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1 **The Greenhouse Gas Climate Change Initiative (GHG-CCI): comparison and quality**
2 **assessment of near-surface-sensitive satellite-derived CO₂ and CH₄ global data sets**

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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 CO₂
46 and CH₄ - with a quality sufficient to obtain information on regional CO₂ and CH₄ 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 CO₂ and CH₄, denoted XCO₂ and XCH₄, to
50 meet the demanding user requirements. GHG-CCI focusses on four core data products: XCO₂ from
51 SCIAMACHY and TANSO and XCH₄ 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 XCO₂ (< 3 ppm) and TANSO XCH₄ (< 17 ppb). The achieved
62 relative accuracy for XCH₄ 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 XCO₂ 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 (CO₂) is the most important anthropogenic greenhouse gas (GHG) contributing to
73 global warming (Solomon et al., 2007). Despite its importance, our knowledge of the CO₂ sources and
74 sinks has significant gaps (e.g., Stephens et al., 2007, Canadell et al., 2010) and despite efforts to
75 reduce CO₂ emissions, atmospheric CO₂ 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 CO₂ 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 (CH₄, 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 CO₂ and CH₄ 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 CO₂ and CH₄, 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 CO₂ and CH₄. They also cover
105 the O₂ 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 CO₂ and CH₄, denoted XCO₂ (in ppm) and XCH₄ (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 CH₄ profiles and
111 IASI/METOP for mid/upper tropospheric CO₂ and CH₄ 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 XCO₂ and
116 XCH₄, which is also the focus of this manuscript. Other algorithms, referred to as Additional
117 Constraints Algorithms (ACAs), are algorithms to retrieve CO₂ and/or CH₄ 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 XCO₂. 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 XCO₂ and XCH₄ 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 CO₂
143 and CH₄ 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 XCO₂.
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" XCO₂ and XCH₄ 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 CO₂ and CH₄ 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 XCO₂. 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 CO₂ 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 XCH₄ are also challenging but somewhat less demanding than those for XCO₂.
201 The main reason is that XCH₄ is more variable compared to XCO₂ 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 XCO₂ (in ppm) and XCH₄ (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 XCO₂ and the bottom panel XCH₄ time series. As can be
214 seen, the various XCO₂ 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 XCH₄ product generated with the IMAP algorithm (Frankenberg et al., 2011) suffers
223 from a significant high bias (relative to several other TANSO/GOSAT XCH₄ 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 XCH₄ 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 XCO₂ this is a
230 challenge because of demanding user requirements and for XCH₄ 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., XCO₂ and/or XCH₄) 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 XCH₄ retrieval using CO₂ as a reference gas. The XCH₄ is
245 essentially obtained from computing the ratio of the retrieved CH₄ column and the retrieved CO₂
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 CH₄/CO₂ column ratio). The disadvantage is that a correction is needed
248 for CO₂ 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 XCO₂ 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 XCO₂ and XCH₄ 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 CO₂ and CH₄ 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 XCO₂ (Heymann et al., 2012a). Recently, an improved version of
265 WFMD has been developed for SCIAMACHY XCO₂ retrieval (Heymann et al., 2012b, see also
266 Figure 2) and the XCO₂ data set generated with this latest version has been used for the GHG-CCI RR.
267 For SCIAMACHY XCH₄ 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 XCO₂ 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 XCO₂.

275 **4.3 TANSO XCO₂ algorithms**

276 Both GHG-CCI TANSO XCO₂ 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 XCH₄ algorithms**

285 For SCIAMACHY XCH₄ 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 XCH₄ 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 XCH₄ algorithms**

293 To overcome the key limitation of the XCH₄ PR algorithms, namely the need to correct the retrieved
294 XCH₄ for CO₂ 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 CH₄. Two TANSO XCH₄ FP retrieval algorithms are being used
297 within GHG-CCI, which are also used for TANSO XCO₂ 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 XCO₂ and XCH₄ 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 XCO₂ 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 XCO₂ or XCH₄ biases when applied to real data.

337 What has been evaluated in detail are the end products, i.e., the quality of the XCO₂ and XCH₄ 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 XCO₂ and
360 XCH₄ 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/; 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 XCO₂ (~0.4 ppm) and 0.2% for XCH₄ (~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 XCO₂ (1-
373 sigma) and 4 ppb (1-sigma) for XCH₄ (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: XCO₂: 2006-2009; XCH₄: 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 XCO₂ and XCH₄ 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 XCO₂ is discussed at Lamont, USA, where the real variability of
396 the CO₂ 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 XCO₂ products from SCIAMACHY and TANSO by adjusting all retrievals to a
400 common *a priori* using the Simple Empirical CO₂ 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 XCO₂ and 0.05 ppm for
403 TCCON XCO₂. 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 XCO₂. 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 XCH₄ 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 XCO₂ (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 CO₂ and CH₄ 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 XCO₂ and Fig. 4 for XCH₄., 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 XCO₂ comparisons with TCCON**

446 The comparison of the two SCIAMACHY XCO₂ 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 XCO₂ 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 XCO₂ 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 XCH₄ comparisons with TCCON**

472 The comparison of the two SCIAMACHY XCH₄ 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 XCH₄ (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 CH₄ 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 XCH₄ 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 XCH₄ 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 XCH₄ has a much higher precision and even the breakthrough precision requirement is met by all
510 algorithms. All TANSO XCH₄ 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 XCO₂ and
517 XCH₄, as described in the following.

518 **5.3 Inter-comparison of XCO₂ data products**

519 Within GHG-CCI two algorithms have been further developed to retrieve XCO₂ from SCIAMACHY,
520 namely WFMD and BESD, and two algorithms to retrieve XCO₂ 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 CO₂ Observations from Space) v2.9 algorithm (O’Dell et al., 2012, Crisp et al., 2012).

528 The global XCO₂ 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 XCO₂ data products all capture the expected large scale variations of atmospheric CO₂ such as the
531 time dependent north-south gradient (Figures 5 and 6, discussed below) and the CO₂ 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 XCO₂ 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 XCO₂, and XCO₂ from NOAA's CO₂ assimilation system CarbonTracker (CT) (Peters et al.,
540 2007). As can be seen, all satellite retrieval algorithms capture the north-south XCO₂ 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 XCO₂ data
551 sets shown in Figures 5 and 6. One approach to further assess the relative quality of the various
552 satellite-derived global XCO₂ 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 XCO₂ 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 XCO₂ 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 XCO₂ data products, which can be used for comparison with the individual
566 data products, e.g., to identify outliers. However, the EMMA XCO₂ product has also been generated to
567 be useful as a stand-alone XCO₂ 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 XCO₂ 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 XCH₄ in the early part of the Bialystok time series that occurred due to
574 missing fits in one of the CH₄ 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 XCO₂
580 products shown in Figs. 6 and 7 and generates a Level 2 product (i.e., a product containing the XCO₂
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 XCO₂ 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 XCO₂ 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 XCO₂ 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 XCO₂ 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 XCO₂ 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 XCH₄ data products**

623 The multi-year global retrievals obtained from the two SCIAMACHY XCH₄ 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 XCH₄ 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 XCH₄ 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 XCH₄ data products**

654 Within GHG-CCI, four TANSO XCH₄ 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 CH₄ to CO₂ columns, followed
659 by a model-based CO₂ correction to compute XCH₄, the column ratios have been compared as well as
660 the final XCH₄ product. As expected, it has been found that the agreement between the ratios is
661 typically somewhat better compared to the XCH₄ products due to differences between the model-based
662 CO₂ 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 XCH₄ 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 XCO₂**

688 Within GHG-CCI, two SCIAMACHY and two TANSO XCO₂ 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 XCO₂ data products generated outside of this project: with the two
691 TANSO XCO₂ 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 XCO₂ 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 XCO₂ 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 XCO₂ algorithms and to add the EMMA data product to the
710 GHG-CCI product portfolio.

711 **5.6.2 Selection results: SCIAMACHY XCH₄**

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 XCH₄**

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 XCH₄ 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 XCH₄ algorithms
742 depend on a CO₂ correction using model data. The long-term goal of GHG-CCI is to use a FP
743 algorithm that is independent of a CO₂ 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 XCH₄ 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 CO₂ and/or CH₄ 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 CO₂ and/or CH₄ 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 XCO₂ and XCH₄ 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 CO₂ and CH₄ 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 XCO₂ and XCH₄ 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 XCO₂ and XCH₄ 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 XCO₂ and 10 ppb for XCH₄. 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 CO₂ and CH₄ 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.

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842 **10. References**

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1141 **11. Tables**

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1143 **Table 1:** GHG-CCI XCO₂ and XCH₄ 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).

Requirements for regional CO₂ and CH₄ source/sink determination using SCIAMACHY/ENVISAT and TANSO/GOSAT					
Parameter	Requirement type	Random error		Systematic error	Stability
		Single observation	1000² km², monthly		
XCO ₂	G	< 1 ppm	< 0.3 ppm	< 0.2 ppm (absolute)	As systematic error but per year
	B	< 3 ppm	< 1.0 ppm	< 0.3 ppm (relative)	--
	T	< 8 ppm	< 1.3 ppm	< 0.5 ppm (relative)	--
XCH ₄	G	< 9 ppb	< 3 ppb	< 1 ppb (absolute)	As systematic error but per year
	B	< 17 ppb	< 5 ppb	< 5 ppb (relative)	--
	T	< 34 ppb	< 11 ppb	< 10 ppb (relative)	--

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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”)).

GHG-CCI ECV Core Algorithms (ECAs)				
Algorithm ID	Data product	Sensor	Algorithm short name	References
CO2_SCI_WFMD	XCO ₂	SCIAMACHY/ ENVISAT	WFMD (WFM-DOAS)	<i>Schneising et al., 2011, 2012;</i> <i>Heymann et al., 2012b</i>
CO2_SCI_BESD	XCO ₂	SCIAMACHY	BESD	<i>Reuter et al., 2010, 2011</i>
CO2_GOS_OCFP	XCO ₂	TANSO/GOSAT	OCFP (UoL-FP)	<i>Cogan et al., 2012</i>
CO2_GOS_SRFPP	XCO ₂	TANSO/GOSAT	SRFP (RemoteC)	<i>Butz et al., 2011</i>
CH4_SCI_WFMD	XCH ₄	SCIAMACHY	WFMD (WFM-DOAS)	<i>Schneising et al., 2010, 2011</i>
CH4_SCI_IMAP	XCH ₄	SCIAMACHY	IMAP	<i>Frankenberg et al., 2011</i>
CH4_GOS_OCFP	XCH ₄	TANSO/GOSAT	OCFP	<i>Parker et al., 2011</i>
CH4_GOS_OCPR	XCH ₄	TANSO/GOSAT	OCPR	<i>Parker et al., 2011</i>
CH4_GOS_SRFPP	XCH ₄	TANSO/GOSAT	SRFP	<i>Butz et al., 2011</i>
CH4_GOS_SRPR	XCH ₄	TANSO/GOSAT	SRPR	<i>Schepers et al., 2012</i>

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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 2nd 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.

GHG-CCI Additional Constraints Algorithms (ACAs)				
Algorithm ID	Data product	Sensor	Algorithm	References
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>

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1168 **Table 4:** TCCON sites as used for the validation of the satellite-derived XCH₄ and XCO₂ Round

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

TCCON validation sites used for GHG-CCI Round Robin					
Name	ID	Latitude [deg]	Longitude [deg]	Altitude [km]	Time coverage MM/YYYY-MM/YYYY
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

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Table 5: Estimated precision and biases of the satellite XCO₂ (top) and XCH₄ (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).

Comparison of GHG-CCI core data products (ECAs) with TCCON				
XCO₂ [ppm]				
Algorithm	Sensor	Estimated precision single observation	Estimated relative biases	Number of satellite obs.
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)	-
XCH₄ [ppb]				
Algorithm	Sensor	Estimated precision single observation	Estimated relative biases	Number of satellite obs.
WFMD v2.3	SCIAMACHY	82 (~30 [#])	11 (~3 [§]) [4-12 [#]]	37628
IMAP v6.0	SCIAMACHY	50 (~30 [#])	15 [4-13 [#]]	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)	-

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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.

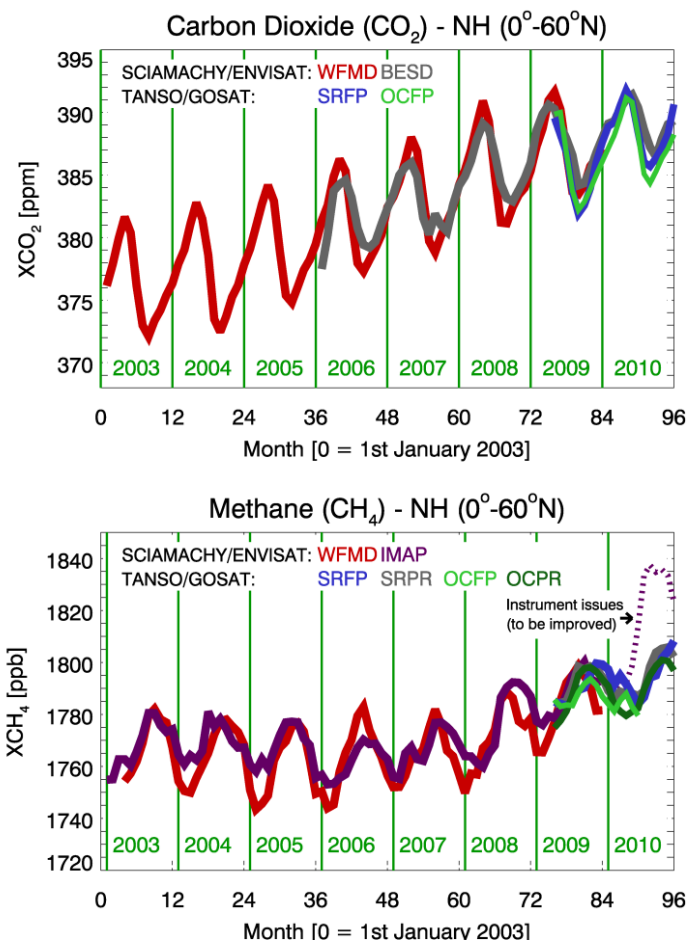
Planned content of the GHG-CCI Climate Research Data Package (CRDP)				
Data products generated with ECV Core Algorithms (ECAs)				
Product ID	Product (Level 2, mixing ratios)	Algorithm §)	Coverage	Comment
XCO2_SCIA	XCO ₂	BESD	Global, land, 2003-2010 ^{*)}	-
XCO2_GOSAT	XCO ₂	OCFP and SRFP	Global, mid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

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1193 **12. Figures**

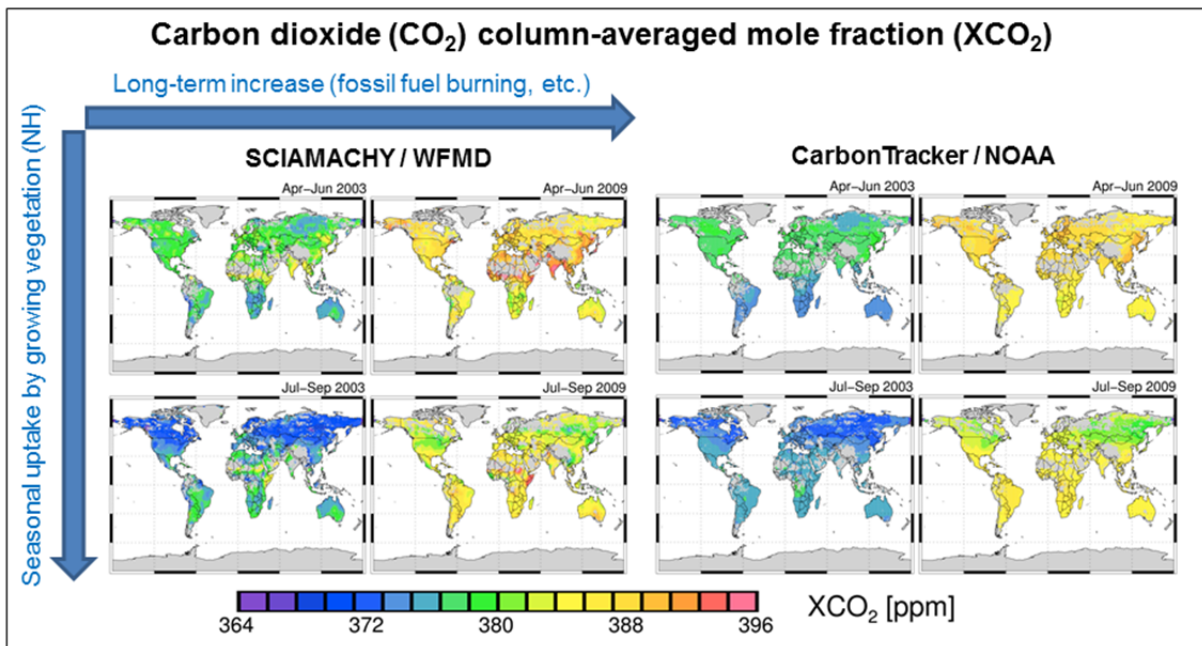


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1195 **Figure 1:** Top: Northern hemispheric monthly mean XCO₂ time series retrieved from
1196 SCIAMACHY/ENVISAT (algorithms: WFMD and BESD) and TANSO/GOSAT (algorithms: SRFP
1197 and OCFP) satellite data. Shown are monthly mean values for the 0°-60°N latitude range. Clearly
1198 visible is the CO₂ increase primarily caused by the burning of fossil fuels and the seasonal cycle
1199 primarily caused by uptake and release of CO₂ by the terrestrial biosphere. Bottom: As top panel but
1200 for XCH₄ (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.

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1209 **Figure 2:** Global XCO₂ 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.

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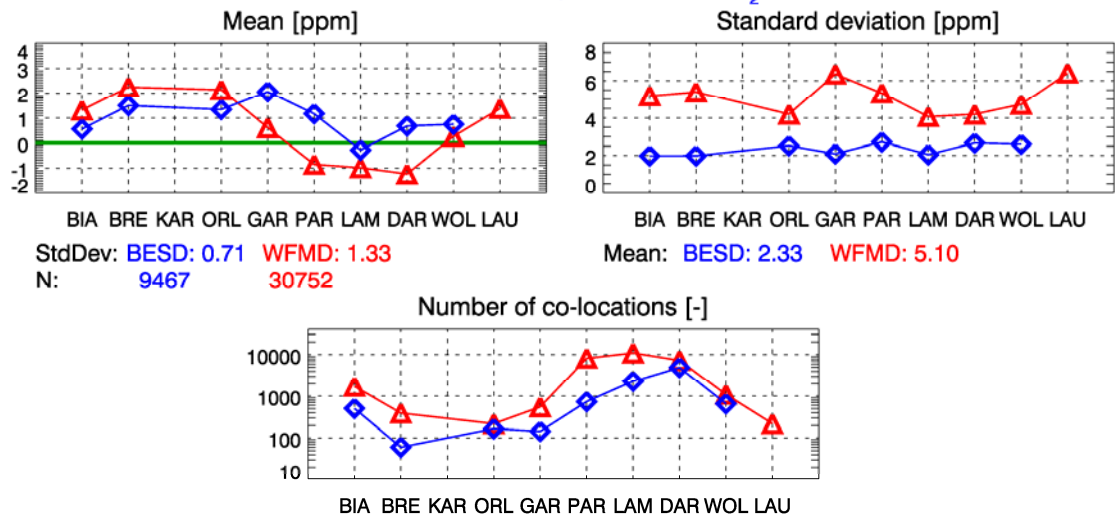
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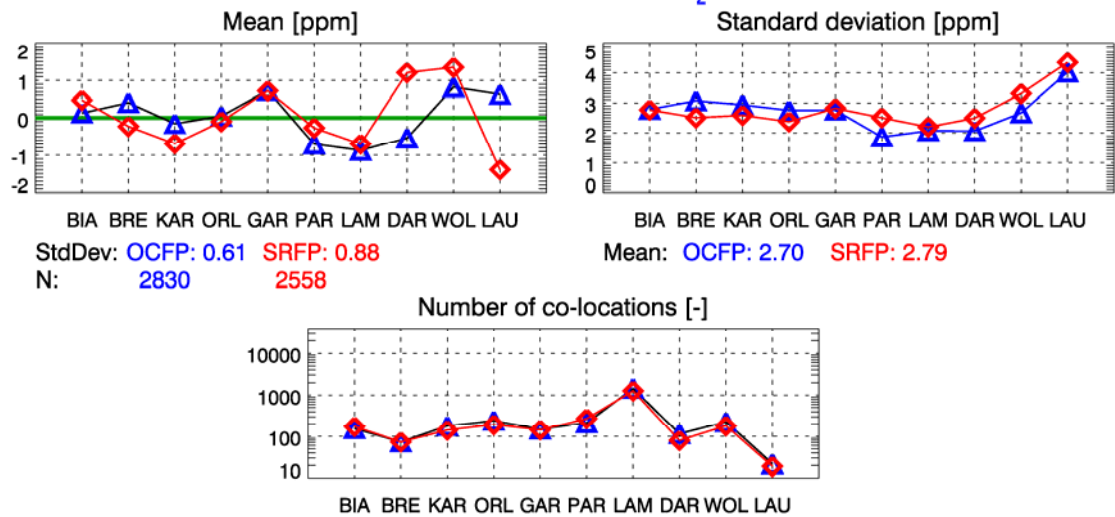
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Satellite - TCCON differences: XCO₂

SCIAMACHY/ENVISAT XCO₂



TANSO/GOSAT XCO₂



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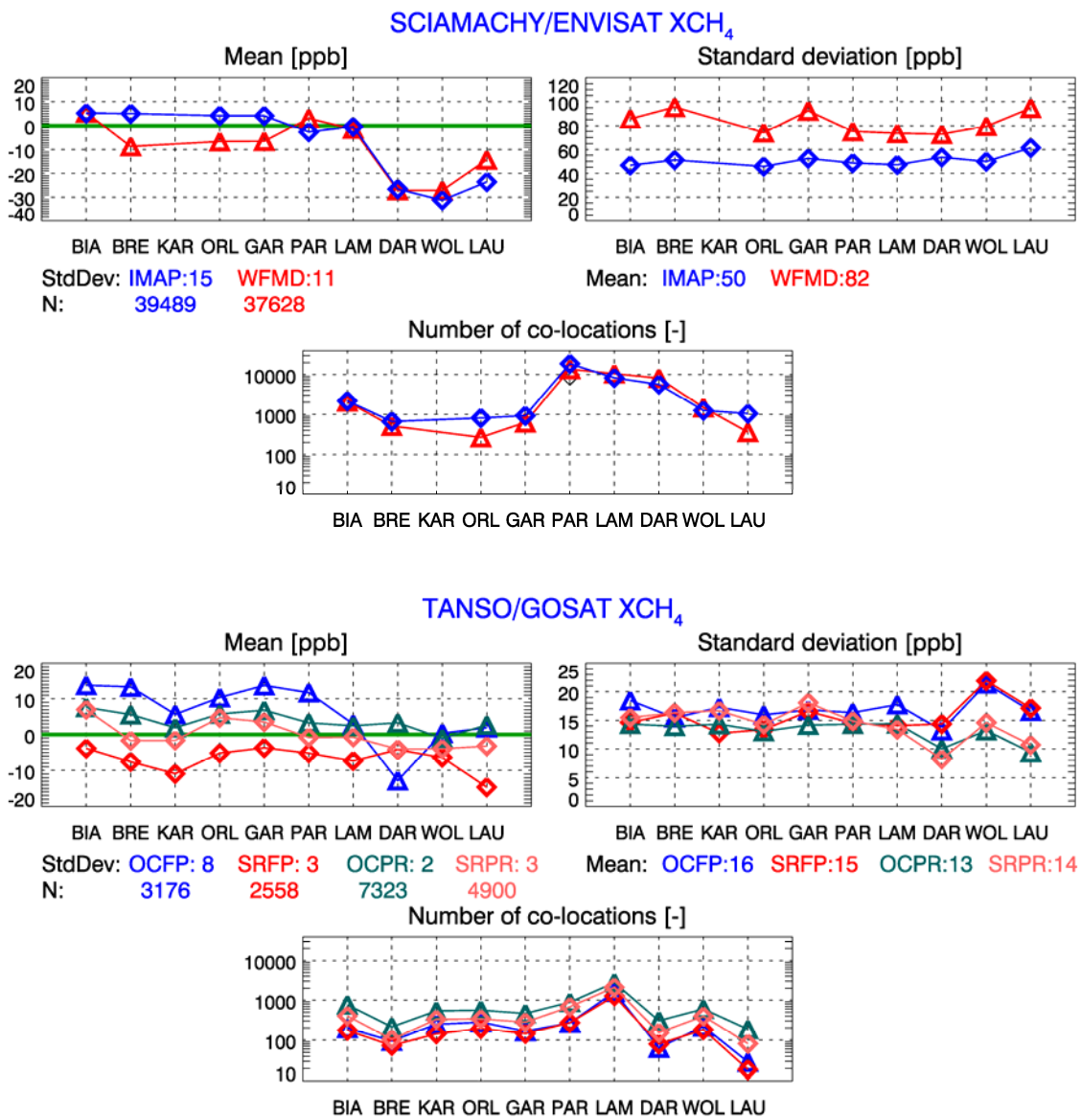
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1221 **Figure 3:** Comparison of the GHG-CCI core ECV XCO₂ data products from
1222 SCIAMACHY/ENVISAT (top half, i.e., first 3 panels) and TANSO/GOSAT (bottom half) with
1223 TCCON ground-based observations (see Table 4 for details on the TCCON sites). 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.

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Satellite - TCCON differences: XCH₄

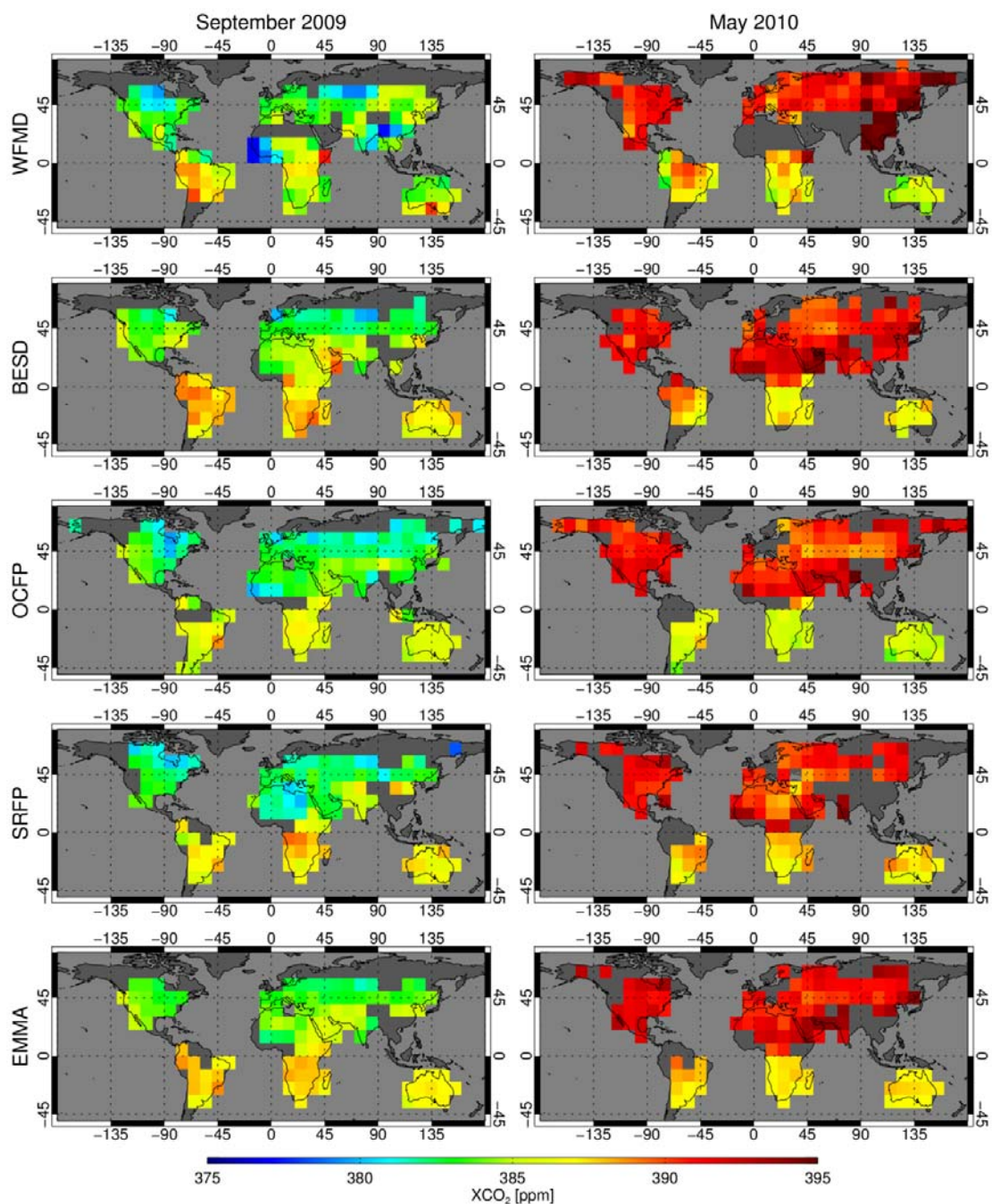


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1240 **Figure 4:** As Fig. 3 but for the GHG-CCI XCH₄ data products.

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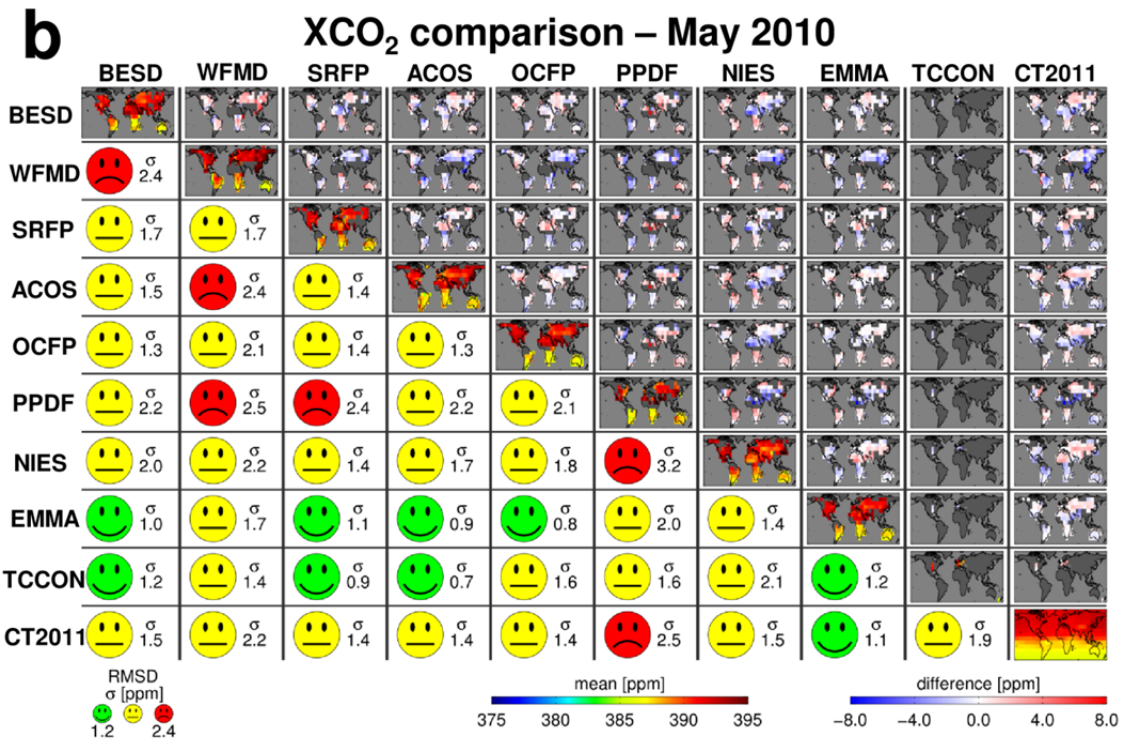
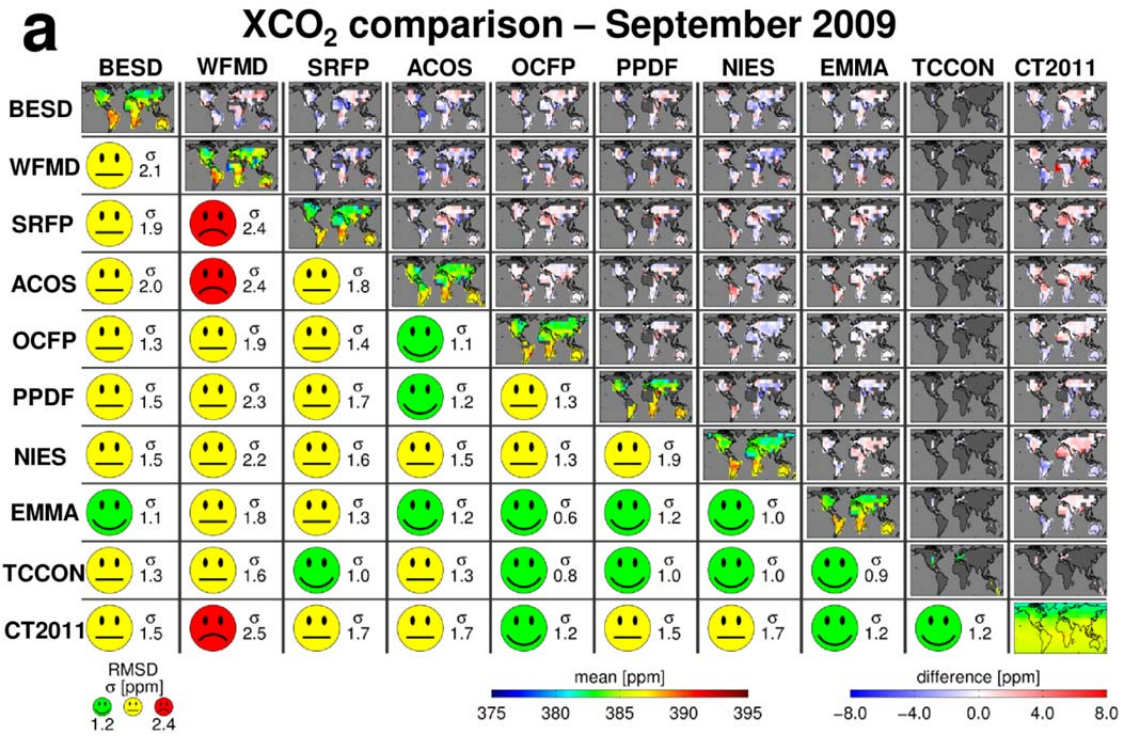
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1245 **Figure 5:** Maps of monthly mean XCO₂ at 10°x10° resolution as obtained using different GHG-CCI
 1246 retrieval algorithms: WFMD and BESD for SCIAMACHY, OCFP and SRFP for TANSO and
 1247 SCIAMACHY and TANSO merged using EMMA for September 2009 (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.

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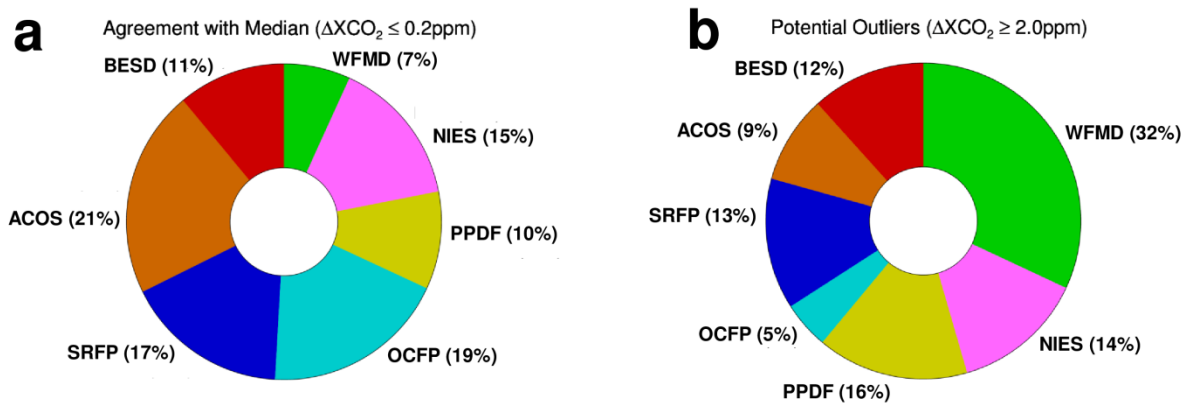


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1254 **Figure 6:** Comparison matrix of monthly XCO₂ maps for September 2009 (top (a)) and May 2010
1255 (bottom (b)) generated using several individual satellite retrieval algorithms: BESD and WFMD for
1256 SCIAMACHY and SRFP, ACOS, OCFP, PPDF, NIES for TANSO. The EMMA data product has
1257 been generated from the ensemble of the individual SCIAMACHY and TANSO XCO₂ data products
1258 (see main text for details). Also shown is XCO₂ from TCCON and NOAA's CarbonTracker (CT,
1259 v2011). The diagonal elements show the monthly XCO₂ maps (using color bar "mean"). The above
1260 diagonal elements show the XCO₂ 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.

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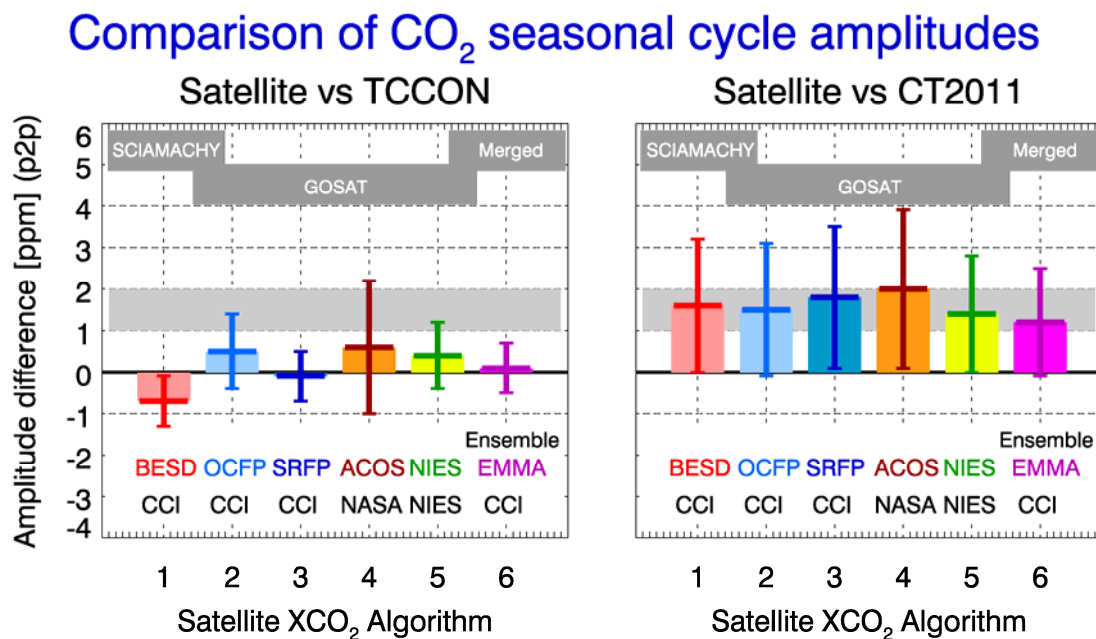
1266

1267 **Figure 7:** Pie charts showing the agreement (left) and disagreement (right) with the EMMA median
1268 obtained using the listed satellite XCO₂ 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 XCO₂ 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.

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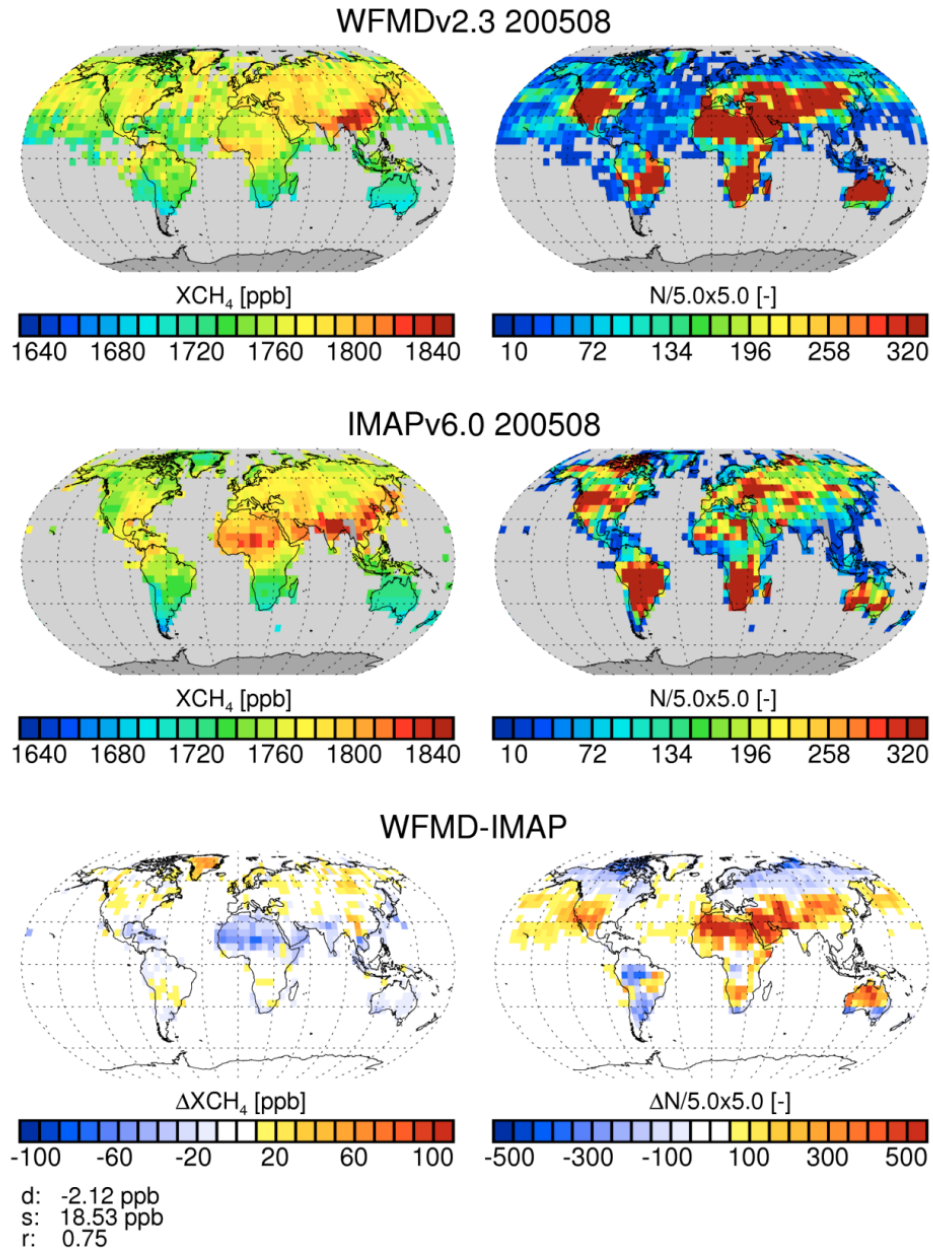


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1285 **Figure 8:** Comparison of the XCO₂ seasonal cycle amplitude (peak-to-peak) of the individual XCO₂
 1286 algorithms and EMMA with TCCON (left) and CarbonTracker (v2011) (right). The figure has been
 1287 adapted from Reuter et al., 2013, where results for all investigated XCO₂ 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 XCO₂ satellite data suggest that the amplitude of the CO₂
 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.

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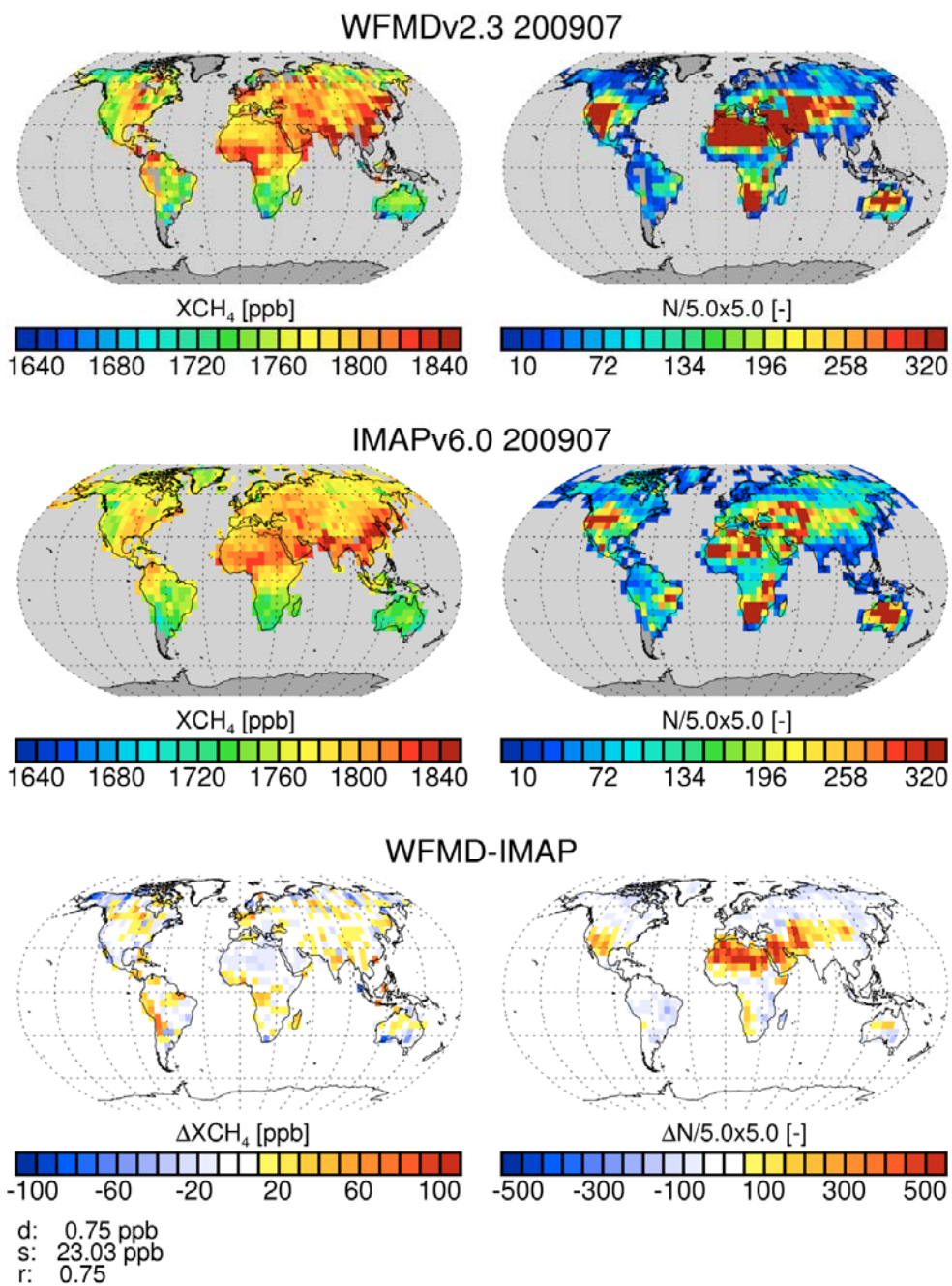
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1296 **Figure 9:** Comparison of two SCIAMACHY XCH₄ data products retrieved using WFMD (top) and
 1297 IMA Pv6.0 (middle) for August 2005. Global maps of the retrieved XCH₄ are shown on the left and the
 1298 number of retrievals per 5°x5° grid cell 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.

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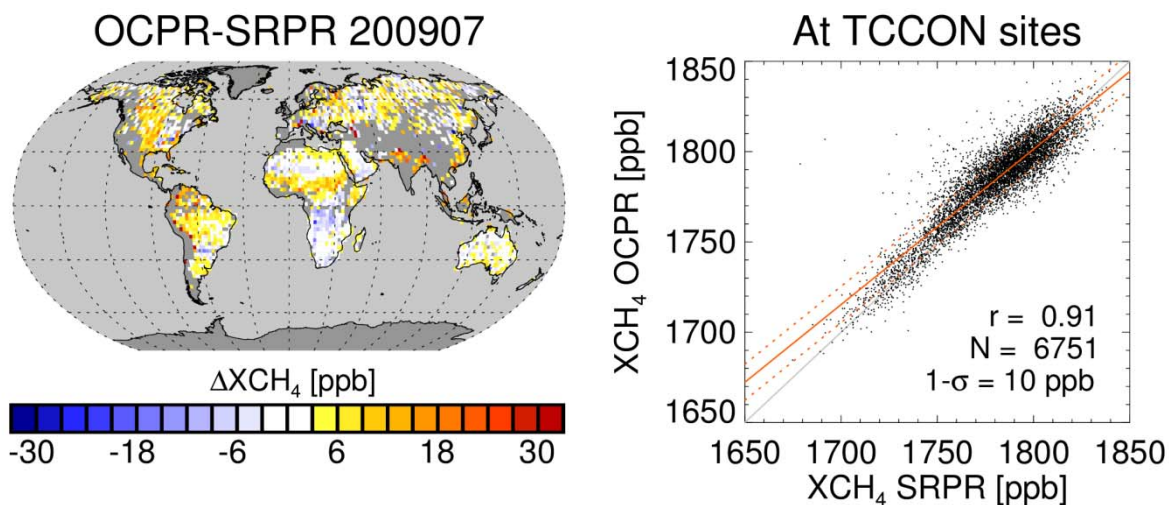
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1305 **Figure 10:** As Fig. 9 but for July 2009.

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1311 **Figure 11:** Comparison of the two GHG-CCI TANSO XCH₄ PR data products retrieved using the
1312 OCPR and SRPR retrieval algorithms. Left: Percentage XCH₄ 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.

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