Report,  
887 pp. 192, version 0 (AIECARv0), 22. August 2011, available from <http://www.esa-ghg-cci.org>.

888 Buchwitz, M., Reuter, M., Schneising, O., Parker, R., Guerlet, Noël, S., S. Crevoisier, C., Laeng, A.  
889 (2012a), Algorithm Inter-comparison and Error Characterization & Analysis Report

890 (AIECAR) of the GHG-CCI project of ESA's Climate Change Initiative, Technical Report,  
891 version 1 (AIECARv1), 28. August 2012, available from <http://www.esa-ghg-cci.org>.

892 Buchwitz, M., Chevallier, F., Bergamaschi, P., Kaminski, T. (2012b), Algorithm Selection Report  
893 (ASR) of the GHG-CCI project of ESA's Climate Change Initiative, Technical Report, 29.  
894 August 2012, available from <http://www.esa-ghg-cci.org>.

895 Butz, A., Guerlet, S., Hasekamp, O., Schepers, D., Galli, A., Aben, I., Frankenberg, C., Hartmann, J.-  
896 M., Tran, H., Kuze, A., Keppel-Aleks, G., Toon, G., Wunch, D., Wennberg, P., Deutscher,  
897 N., Griffith, D., Macatangay, R., Messerschmidt, J., Notholt, J., Warneke, T. (2011),  
898 Towards accurate CO<sub>2</sub> and CH<sub>4</sub> observations from GOSAT, *Geophys. Res. Lett.*,  
899 doi:10.1029/2011GL047888.

900 Butz, A., Galli, A., Hasekamp, O., Landgraf, J., Tol, J. P., Aben, I. (2012), TROPOMI aboard  
901 Sentinel-5 Precursor: Prospective performance of CH<sub>4</sub> retrievals for aerosol and cirrus loaded  
902 atmospheres, *Remote Sensing of Environment*, 120, 267 – 276.

903 Canadell, J. G., Ciais, P., Dhakal, S., Dolman, H., Friedlingstein, P., Gurney, K. R., Held, A., Jackson,  
904 R. B., Le Quéré, C., Malone, E. L., Ojima, D. S., Patwardhan, A., Peters, G. P., Raupach, M.  
905 R. (2010), Interactions of the carbon cycle, human activity, and the climate system: a research  
906 portfolio, *Current Opinion in Environmental Sustainability*, 2, 301–311, available online at  
907 [www.sciencedirect.com](http://www.sciencedirect.com).

908 Chevallier, F., Engelen, R. J., Peylin, P. (2005), The contribution of AIRS data to the estimation of  
909 CO<sub>2</sub> sources and sinks. *Geophys. Res. Lett.*, 32, L23801, doi:10.1029/2005GL024229.

910 Chevallier, F., Bréon, F.-M., and Rayner, P. J. (2007), Contribution of the Orbiting Carbon  
911 Observatory to the estimation of CO<sub>2</sub> sources and sinks: Theoretical study in a variational data  
912 assimilation framework, *J. Geophys. Res.*, 112, D09307, doi:10.1029/2006JD007375.

913 Cogan, A., Boesch, H., Parker, R., Feng, L., Palmer, P., Blavier, J.-F., Deutscher, N., Macatangay, R.,  
914 Notholt, J., Roehl, C. M., Warneke, T., Wunch, D. (2012), Atmospheric carbon dioxide  
915 retrieved from the Greenhouse gases Observing SATellite: Comparison with ground-based

916 TCCON observations and GEOS-Chem model calculations, *J. Geophys. Res.*, 117, D21,  
917 doi:10.1029/2012JD018087.

918 Crevoisier, C., Heilliette, S., Chédin, A., Serrar, S., Armante, R., Scott, N.A. (2004), Midtropospheric  
919 CO<sub>2</sub> concentration retrieval from AIRS observations in the tropics, *Geophys. Res. Lett.*, 31,  
920 L17106, doi:10.1029/2004GL020141.

921 Crevoisier, C., Chédin, A., Matsueda, H., Machida, T., Armante, R., Scott, N. A. (2009a), First year of  
922 upper tropospheric integrated content of CO<sub>2</sub> from IASI hyperspectral infrared observations,  
923 *Atmos. Chem. Phys.*, 9, 4797–4810.

924 Crevoisier, C., Nobileau, D., Fiore, A., Armante, R., Chédin, A., Scott, N. A. (2009b), Tropospheric  
925 methane in the tropics – first year from IASI hyperspectral infrared observations, *Atmos.*  
926 *Chem. Phys.*, 9, 6337–6350.

927 Crisp, D., Atlas, R. M., Bréon, F.-M., Brown, L. R., Burrows, J. P., Ciais, P., Connor, B. J., Doney, S.  
928 C., Fung, I. Y., Jacob, D. J., Miller, C. E., O'Brien, D., Pawson, S., Randerson, J. T., Rayner,  
929 P., Salawitch, R. S., Sander, S. P., Sen, B., Stephens, G. L., Tans, P. P., Toon, G. C.,  
930 Wennberg, P. O., Wofsy, S. C., Yung, Y. L., Kuang, Z., Chudasama, B., Sprague, G., Weiss,  
931 P., Pollock, R., Kenyon, D., Schroll, S. (2004), The Orbiting Carbon Observatory (OCO)  
932 mission, *Adv. Space Res.*, 34, 700-709.

933 Crisp, D., Fisher, B. M., O'Dell, C., Frankenberg, C., Basilio, R., Boesch, H. L. R. Brown, R.  
934 Castano, B. Connor, N. M. Deutscher, A. Eldering, D. Griffith, M. Gunson, A. Kuze, L.  
935 Mandrake, J. McDuffie, J. Messerschmidt, C. E. Miller, I. Morino, V. Natraj, J. Notholt, D. M.  
936 O'Brien, F. Oyafuso, I. Polonsky, J. Robinson, R. Salawitch, V. Sherlock, M. Smyth, H. Suto,  
937 T. E. Taylor, D. R. Thompson, P. O. Wennberg, D. Wunch, Y. L. Yung (2012), The ACOS CO<sub>2</sub>  
938 retrieval algorithm – Part II: Global XCO<sub>2</sub> data characterization, *Atmos. Meas. Tech.*, 5, 687–  
939 707.

940 Deutscher, N. M., Griffith, D. W. T., Bryant, G. W., Wennberg, P. O., Toon, G. C., Washenfelder, R.  
941 A., Keppel-Aleks, G., Wunch, D., Yavin, Y. G., Allen, N. T., Blavier, J.-F. L., Jiménez, R.,

942 Daube, B. C., Bright, A. V, Matross, D. M., Wofsy, S. C., Park, S. (2010), Total column CO<sub>2</sub>  
943 measurements at Darwin, Australia – site description and calibration against in situ aircraft  
944 profiles, *Atmos. Meas. Tech.*, 3(4), 947–958, doi:10.5194/amt-3-947-2010.

945 Dlugokencky, E. J., Bruhwiler, L., White, J. W. C., Emmons, L. K., Novelli, P. C., Montzka, S. A.,  
946 Masarie, K. A., Lang, P. M., Crotwell, A. M., Miller, J. B., Gatti, L. V. (2009), Observational  
947 constraints on recent increases in the atmospheric CH<sub>4</sub> burden, *Geophys. Res. Lett.*, 36,  
948 L18803, doi:10.1029/2009GL039780.

949 Sussmann, R., Ostler, A., Forster, F., Rettinger, M., Deutscher, N. M., Griffith, D. W. T., Hannigan, J.  
950 W., Jones, N., Patra, P. K. (2013), First intercalibration of column-averaged methane from the  
951 Total Carbon Column Observing Network and the Network for the Detection of Atmospheric  
952 Composition Change, *Atmos. Meas. Tech.*, 6, 397–418.

953 Foucher, P. Y., Chédin, A., Dufour, G., Capelle, V., Boone, C. D., Bernath, P. (2009), Technical Note:  
954 Feasibility of CO<sub>2</sub> profile retrieval from limb viewing solar occultation made by the ACE-FTS  
955 instrument, *Atmos. Chem. Phys.*, 9, 2873–2890.

956 Frankenberg, C., Meirink, J. F., van Weele, M., Platt, U., Wagner, T. (2005), Assessing methane  
957 emissions from global spaceborne observations, *Science*, 308, 1010–1014.

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

962 GCOS (Global Climate Observing System) (2006), Systematic Observation Requirements for  
963 Satellite-based products for Climate – Supplemental Details to the GCOS Implementation  
964 Plan, GCOS 107, September 2006.

965 Geibel, M. C., Messerschmidt, J., Gerbig, C., Blumenstock, T., Chen, H., Hase, F., Kolle, O., Lavric,  
966 J. V., Notholt, J., Palm, M., Rettinger, M., Schmidt, M., Sussmann, R., Warneke, T., Feist, D.  
967 G. (2012), Calibration of column-averaged CH<sub>4</sub> over European TCCON FTS sites with

968 airborne in-situ measurements, *Atmos. Chem. Phys.*, 12, 8763–8775, doi:10.5194/acp-12-  
969 8763-2012.

970 Heymann, J., Schneising, O., Reuter, M., Buchwitz, M., Rozanov, V. V., Velazco, V. A.,  
971 Bovensmann, H., Burrows, J. P. (2012a), SCIAMACHY WFM-DOAS XCO<sub>2</sub>: comparison  
972 with CarbonTracker XCO<sub>2</sub> focusing on aerosols and thin clouds, *Atmos. Meas. Tech.*, 5, 1935-  
973 1952, 2012.

974 Heymann, J., Bovensmann, H., Buchwitz, M., Burrows, J. P., Deutscher, N. M., Notholt, J., Rettinger,  
975 M., Reuter, M., Schneising, O., Sussmann, R., Warneke, T. (2012b), SCIAMACHY WFM-  
976 DOAS XCO<sub>2</sub>: reduction of scattering related errors, *Atmos. Meas. Tech.*, 5, 2375-2390, 2012.

977 Kaminski, T., Scholze, M., Houweling, S. (2010), Quantifying the Benefit of A-SCOPE  
978 Data for Reducing Uncertainties in Terrestrial Carbon Fluxes in CCDAS. *Tellus B*,  
979 doi:10.1111/j.1600-0889.2010.00483.x

980 Kaminski, T., Knorr, W., Scholze, M., Gobron, N., Pinty, R., Giering, R., Mathieu, P.-P. (2012),  
981 Consistent Assimilation of MERIS FAPAR and atmospheric CO<sub>2</sub> into a Terrestrial Vegetation  
982 Model and Interactive Mission Benefit Analysis. *Biogeosciences*, 9(8):3173-3184.

983 Knutti, R., R. Furrer, C. Tebaldi, J. Cermak, G. A. Meehl (2010), Challenges in Combining  
984 Projections from Multiple Climate Models. *J. Climate*, 23, 2739–2758. doi:  
985 <http://dx.doi.org/10.1175/2009JCLI3361.1>

986 Kuze, A., Suto, H., Nakajima, M., and Hamazaki, T. (2009), Thermal and near infrared sensor for  
987 carbon observation Fourier-transform spectrometer on the Greenhouse Gases Observing  
988 Satellite for greenhouse gases monitoring, *Appl. Opt.*, 48, 6716–6733.

989 Meirink, J. F., Eskes, H. J., and Goede, A. P. H. (2006), Sensitivity analysis of methane emissions  
990 derived from SCIAMACHY observations through inverse modelling, *Atmos. Chem. Phys.*, 6,  
991 1275–1292.

992 Messerschmidt, J., Geibel, M. C., Blumenstock, T., Chen, H., Deutscher, N. M., Engel, A., Feist, D.  
993 G., Gerbig, C., Gisi, Hase, M. F., Katrynski, K., Kolle, O., Lavric, J. V., Notholt, J., Palm, M.,

994 Ramonet, M., Rettinger, M., Schmidt, M., Sussmann, R., Toon, G. C., F. Truong, F., Warneke,  
995 T., Wennberg, P. O., Wunch, D., Xueref-Remy, I. (2012), Calibration of TCCON column-  
996 averaged CO<sub>2</sub>: the first aircraft campaign over European TCCON sites, *Atmos. Chem. Phys.*,  
997 11, 10765-10777.

998 Noël, S., Bramstedt, K., Rozanov, A., Bovensmann, H., Burrows, J. P. (2011), Stratospheric methane  
999 profiles from SCIAMACHY solar occultation measurements derived with onion peeling  
1000 DOAS, *Atmos. Meas. Tech.*, 4, 2567-2577.

1001 Notholt, J., Dils, B., Blumenstock, T., Brunner, D., Buchmann, B., De Mazière, M., Popp, C.,  
1002 Sussmann, R. (2012), Product Validation and Algorithm Selection Report (PVASR) of the  
1003 GHG-CCI project of ESA's Climate Change Initiative, Technical Report, 22. August 2012,  
1004 available from <http://www.esa-ghg-cci.org>.

1005 O'Dell, C. W., Connor, B., Boesch, H., O'Brien, D., Frankenberg, C., Castano, R., Christi, M.,  
1006 Eldering, D., Fisher, B., Gunson, M., McDuffie, J., Miller, C. E., Natraj, V., Oyafuso, F.,  
1007 Polonsky, I., Smyth, M., Taylor, T., Toon, G. C., Wennberg, P. O., Wunch, D., (2012), The  
1008 ACOS CO<sub>2</sub> retrieval algorithm – Part 1: Description and validation against synthetic  
1009 observations, *Atmos. Meas. Tech.*, 5, 99–121, 2012.

1010 Oshchepkov S., Bril, A., Yokota, T. (2008), PPDF-based method to account for atmospheric light  
1011 scattering in observations of carbon dioxide from space. *J. Geophys. Res.*, 113, D23210.

1012 Oshchepkov S., Bril, A., Yokota, T. (2009), An improved photon path length probability density  
1013 function-based radiative transfer model for space-based observation of greenhouse gases. *J.*  
1014 *Geophys. Res.*, 114, D19207.

1015 Oshchepkov, S., Bril, A., Maksyutov, S., Yokota, T. (2011), Detection of optical path in spectroscopic  
1016 space-based observations of greenhouse gases: Application to GOSAT data processing, *J.*  
1017 *Geophys. Res.*, 116, D14304, doi:10.1029/2010JD015352.

1018 Oshchepkov, S., Bril, A., Yokota, T., Morino, I., Yoshida, Y., Matsunaga, T., Belikov, D., Wunch, D.,  
1019 Wennberg, P., Toon, G., O'Dell, C., Butz, A., Guerlet, S., Cogan, A., Boesch, H., Eguchi, N.,  
1020 Deutscher, N., Griffith, G., Macatangay, R., Notholt, J., Sussmann, R., Rettinger, M.,



1021 Sherlock, V., Robinson, J., Kyrö, E., Heikkinen, P., Feist, D. G., Nagahama, T., Kadygrov, N.,  
1022 Maksyutov, S., Uchino, O., Watanabe, H. (2012), Effects of atmospheric light scattering on  
1023 spectroscopic observations of greenhouse gases from space: Validation of PPDF-based CO<sub>2</sub>  
1024 retrievals from GOSAT, *J. Geophys. Res.*, 117, D12305, doi:10.1029/2012JD017505.

1025 Parker, R., Boesch, H., Cogan, A., Fraser, A., Feng, L., Palmer, P., Messerschmidt, J., Deutscher, N.,  
1026 Griffith, D., Notholt, J., Wennberg, P. Wunch, D. (2011), Methane Observations from the  
1027 Greenhouse gases Observing SATellite: Comparison to ground-based TCCON data and Model  
1028 Calculations, *Geophys. Res. Lett.*, doi:10.1029/2011GL047871.

1029 Peters, W., Jacobson, A. R., Sweeney, C., Andrews, A. E., Conway, T. J., Masarie, K., Miller, J. B.,  
1030 Bruhwiler, L. M. P., Petron, G., Hirsch, A. I., Worthy, D. E. J., van der Werf, G. R.,  
1031 Randerson, J. T., Wennberg, P. O., Krol, M. C., Tans, P. P. (2007): An atmospheric  
1032 perspective on North American carbon dioxide exchange: CarbonTracker, Proceedings of the  
1033 National Academy of Sciences (*PNAS*) of the United States of America, 27 Nov. 2007,  
1034 104(48), 18925-18930.

1035 Reuter, M., Buchwitz, M., Schneising, O., Heymann, J., Bovensmann, H., Burrows, J. P. (2010), A  
1036 method for improved SCIAMACHY CO<sub>2</sub> retrieval in the presence of optically thin clouds,  
1037 *Atmos. Meas. Tech.*, 3, 209-232.

1038 Reuter, M., Bovensmann, H., Buchwitz, M., Burrows, J. P., Connor, B. J., Deutscher, N. M., Griffith,  
1039 D. W. T., Heymann, J., Keppel-Aleks, G., Messerschmidt, J., Notholt, J., Petri, C., Robinson,  
1040 J., Schneising, O., Sherlock, V., Velazco, V., Warneke, T., Wennberg, P. O., Wunch, D.  
1041 (2011), Retrieval of atmospheric CO<sub>2</sub> with enhanced accuracy and precision from  
1042 SCIAMACHY: Validation with FTS measurements and comparison with model results, *J.*  
1043 *Geophys. Res.*, 116, D04301, doi:10.1029/2010JD015047.

1044 Reuter, M., Schneising, O., Parker, R., Guerlet, S., Noël, S., Crevoisier, C., Laeng, A. (2012a),  
1045 Algorithm Theoretical Basis Document (ATBD) of the GHG-CCI project of ESA's Climate  
1046 Change Initiative, Technical Report, pp. 486, version 1 (ATBDv1), 15. March 2012, available  
1047 from <http://www.esa-ghg-cci.org>.

1048 Reuter, M., Buchwitz, M., Schneising, O., Hase, F., Heymann, J., Guerlet, S., Cogan, A. J.,  
1049 Bovensmann, H., Burrows, J. P., (2012b), A simple empirical model estimating atmospheric  
1050 CO<sub>2</sub> background concentrations, *Atmos. Meas. Tech.*, 5, 1349-1357.

1051 Reuter, M., Boesch, H., Bovensmann, H., Bril, A., Buchwitz, M., Butz, A., Burrows, J. P., O'Dell, C.  
1052 W., Guerlet, S., Hasekamp, O., Heymann, J., Kikuchi, S. Oshchepkov, S., Parker, R., Pfeifer,  
1053 S., Schneising, O., Yokota, T., Yoshida, Y. (2013), A joint effort to deliver satellite retrieved  
1054 atmospheric CO<sub>2</sub> concentrations for surface flux inversions: The ensemble median algorithm  
1055 EMMA, *Atmos. Chem. Phys.*, 13, 1771-1780.

1056 Rigby, M., Prinn, R. G., Fraser, P. J., Simmonds, P. G., Langenfelds, R. L., Huang, J., Cunnold, D. M.,  
1057 Steele, L. P., Krummel, P. B., Weiss, R. F., O'Doherty, S., Salameh, P. K., Wang, H. J., Harth,  
1058 C. M., Mühle, J., Porter, L. W. (2008), Renewed growth of atmospheric methane, *Geophys.*  
1059 *Res. Lett.*, 35, L22805, doi:10.1029/2008GL036037.

1060 Rodgers, C. D. (2000), Inverse Methods for Atmospheric Sounding: Theory and Practice, *World*  
1061 *Scientific Publishing*.

1062 Schepers, D., Guerlet, S., Butz, A., Landgraf, J., Frankenberg, C., Hasekamp, O., Blavier, J.-F.,  
1063 Deutscher, N. M., Griffith, D. W. T., Hase, F., Kyro, E., Morino, I., Sherlock, V., Sussmann,  
1064 R., Aben, I. (2012), Methane retrievals from Greenhouse Gases Observing Satellite (GOSAT)  
1065 shortwave infrared measurements: Performance comparison of proxy and physics retrieval  
1066 algorithms, *J. Geophys. Res.*, 117, D10307, doi:10.1029/2012JD017549.

1067 Schneising, O., Buchwitz, M., Burrows, J. P., Bovensmann, H., Reuter, M., Notholt, J., Macatangay,  
1068 R., Warneke, T. (2008), Three years of greenhouse gas column-averaged dry air mole  
1069 fractions retrieved from satellite - Part 1: Carbon dioxide, *Atmos. Chem. Phys.*, 8, 3827-3853,  
1070 2008.

1071 Schneising, O., Buchwitz, M., Burrows, J. P., Bovensmann, H., Bergamaschi, P., Peters, W. (2009),  
1072 Three years of greenhouse gas column-averaged dry air mole fractions retrieved from satellite  
1073 - Part 2: Methane, *Atmos. Chem. Phys.*, 9, 443-465.

1074 Schneising, O., Buchwitz, M., Reuter, M., Heymann, J., Bovensmann, H., and Burrows, J. P. (2011),  
1075 Long-term analysis of carbon dioxide and methane column-averaged mole fractions retrieved  
1076 from SCIAMACHY, *Atmos. Chem. Phys.*, 11, 2881-2892.

1077 Schneising, O., Bergamaschi, P., Bovensmann, H., Buchwitz, M., Burrows, J. P., Deutscher, N. M.,  
1078 Griffith, D. W. T., Heymann, J., Macatangay, R., Messerschmidt, J., Notholt, J., Rettinger, M.,  
1079 Reuter, M., Sussmann, R., Velazco, V. A., Warneke, T., Wennberg, P. O., Wunch, D. (2012),  
1080 Atmospheric greenhouse gases retrieved from SCIAMACHY: comparison to ground-based  
1081 FTS measurements and model results, *Atmos. Chem. Phys.*, 12, 1527-1540.

1082 Simpson, I. J., Sulbaek Andersen, M. P., Meinardi, S., Bruhwiler, L., Blake, N. J., Helmig, D.,  
1083 Rowland, F. S., Blake, D. R. (2012), Long-term decline of global atmospheric ethane concentrations  
1084 and implications for methane, *Nature*, [www.nature.com/doi/10.1038/nature11342](http://www.nature.com/doi/10.1038/nature11342)

1085 Solomon, S., Qin, D., Manning, M., Chen, Z., Marquis, M., Averyt, K. B., Tignor, M., and Miller, H.  
1086 L. (Eds.): *Climate Change 2007: The Physical Science Basis*, Contribution of Working Group  
1087 I to the Fourth Assessment Report of the Intergovernmental Panel on Climate Change (IPCC),  
1088 *Cambridge University Press*, Cambridge, United Kingdom and New York, NY, USA, 2007.

1089 Stephens, B. B., Gurney, K. R., Tans, P. P., Sweeney, C., Peters, W., Bruhwiler, L., Ciais, P.,  
1090 Ramonet, M., Bousquet, P., Nakazawa, T., Aoki, S., Machida, T., Inoue, G., Vinnichenko, N.,  
1091 Lloyd, J., Jordan, A., Heimann, M., Shibistova, O., Langenfelds, R. L., Steele, L. P., Francey,  
1092 R. J., and Denning, A. S. (2007), Weak northern and strong tropical land carbon uptake from  
1093 vertical profiles of atmospheric CO<sub>2</sub>, *Science*, 316, 1732–1735.

1094 Toon, G. (1991), The JPL MkIV interferometer, *Optics Photonics News*, 2, 19–21.

1095 von Clarmann, T., Höpfner, M., Kellmann, S., Linden, A., Chauhan, S., Funke, B., Grabowski, U.,  
1096 Glatthor, N., Kiefer, M., Schieferdecker, T., Stiller, G., Versick, S. (2009), Retrieval of  
1097 temperature, H<sub>2</sub>O, O<sub>3</sub>, HNO<sub>3</sub>, CH<sub>4</sub>, N<sub>2</sub>O, ClONO<sub>2</sub> and ClO from MIPAS reduced resolution  
1098 nominal mode limb emission measurements, *Atmos. Meas. Tech.*, 2, 159-175.

1099 Wecht, K. J., Jacob, D. J., Wofsy, S. C., Kort, E. A., Worden, J. R., Kulawik, S. S., Henze, D. K., M.  
1100 Kopacz, M., H. Payne, V. H. (2012), Validation of TES methane with HIPPO aircraft

1101 observations: implications for inverse modeling of methane sources, *Atmos. Chem. Phys.*, 12,  
1102 1823–1832.

1103 Wofsy, S. C., Daube, B. C., Jimenez, R., Kort, E., Pittman, J. V., Park, S., Commane, R., Xiang, B.,  
1104 Santoni, G., Jacob, D., Fisher, J., Pickett-Heaps, C., Wang, H., Wecht, K., Wang, Q.-Q.,  
1105 Stephens, B. B., Schertz, S., Romashkin, P., Campos, T., Haggerty, J., Cooper, W. A., Rogers,  
1106 D., Beaton, S., Elkins, J. W., Fahey, D., Gao, R., Moore, F., Montzka, S. A., Schwartz, J. P.,  
1107 Hurst, D., Miller, B., Sweeney, C., Oltmans, S., Nance, D., Hints, E., Dutton, G., Watts, L.  
1108 A., Spackman, R., Rosenlof, K., Ray, E., Zondlo, M., Diao, M., Mahoney, M. J., Chahine, M.,  
1109 Olsen, E., Keeling, R., Bent, J., Atlas, E. A., Lueb, R., Patra, P., Ishijima, K., Engelen, R.,  
1110 Nassar, R., Jones, D. B., Mikaloff-Fletcher, S. (2011), HIAPER Pole-to-Pole Observations  
1111 (HIPPO): Fine grained, global scale measurements for determining rates for transport, surface  
1112 emissions, and removal of climatically important atmospheric gases and aerosols, *Philos. T.*  
1113 *Roy. Soc. A*, 369, 2073–2086, doi:10.1098/rsta.2010.0313, 2011.

1114 Wunch, D., Toon, G. C., Wennberg, P. O., Wofsy, S. C., Stephens, B. B., Fischer, M. L., Uchino, O.,  
1115 Abshire, J. B., Bernath, P., Biraud, S. C., Blavier, J.-F. L., Boone, C., Bowman, K. P.,  
1116 Browell, E. V., Campos, T., Connor, B. J., Daube, B. C., Deutscher, N. M., Diao, M., Elkins,  
1117 J. W., Gerbig, C., Gottlieb, E., Griffith, D. W. T., Hurst, D. F., Jimenez, R., Keppel-Aleks, G.,  
1118 Kort, E. A., Macatangay, R., Machida, T., Matsueda, H., Moore, F., Morino, I., Park, S.,  
1119 Robinson, J., Roehl, C. M., Sawa, Y., Sherlock, V., Sweeney, C., Tanaka, T., Zondlo, M. A.  
1120 (2010), Calibration of the Total Carbon Column Observing Network using aircraft profile  
1121 data, *Atmos. Meas. Tech.*, 3, 1351–1362, doi:10.5194/amt-3-1351-2010, [http://www.atmos-](http://www.atmos-meas-tech.net/3/1351/2010/)  
1122 [meas-tech.net/3/1351/2010/](http://www.atmos-meas-tech.net/3/1351/2010/).

1123 Wunch, D., Toon, G. C., Blavier, J.-F. L., Washenfelder, R. A., Notholt, J., Connor, B. J., Griffith, D.  
1124 W. T., Sherlock, V., Wennberg, P. O. (2011a), The Total Carbon Column Observing Network,  
1125 *Phil. Trans. R. Soc. A*, 369, 2087–2112, doi:10.1098/rsta.2010.0240.

1126 Wunch, D., Wennberg, P. O., Toon, G. C., Connor, B. J., Fisher, B., Osterman, G. B., Frankenberg,  
1127 C., Mandrake, L., O'Dell, C., Ahonen, P., Biraud, S. C., Castano, R., Cressie, N., Crisp, D.,

1128 Deutscher, N. M., Eldering, A., Fisher, M. L., Griffith, D. W. T., Gunson, M., Heikkinen, P.,  
1129 Keppel-Aleks, G., Kyrö, E., Lindenmaier, R., Macatangay, R., Mendonca, J., Messerschmidt,  
1130 J., Miller, C. E., Morino, I., Notholt, J., Oyafuso, F. A., Rettinger, M., Robinson, J., Roehl,  
1131 C. M., Salawitch, R. J., Sherlock, V., Strong, K., Sussmann, R., Tanaka, T., Thompson, D. R.,  
1132 Uchino, O., Warneke, T., Wofsy, S. C. (2011b), A method for evaluating bias in global  
1133 measurements of CO<sub>2</sub> total columns from space, *Atmos. Chem. Phys.*, 11, 12317-12337.

1134 Yoshida, Y., Ota, Y., Eguchi, N., Kikuchi, N., Nobuta, K., Tran, H., Morino, I., Yokota, T. (2011):  
1135 Retrieval algorithm for CO<sub>2</sub> and CH<sub>4</sub> column abundances from short-wavelength infrared  
1136 spectral observations by the Greenhouse gases observing satellite, *Atmos. Meas. Tech.*, 4, 717–  
1137 734, doi:10.5194/amt-4-717-2011.

1138

1139

1140

1141 **11. Tables**

1142

1143 **Table 1:** GHG-CCI XCO<sub>2</sub> and XCH<sub>4</sub> random and systematic uncertainty requirements for  
 1144 measurements over land. Abbreviations: G=Goal requirement (the maximum that needs to be  
 1145 achieved; better performance likely not needed as other errors (e.g., modelling errors) will dominate),  
 1146 B=Breakthrough requirement (“good” performance somewhere between G and T), T=Threshold  
 1147 requirement (the minimum that needs to be achieved for the specified application, here: global  
 1148 regional-scale surface flux inverse modelling). See also main text for a detailed explanation. From  
 1149 GHG-CCI User Requirements Document (URD, Buchwitz et al., 2011a).

<b>Requirements for regional CO<sub>2</sub> and CH<sub>4</sub> source/sink determination using SCIAMACHY/ENVISAT and TANSO/GOSAT</b>					
<b>Parameter</b>	<b>Requirement type</b>	<b>Random error</b>		<b>Systematic error</b>	<b>Stability</b>
		<b>Single observation</b>	<b>1000<sup>2</sup> km<sup>2</sup>, monthly</b>		
XCO <sub>2</sub>	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 <sub>4</sub>	G	< 9 ppb	< 3 ppb	< 1 ppb (absolute)	As systematic error but per year
	B	< 17 ppb	< 5 ppb	< 5 ppb (relative)	--
	T	< 34 ppb	< 11 ppb	< 10 ppb (relative)	--

1150

1151

1152

1153

1154 **Table 2:** Overview GHG-CCI ECV Core Algorithms (ECAs). Details on each of these algorithms are  
 1155 also given in the GHG-CCI ATBD (Reuter et al., 2012a) and in Buchwitz et al., 2012a. Column  
 1156 “Algorithm short name” lists the GHG-CCI algorithm identifiers (names in brackets are names (also)  
 1157 used in the literature (see column “References”)).

<b>GHG-CCI ECV Core Algorithms (ECAs)</b>				
<b>Algorithm ID</b>	<b>Data product</b>	<b>Sensor</b>	<b>Algorithm short name</b>	<b>References</b>
CO2_SCI_WFMD	XCO <sub>2</sub>	SCIAMACHY/ ENVISAT	WFMD (WFM-DOAS)	<i>Schneising et al., 2011, 2012;</i> <i>Heymann et al., 2012b</i>
CO2_SCI_BESD	XCO <sub>2</sub>	SCIAMACHY	BESD	<i>Reuter et al., 2010, 2011</i>
CO2_GOS_OCFP	XCO <sub>2</sub>	TANSO/GOSAT	OCFP (UoL-FP)	<i>Cogan et al., 2012</i>
CO2_GOS_SRFP	XCO <sub>2</sub>	TANSO/GOSAT	SRFP (RemoteC)	<i>Butz et al., 2011</i>
CH4_SCI_WFMD	XCH <sub>4</sub>	SCIAMACHY	WFMD (WFM-DOAS)	<i>Schneising et al., 2010, 2011</i>
CH4_SCI_IMAP	XCH <sub>4</sub>	SCIAMACHY	IMAP	<i>Frankenberg et al., 2011</i>
CH4_GOS_OCFP	XCH <sub>4</sub>	TANSO/GOSAT	OCFP	<i>Parker et al., 2011</i>
CH4_GOS_OCPR	XCH <sub>4</sub>	TANSO/GOSAT	OCPR	<i>Parker et al., 2011</i>
CH4_GOS_SRFP	XCH <sub>4</sub>	TANSO/GOSAT	SRFP	<i>Butz et al., 2011</i>
CH4_GOS_SRPR	XCH <sub>4</sub>	TANSO/GOSAT	SRPR	<i>Schepers et al., 2012</i>

1158

1159

1160 **Table 3:** Overview GHG-CCI Additional Constraints Algorithms (ACAs). (\*) Note that  
1161 CO2\_SCI\_ONPD is a new algorithm “similar” as the one described in Noël et al., 2011, which has  
1162 been added in the 2<sup>nd</sup> year of GHG-CCI. Details on each of these algorithms are also given in the  
1163 GHG-CCI ATBD (Reuter et al., 2012a) and in Buchwitz et al., 2012a.

<b>GHG-CCI Additional Constraints Algorithms (ACAs)</b>				
<b>Algorithm ID</b>	<b>Data product</b>	<b>Sensor</b>	<b>Algorithm</b>	<b>References</b>
CO2_AIR_NLIS	Mid/upper trop. column	AIRS	NLIS	<i>Crevoisier et al., 2004</i>
CO2_IAS_NLIS	Mid/upper trop. column	IASI	NLIS	<i>Crevoisier et al., 2009a</i>
CO2_ACE_CLRS	Upper trop. / strat. profile	ACE-FTS	CLRS	<i>Foucher et al., 2009</i>
CO2_SCI_ONPD	Stratospheric profile	SCIAMACHY	ONPD	<i>(Noël et al., 2011) (*)</i>
CH4_IAS_NLIS	Upper trop. / strat. profile	IASI	NLIS	<i>Crevoisier et al., 2009b</i>
CH4_MIP_IMK	Upper trop. / strat. profile	MIPAS	KIT/IMK MIPAS	<i>von Clarmann et al., 2009</i>
CH4_SCI_ONPD	Stratospheric profile	SCIAMACHY	ONPD	<i>Noël et al., 2011</i>

1164

1165

1166



1167

1168 **Table 4:** TCCON sites as used for the validation of the satellite-derived XCH<sub>4</sub> and XCO<sub>2</sub> Round

1169 Robin (RR) data products by the GHG-CCI validation team (from Notholt et al., 2012).

<b>TCCON validation sites used for GHG-CCI Round Robin</b>					
<b>Name</b>	<b>ID</b>	<b>Latitude</b> <b>[deg]</b>	<b>Longitude</b> <b>[deg]</b>	<b>Altitude</b> <b>[km]</b>	<b>Time coverage</b> <b>MM/YYYY-MM/YYYY</b>
Bialystok	BIA	53.231	23.025	0.183	03/2009 - 03/2011
Bremen	BRE	53.104	8.850	0.027	01/2009 - 12/2010
Karlsruhe	KAR	49.102	8.440	0.110	04/2010 - 05/2011
Orleans	ORL	47.965	2.113	0.132	08/2009 - 11/2010
Garmisch	GAR	47.476	11.063	0.744	05/2009 - 12/2010
ParkFalls	PAR	45.945	-90.273	0.442	06/2004 - 04/2011
Lamont	LAM	36.604	-97.486	0.320	07/2008 - 05/2011
Darwin	DAR	-12.425	130.891	0.030	08/2005 - 02/2011
Wollongong	WOL	-34.406	150.879	0.030	06/2008 - 03/2011
Lauder	LAU	-45.050	169.680	0.370	06/2004 - 06/2011

1170

1171

1172

1173  
 1174  
 1175  
 1176  
 1177  
 1178  
 1179  
 1180  
 1181  
 1182  
 1183

**Table 5:** Estimated precision and biases of the satellite XCO<sub>2</sub> (top) and XCH<sub>4</sub> (bottom) GHG-CCI core data products retrieved with ECAs obtained from comparisons with ground-based TCCON retrievals (see Figure 3 and 4 for details). \*) The exact version number for BESD is v01.00.01. Numbers in curved brackets are for SCIAMACHY methane retrievals during 2003-2005, i.e., before significant detector degradation of the methane channel: values from Buchwitz et al., 2012a, are indicated by #) and value from Schneising et al., 2012, is indicated by §). Values in square brackets for SCIAMACHY methane retrieval are from Buchwitz et al., 2012a, based on an analysis of all available retrievals (all years) and using a different assessment method. Also listed are the GHG-CCI user requirements as given the GHG-CCI User Requirements Document (URD (Buchwitz et al., 2011a), see also Table 1, e.g., for the explanation of T, B, G).

<b>Comparison of GHG-CCI core data products (ECAs) with TCCON</b>				
<b>XCO<sub>2</sub> [ppm]</b>				
<b>Algorithm</b>	<b>Sensor</b>	<b>Estimated precision single observation</b>	<b>Estimated relative biases</b>	<b>Number of satellite obs.</b>
WFMD v2.2	SCIAMACHY	5.1	1.3	30752
BESD v1 *)	SCIAMACHY	2.3	0.7	9467
OCFP v3.0	TANSO	2.7	0.6	2830
SRFP v1.1	TANSO	2.8	0.9	2558
Required (URD):		< 8(T), 3(B), 1(G)	< 0.5(T), 0.3(B), 0.2(G)	-
<b>XCH<sub>4</sub> [ppb]</b>				
<b>Algorithm</b>	<b>Sensor</b>	<b>Estimated precision single observation</b>	<b>Estimated relative biases</b>	<b>Number of satellite obs.</b>
WFMD v2.3	SCIAMACHY	82 (~30 <sup>#</sup> )	11 (~3 <sup>§</sup> ) [4-12 <sup>#</sup> ]	37628
IMAP v6.0	SCIAMACHY	50 (~30 <sup>#</sup> )	15 [4-13 <sup>#</sup> ]	39489
OCFP v3.2	TANSO	16	8	3176
SRFP v1.1	TANSO	15	3	2558
OCPR v3.2	TANSO	13	2	7323
SRPR v1.1	TANSO	14	3	4900
Required (URD):		< 34(T), 17(B), 9(G)	< 10(T), 5(B), 3(G)	-

1184  
 1185

1186

1187 **Table 6:** Overview of the planned content of the GHG-CCI CRDP. §) see Table 2 and Table 3, \*) may

1188 end later, +) may start earlier, #) mainly high latitudes. Products: (1) mid/upper tropospheric columns,

1189 (2) (primarily) stratospheric vertical profiles.

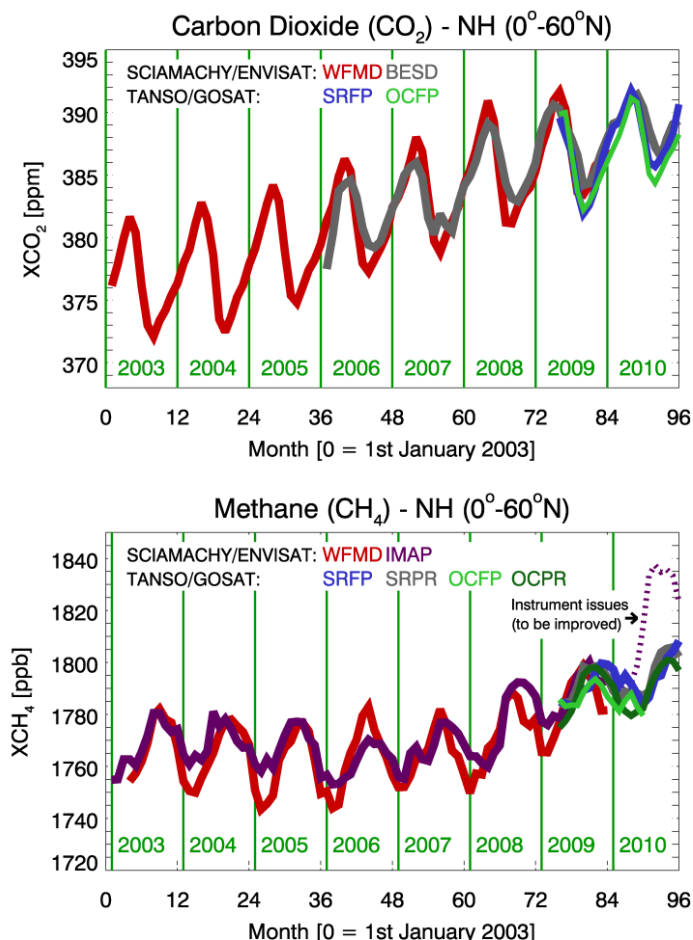
<b>Planned content of the GHG-CCI Climate Research Data Package (CRDP)</b>				
<b>Data products generated with ECV Core Algorithms (ECAs)</b>				
<b>Product ID</b>	<b>Product</b> (Level 2, mixing ratios)	<b>Algorithm §)</b>	<b>Coverage</b>	<b>Comment</b>
XCO2_SCIA	XCO <sub>2</sub>	BESD	Global, land, 2003-2010 <sup>*)</sup>	-
XCO2_GOSAT	XCO <sub>2</sub>	OCFP and SRFP	Global, mid 2009-2010 <sup>*)</sup>	2 alternative products
XCO2_EMMA	XCO <sub>2</sub>	EMMA	Global, mid 2009-2010 <sup>*)</sup>	Merged SCIA and GOSAT
XCH4_SCIA	XCH <sub>4</sub>	IMAP and WFMD	Global, 2003-2010 <sup>*)</sup>	2 alternative products
XCH4_GOSAT	XCH <sub>4</sub>	SRFP and OCPR	Global, mid 2009-2010 <sup>*)</sup>	2 alternative products
<b>Data products generated with Additional Constraints Algorithms (ACAs)</b>				
<b>Product ID</b>	<b>Product</b> (Level 2, mixing ratios)	<b>Algorithm §)</b>	<b>Coverage</b>	<b>Comment</b>
CO2_AIRS	CO <sub>2</sub> (1)	NLIS	Tropics, 2003-2007	-
CO2_IASI	CO <sub>2</sub> (1)	NLIS	Tropics, 2007-2010 <sup>*)</sup>	-
CH4_IASI	CH <sub>4</sub> (1)	NLIS	Tropics, 2007-2010 <sup>*)</sup>	-
CH4_SCIA_OCC	CH <sub>4</sub> (2)	ONPD	NH mid/high lat., 2003-2010 <sup>*)</sup>	-
CO2_SCI_OCC	CO <sub>2</sub> (2)	ONPD	NH mid/high lat., 2003-2010 <sup>*)</sup>	-
CH4_MIPAS	CH <sub>4</sub> (2)	KIT/IMK MIPAS	Global, 2005 <sup>+) -2010<sup>*)</sup></sup>	-
CO2_ACEFTS	CO <sub>2</sub> (2)	CLRS	Global <sup>#)</sup> , 2004-2010 <sup>*)</sup>	-

1190

1191

1192

1193 **12. Figures**

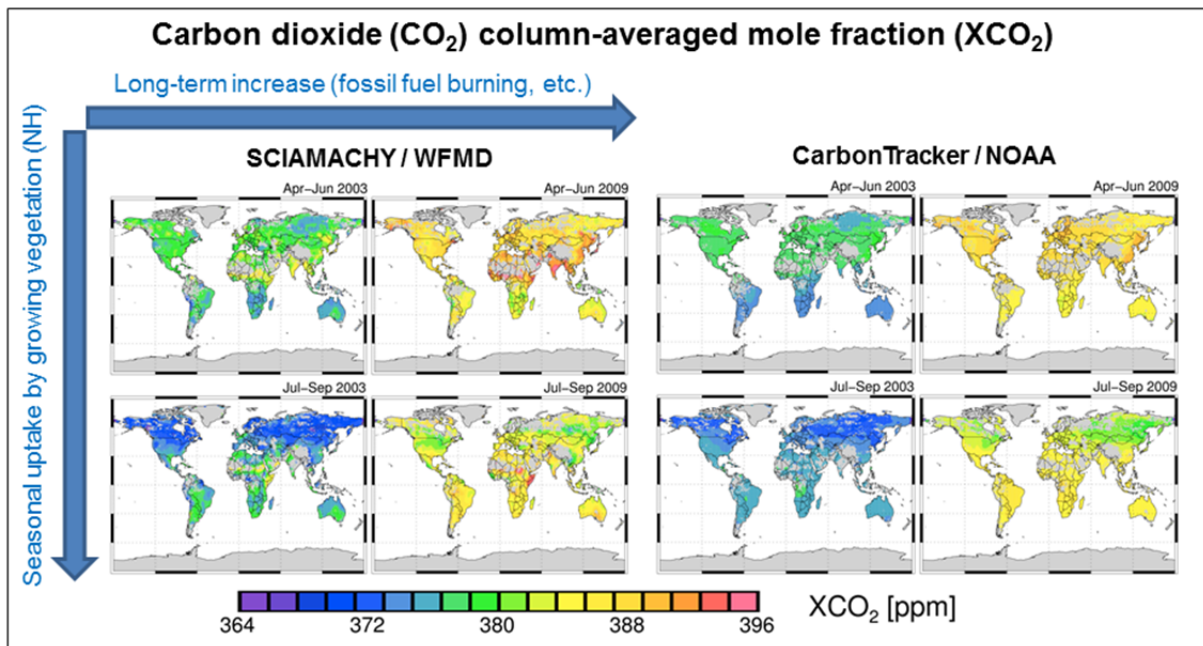


1194

1195 **Figure 1:** Top: Northern hemispheric monthly mean XCO<sub>2</sub> time series retrieved from  
1196 SCIAMACHY/ENVISAT (algorithms: WFMD and BESD) and TANSO/GOSAT (algorithms: SRFP  
1197 and OCFP) satellite data. Shown are monthly mean values for the 0°-60°N latitude range. Clearly  
1198 visible is the CO<sub>2</sub> increase primarily caused by the burning of fossil fuels and the seasonal cycle  
1199 primarily caused by uptake and release of CO<sub>2</sub> by the terrestrial biosphere. Bottom: As top panel but  
1200 for XCH<sub>4</sub> (algorithms: SCIAMACHY: WFMD and IMAP, TANSO: SRFP, SRPR, OCFP, OCPR).  
1201 The seasonal cycle of methane is primarily due to wetland emissions, which are largest in summer /  
1202 early autumn, when soils are warm and humid. Also clearly visible is the not yet well understood  
1203 recent methane increase. For a color version of this figure please have a look at the on-line version of  
1204 this publication.

1205

1206



1207

1208

1209 **Figure 2:** Global XCO<sub>2</sub> maps from SCIAMACHY (left) and CarbonTracker (right) for two seasons

1210 (April-June, top, and July-September, bottom) and two years (2003 and 2009). The CarbonTracker

1211 model data have been sampled according to the SCIAMACHY measurements and the SCIAMACHY

1212 averaging kernels have been applied to CarbonTracker. Figure adapted from Heymann et al., 2012b.

1213 For a color version of this figure please have a look at the on-line version of this publication.

1214

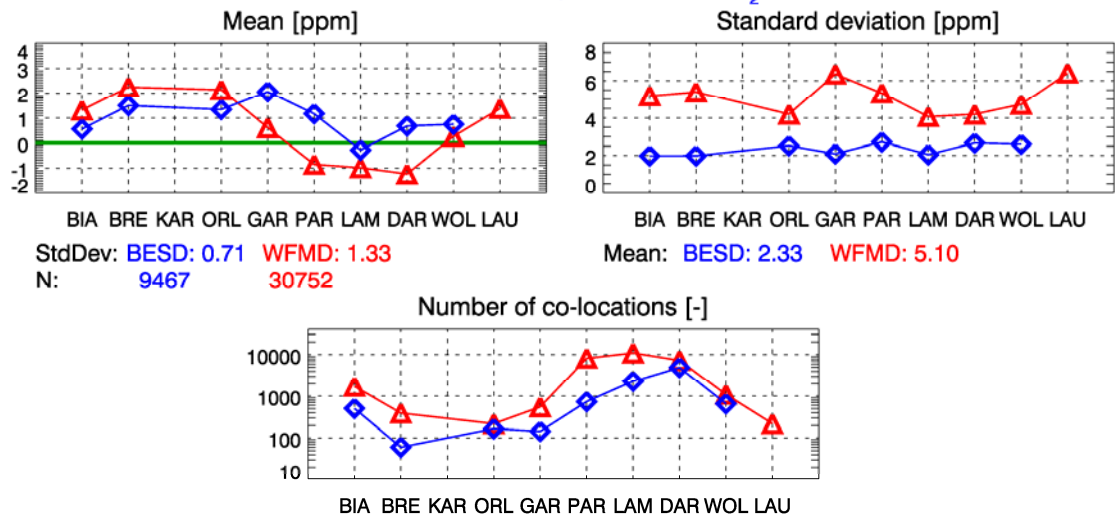
1215

1216

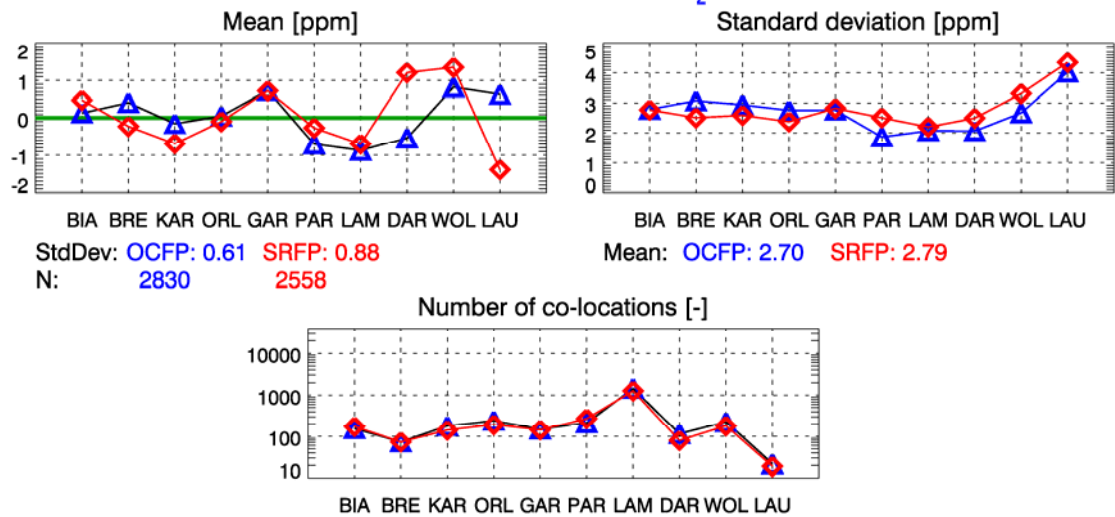
1217

### Satellite - TCCON differences: XCO<sub>2</sub>

#### SCIAMACHY/ENVISAT XCO<sub>2</sub>



#### TANSO/GOSAT XCO<sub>2</sub>



1218

1219

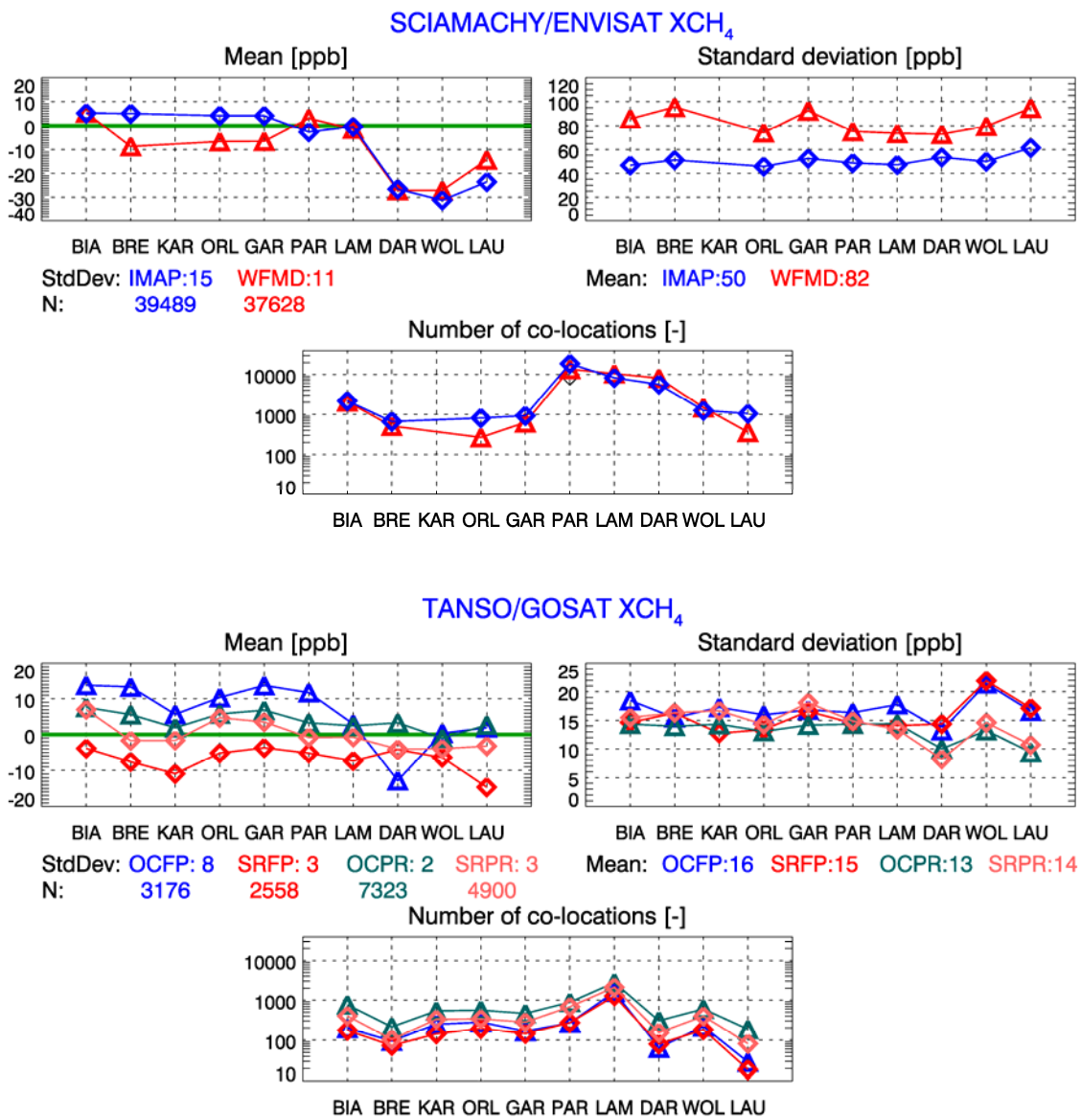
1220

1221 **Figure 3:** Comparison of the GHG-CCI core ECV XCO<sub>2</sub> data products from  
1222 SCIAMACHY/ENVISAT (top half, i.e., first 3 panels) and TANSO/GOSAT (bottom half) with  
1223 TCCON ground-based observations (see Table 4 for details on the TCCON sites). Shown are the mean  
1224 difference (“Mean” in ppm) with respect to TCCON (left), the standard deviation of the difference  
1225 (right), and the number of co-locations (middle). A 500 km / 2 hour spatio-temporal co-location  
1226 criterion has been used to compute the satellite – TCCON differences. The numerical values listed are:  
1227 Left: “StdDev” is the standard deviation of the mean differences as obtained at the TCCON sites, i.e.,  
1228 a measure of the station-to-station bias, and can be interpreted as relative accuracy (relative bias) of  
1229 the satellite retrievals. “N” is the number of satellite data used for comparison (only those data points  
1230 are shown where at least 10 satellite observations are available for a given site). Right: “Mean” is the  
1231 mean value of the standard deviations show by the symbols and is a measure of the achieved overall  
1232 precision. Note that the number of co-locations is significantly different for the different TCCON sites,  
1233 e.g., due to clouds. For a color version of this figure please have a look at the on-line version of this  
1234 publication.

1235

1236  
1237

Satellite - TCCON differences: XCH<sub>4</sub>



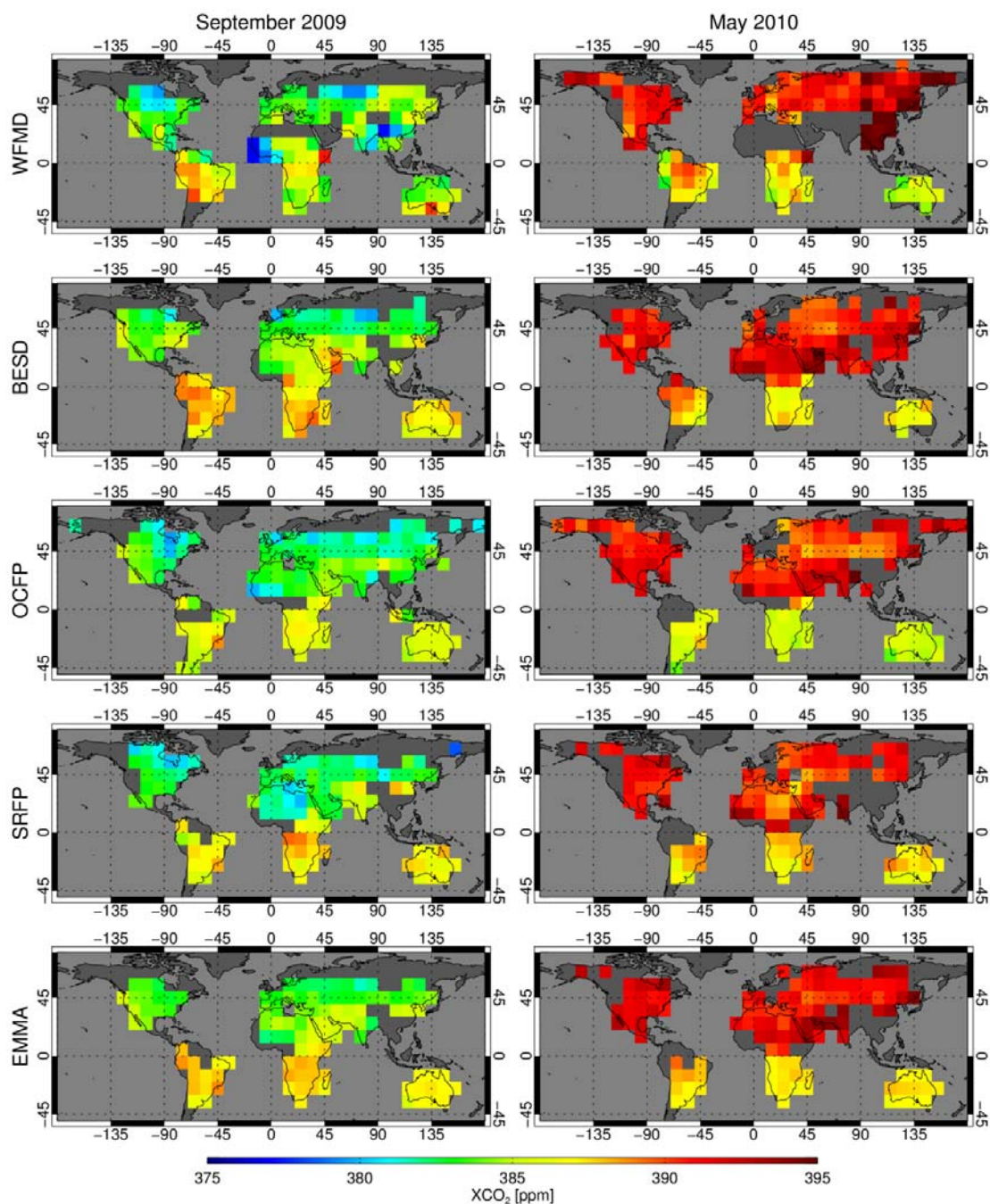
1238  
1239

1240 **Figure 4:** As Fig. 3 but for the GHG-CCI XCH<sub>4</sub> data products.

1241

1242

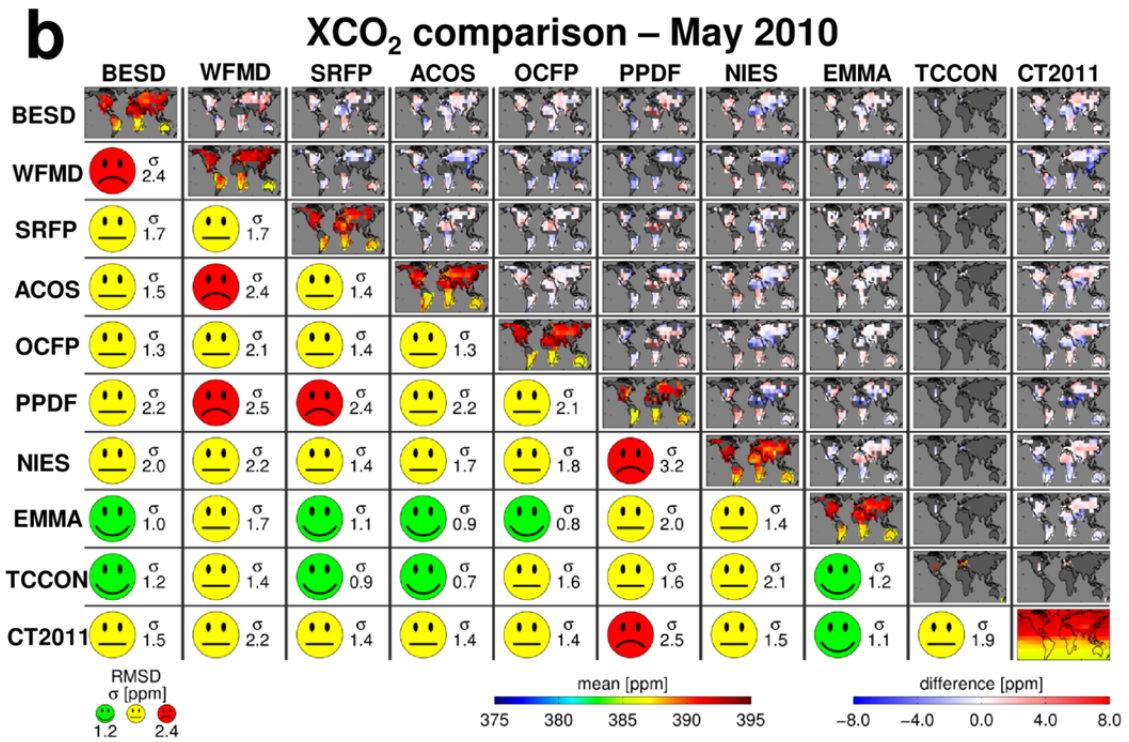
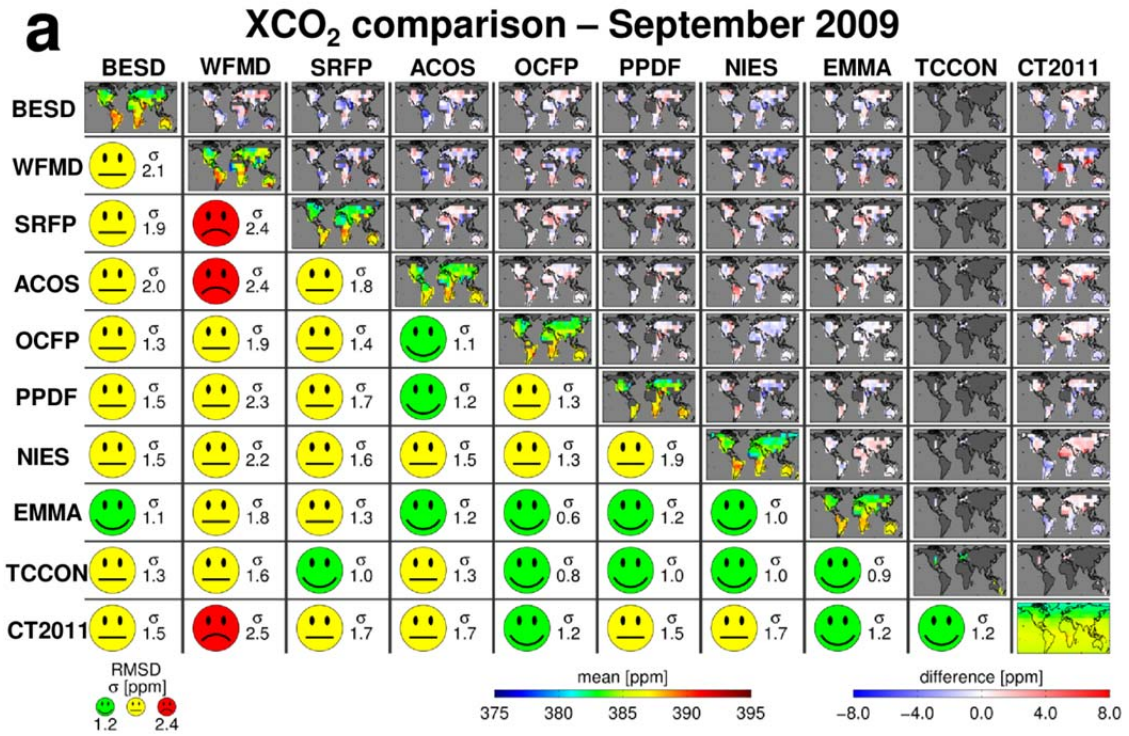




1244

1245 **Figure 5:** Maps of monthly mean XCO<sub>2</sub> at 10°x10° resolution as obtained using different GHG-CCI  
 1246 retrieval algorithms: WFMD and BESD for SCIAMACHY, OCFP and SRFP for TANSO and  
 1247 SCIAMACHY and TANSO merged using EMMA for September 2009 (left) and May 2012 (right).  
 1248 For a color version of this figure please have a look at the on-line version of this publication.

1249

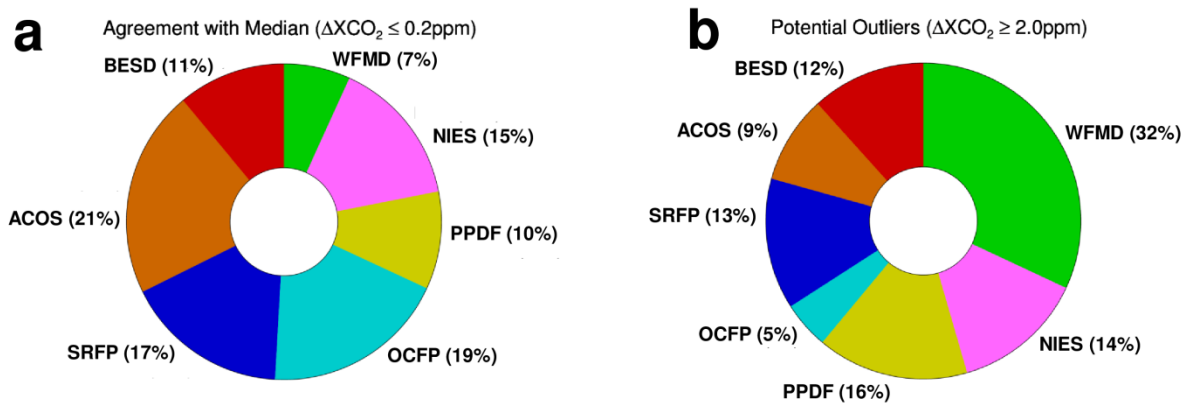


1253

1254 **Figure 6:** Comparison matrix of monthly XCO<sub>2</sub> maps for September 2009 (top (a)) and May 2010  
1255 (bottom (b)) generated using several individual satellite retrieval algorithms: BESD and WFMD for  
1256 SCIAMACHY and SRFP, ACOS, OCFP, PPDF, NIES for TANSO. The EMMA data product has  
1257 been generated from the ensemble of the individual SCIAMACHY and TANSO XCO<sub>2</sub> data products  
1258 (see main text for details). Also shown is XCO<sub>2</sub> from TCCON and NOAA’s CarbonTracker (CT,  
1259 v2011). The diagonal elements show the monthly XCO<sub>2</sub> maps (using color bar “mean”). The above  
1260 diagonal elements show the XCO<sub>2</sub> differences for all combinations (color bar “difference”). The below  
1261 diagonal elements show the numerical values of the Root Mean Square Difference (RMSD) as well as  
1262 color coded smileys of the RMSD (green: RMSD < 1.2 ppm, red: RMSD > 2.4 ppm, otherwise  
1263 yellow). For a color version of this figure please have a look at the on-line version of this publication.

1264

1265



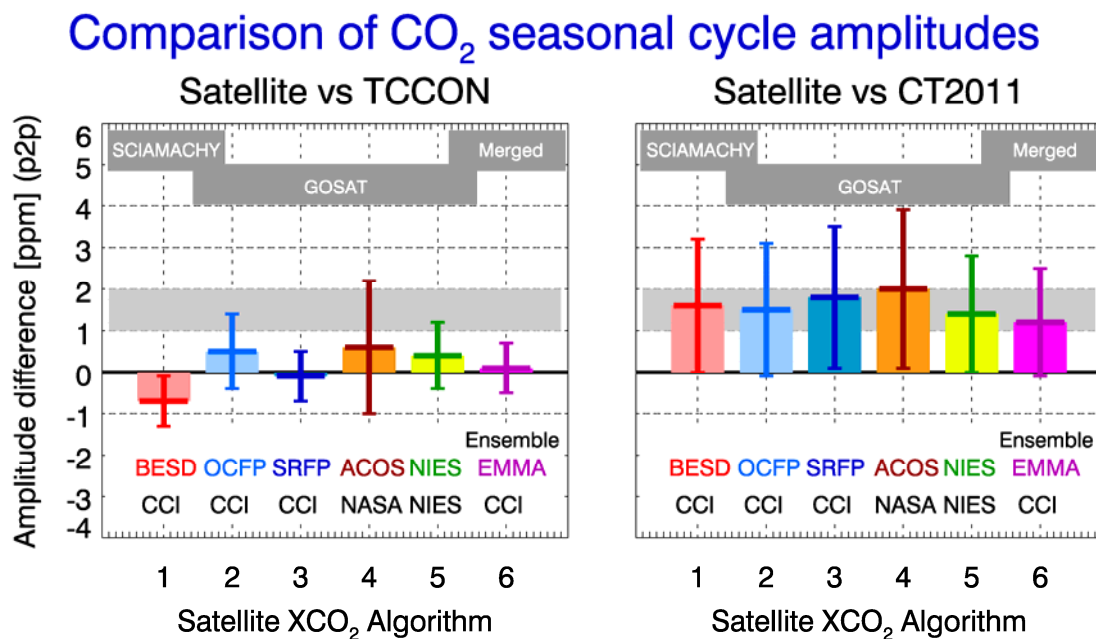
1266

1267 **Figure 7:** Pie charts showing the agreement (left) and disagreement (right) with the EMMA median  
1268 obtained using the listed satellite XCO<sub>2</sub> data products. The figure has been obtained using the EMMA  
1269 Level 3 data product (10°x10°, monthly = 1 voxel). For each voxel the mean XCO<sub>2</sub> value for each  
1270 algorithm has been computed and the median using all algorithms. The “Agreement with the Median”  
1271 (left) has been computed as follows: For algorithm *i* the number of voxels which agree with the  
1272 median within 0.2 ppm have been counted (=  $N_i$ ). 100% corresponds to the sum of these numbers ( $N =$   
1273  $\sum_i N_i$ ). The percentages shown are  $N_i/N * 100\%$ . The percentages of “Potential Outliers” (right) have  
1274 been calculated using the same method except that all voxels have been counted where the differences  
1275 to the median are larger than 2 ppm. As can be seen from the left figure, the data product which  
1276 agrees best with the median is the ACOS product (v2.9, 21% agreement) followed by the similar  
1277 OCFP algorithm (19% agreement). The largest number of potential outliers have the data products  
1278 generated with the two very fast algorithms WFMD (32%) and PPDF (16%). For a color version of  
1279 this figure please have a look at the on-line version of this publication.

1280

1281

1282

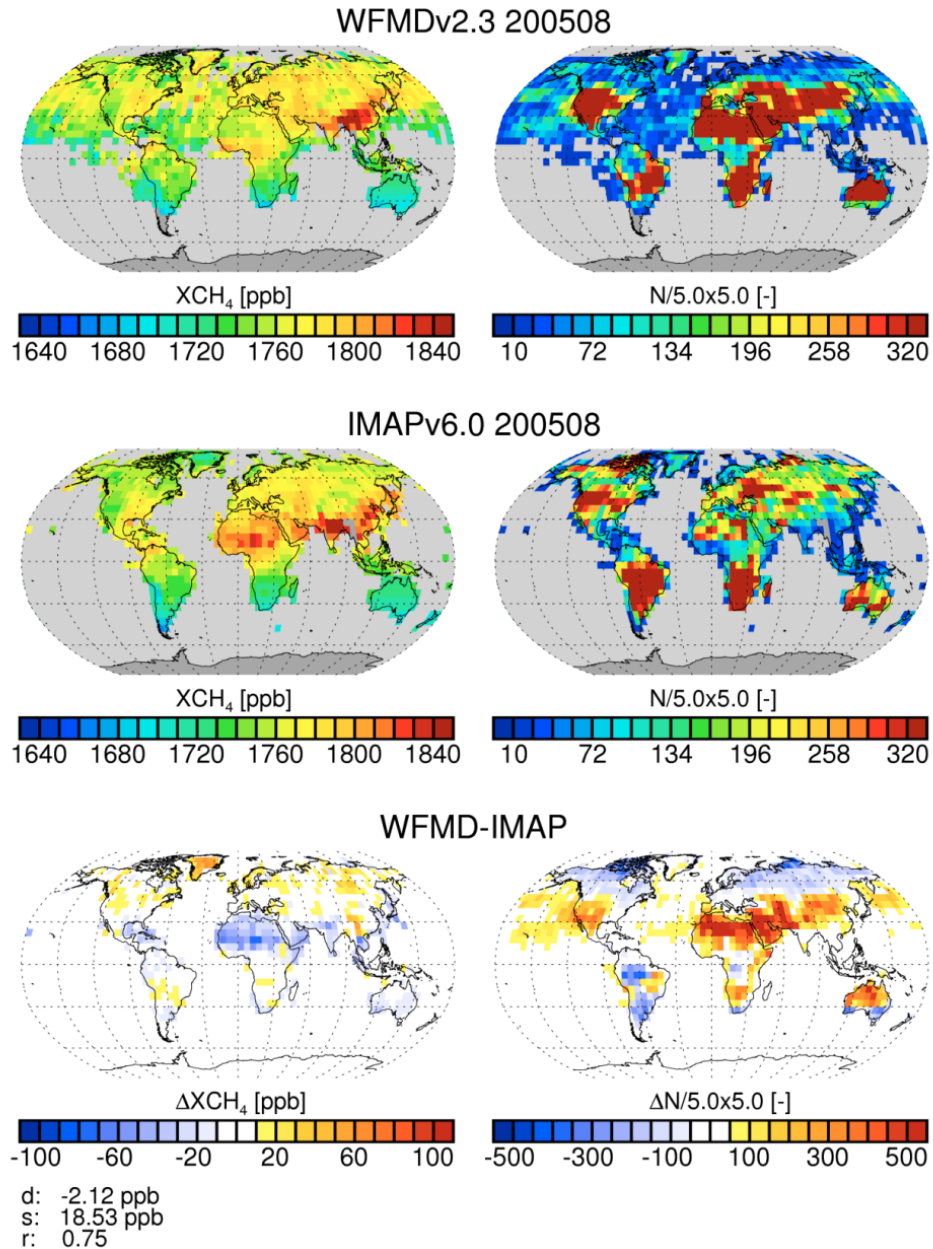


1284

1285 **Figure 8:** Comparison of the XCO<sub>2</sub> seasonal cycle amplitude (peak-to-peak) of the individual XCO<sub>2</sub>  
 1286 algorithms and EMMA with TCCON (left) and CarbonTracker (v2011) (right). The figure has been  
 1287 adapted from Reuter et al., 2013, where results for all investigated XCO<sub>2</sub> data products are shown, i.e.,  
 1288 including WFMD and PPDF, not shown here as their error bars do not indicate good enough  
 1289 agreement with TCCON. As can be seen, all XCO<sub>2</sub> satellite data suggest that the amplitude of the CO<sub>2</sub>  
 1290 seasonal cycle is underestimated by CarbonTracker by approximately 1.5+/-0.5 ppm peak-to-peak. For  
 1291 a color version of this figure please have a look at the on-line version of this publication.

1292

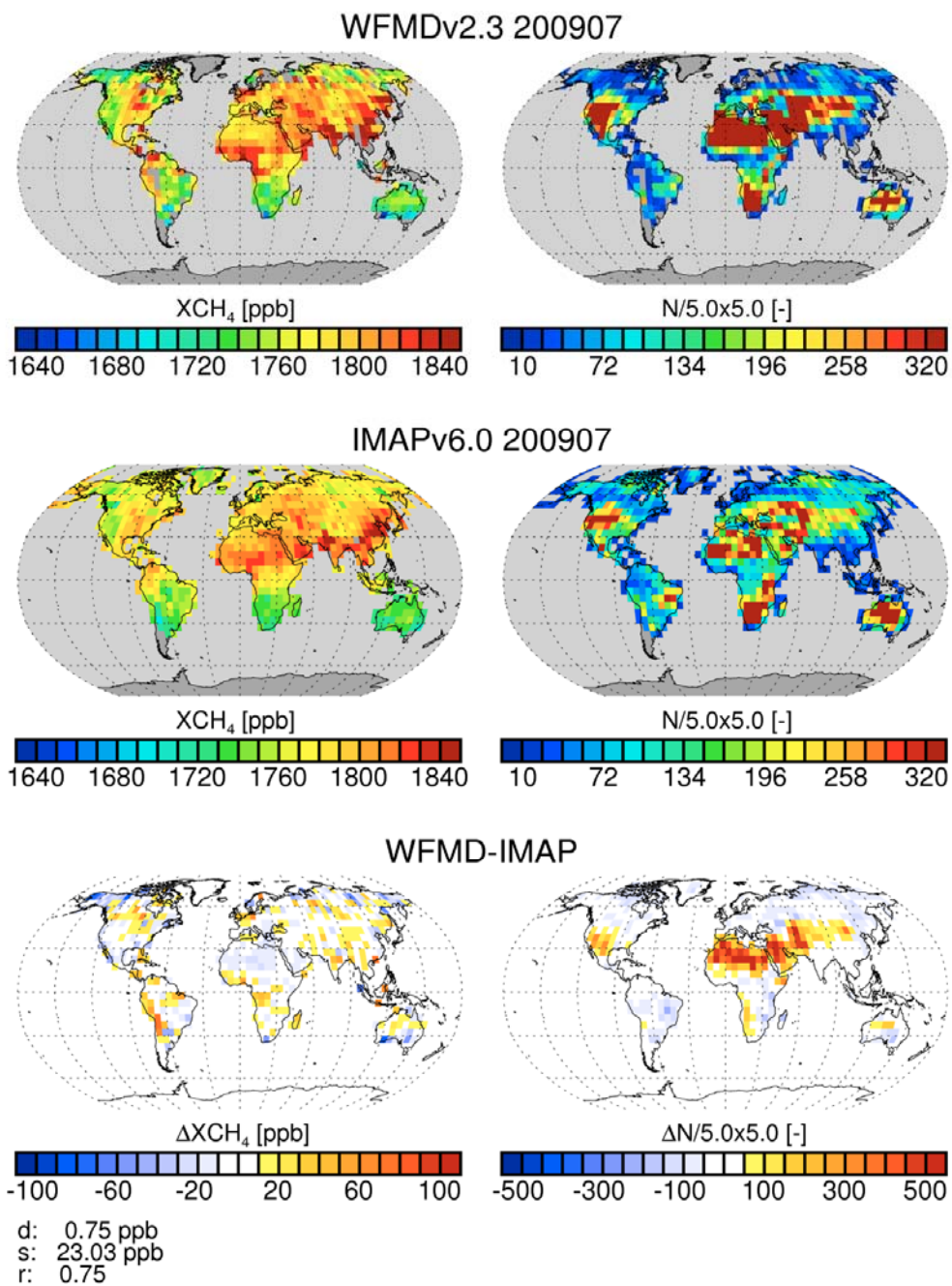
1293



1295

1296 **Figure 9:** Comparison of two SCIAMACHY XCH<sub>4</sub> data products retrieved using WFMD (top) and  
 1297 IMAP (middle) for August 2005. Global maps of the retrieved XCH<sub>4</sub> are shown on the left and the  
 1298 number of retrievals per 5°x5° grid cell on the right. The WFMD-IMAP difference is shown in the  
 1299 bottom row. Listed in the bottom left are the following parameters: d: mean difference (-2.12 ppb), s:  
 1300 standard deviation of the difference (18.53 ppb), r: linear correlation coefficient (0.75). For a color  
 1301 version of this figure please have a look at the on-line version of this publication.

1302



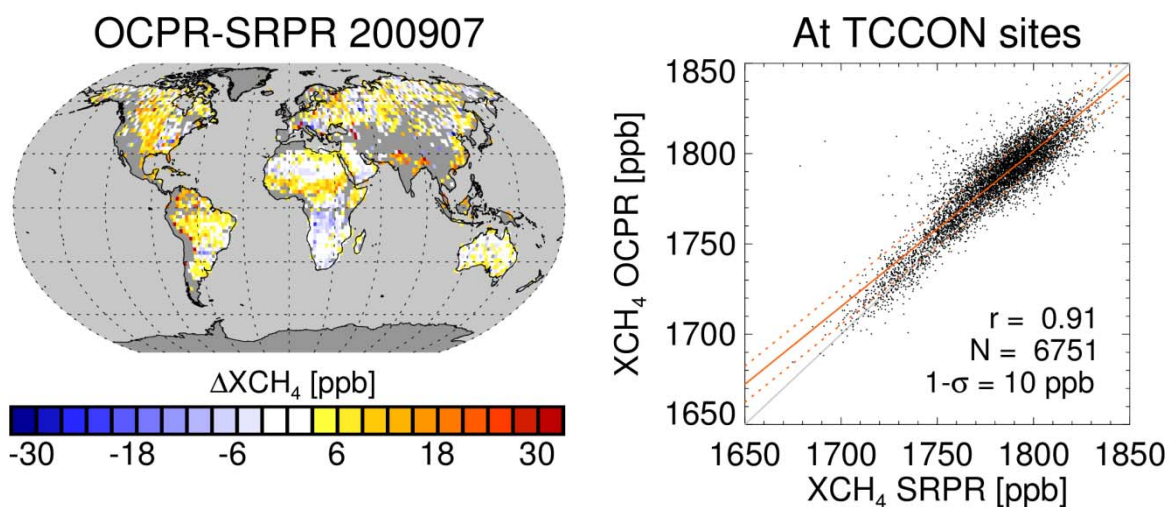
1304

1305 **Figure 10:** As Fig. 9 but for July 2009.

1306

1307

1308



1309

1310

1311 **Figure 11:** Comparison of the two GHG-CCI TANSO XCH<sub>4</sub> PR data products retrieved using the  
1312 OCPR and SRPR retrieval algorithms. Left: Percentage XCH<sub>4</sub> difference OCPR-SRPR for July 2009.  
1313 Right: Scatter plot of 6751 co-located OCPR versus SRPR retrievals at TCCON sites. The standard  
1314 deviation of the difference is 10 ppb (1-sigma) and the linear correlation coefficient is 0.91. For a color  
1315 version of this figure please have a look at the on-line version of this publication.

1316