# ESA EARTH EXPLORER 8 CANDIDATE MISSION CARBONSAT: ERROR BUGDET FOR ATMOSPHERIC CARBON DIOXIDE AND METHANE RETRIEVALS

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#### ABSTRACT

CarbonSat is one of two candidate missions for ESA's Earth Explorer 8 (EE8) satellite; one of them will be selected for implementation in November 2015 for a targeted launch date around 2023. The main goal of CarbonSat is to advance our knowledge of the sources and sinks, both natural and man-made, of the two most important anthropogenic greenhouse gases; carbon dioxide  $(CO_2)$  and methane  $(CH_4)$  from the global via the sub-continental to the local scale. CarbonSat will be the first satellite mission to image local scale emission hot spots of CO<sub>2</sub> (e.g., cities, volcanoes, industrial areas) and CH<sub>4</sub> (e.g., fossil fuel production, landfills, seeps) and to quantify their emissions and discriminate them from surrounding biospheric fluxes. The primary geophysical data products of CarbonSat are atmospheric columnaveraged dry air mole fractions of CO<sub>2</sub> and CH<sub>4</sub>, i.e., XCO<sub>2</sub> (in ppm) and XCH<sub>4</sub> (in ppb), respectively. In addition, CarbonSat will deliver a number of secondary data products, which will also be of good quality, such as vegetation chlorophyll Sun-Induced Fluorescence (SIF) as retrieved from clear solar Fraunhofer lines located at 755 nm; SIF will be retrieved simultaneously with the primary products. Here we present an updated error budget using the latest retrieval algorithm and instrument/mission specification focusing on nadir observations over land.

#### 1. INTRODUCTION

Carbon dioxide  $(CO_2)$  and methane  $(CH_4)$  are the two most important anthropogenic greenhouse gases responsible for global warming [16]. Despite their importance, our knowledge of their sources and sinks is inadequate and does not meet the needs for attribution, mitigation and the accurate prediction of future change



Fig. 1: Satellite-derived Northern Hemispheric XCO<sub>2</sub> 2002-2013. From: <u>http://www.esa-ghg-cci.org/</u> [4, 5].

(e.g., [9, 11-13, 16, 17, 19]), and despite efforts to reduce  $CO_2$  emissions, the atmospheric  $CO_2$  continues to increase with approximately 2 ppm/year (Fig. 1). Satellites help to close important observational gaps by delivering global distributions of atmospheric  $CO_2$  and  $CH_4$ , which are used to obtain source/sink information, e.g., via inverse modelling (e.g., [4-5, 20-23, 25-27] and references given therein). However, none of the existing or planned missions, except CarbonSat [6-8, 10], has been optimized to detect and quantify the emissions of localized emission hot spots such as cities (Fig. 2).



Fig. 2: Assessment of the capability of CarbonSat to quantify the anthropogenic fossil fuel (FF)  $CO_2$  emissions of Berlin. Top left: FF  $CO_2$  emissions of Berlin and surroundings with the two coal-fired power plants Jänschwalde and Schwarze Pumpe. Top right: Corresponding atmospheric  $XCO_2$  including biogenic  $XCO_2$ . Bottom: Random (top panel) and systematic (bottom panel) errors of CarbonSat-inferred FF Berlin  $CO_2$ emissions from single Berlin overpasses for three different swath width. Single overpass random errors ("precision") are typically below ~15% (6 MtCO<sub>2</sub>/year) and systematic errors (e.g., due to aerosols) typically below ~10% (update of Fig. 18 of [7]).

## 2. CARBONSAT OVERVIEW

The unique feature of CarbonSat [2, 6] is its "GHG imaging capability", which is achieved via a combination of high spatial resolution (~6 km<sup>2</sup>) and good spatial coverage (swath width ~180-240 km (goal: 500 km) with contiguous coverage). This capability enables global imaging of localized strong emission sources, such as cities, power plants, methane seeps, landfills and volcanos, and thereby permitting a better disentangling of natural and anthropogenic sources and sinks. For the specification of CarbonSat, extensive experience from past (SCIAMACHY) [2] and present (GOSAT, OCO-2) [1, 18] greenhouse gas satellite missions have been carefully taken into account.

CarbonSat's main mode is the nadir mode but CarbonSat will also measure solar spectra and perform observations under sun-glint conditions, to improve the quality of the observations over water and possibly also over snow and ice covered land surfaces, which are poor reflectors in the Short-Wave-Infra-Red (SWIR) spectral region outside of sun-glint conditions. Here we focus on nadir (i.e., non-glint) observations over land. The orbit is assumed to be sun-synchronous with an equator crossing time around local noon.

The CarbonSat imaging spectrometer will cover three spectral bands (Tab. 1, Fig. 3). The Near-Infra-Red (NIR) band covers the  $O_2$  A-band spectral region (747–773 nm) at 0.1 nm spectral resolution (approx. 1.7 cm<sup>-1</sup>).

This band will be used to obtain information on aerosols, clouds, surface pressure and vegetation chlorophyll Solar-Induced Fluorescence (SIF, e.g., [6, 14, 20]). The first SWIR band (SWIR-1) covers the 1590-1675 nm spectral region at 0.3 nm spectral resolution ( $\sim 1.2 \text{ cm}^{-1}$ ). This spectral region contains important absorption bands of CO<sub>2</sub> and CH<sub>4</sub> but is otherwise quite transparent and therefore permits to retrieve information on CO<sub>2</sub> and CH4 vertical columns with high near-surface sensitivity (Fig. 3 right). The "strong CO<sub>2</sub> band" SWIR-2 covers the 1925–2095 nm region with a spectral resolution of 0.55 nm (~1.4 cm<sup>-1</sup>). It provides additional information on CO<sub>2</sub> but also on water vapor and cirrus clouds - the latter in particular from the saturated water vapour band around 1939 nm [15]. The basic idea is to retrieve CO<sub>2</sub> and CH<sub>4</sub> columns from the transparent SWIR-1 band and to use in addition the partly non-transparent NIR and SWIR-2 bands located at shorter (NIR) and longer (SWIR-2) wavelengths to obtain information on atmospheric scatterers to constrain the CO<sub>2</sub> and CH<sub>4</sub> retrieval in the SWIR-1.

For this study we use the latest specification of the CarbonSat imaging spectrometer. The instrument parameters (Tab. 1) are used in an instrument model, which converts high spectral resolution spectra – as computed with the radiative transfer model SCIATRAN [24] – to simulated CarbonSat observations taking into account the relevant instrument characteristics as listed in Tab. 1.

<b>CarbonSat Spectral Instrument Characteristics</b>					
Parameter	Spectral band				
	NIR	SWIR-1	SWIR-2		
Spectral range [nm]	747 – 773	1590 - 1675	1925 – 2095		
Spectral resolution FWHM [nm]	0.1	0.3	0.55		
Spectral Sampling Ratio (SSR) [1/FWHM]	3	3	3		
Threshold Signal-to-Noise Ratio (SNR) for SZA 50° and vegetation surface [-]	473	347	274		
Radiance for listed SNR in photons/s/nm/cm <sup>2</sup> /steradiant	$2.0 \ge 10^{13}$	4.1 x 10 <sup>12</sup>	9.9 x 10 <sup>11</sup>		

Table 1: CarbonSat instrument parameters. The spectral resolution is specified as Full Width at Half Maximum (FWHM) of the Instrument Spectral Response Function (ISRF). The SSR is the number of spectral elements (detector pixel) per spectral resolution FWHM. An example spectrum is shown in Fig. 3.



Fig. 3: Typical CarbonSat radiance spectra (left and middle panels) and XCO<sub>2</sub> averaging kernel (right, blue curve).

#### **3.** ERROR BUDGET

The latest error budget for CarbonSat XCO<sub>2</sub> and XCH<sub>4</sub> nadir-mode retrievals over land is shown in Tab. 2. A similar table exists for the glint-mode observations (not shown here). Listed are various error sources related to the retrieval algorithm and the instrument. For the instrument the required threshold (i.e., minimum) performance has been assumed. Listed are single observation random errors and systematic errors for monthly regional-scale spatio-temporal resolution. The latter is also referred to as "relative accuracy" implying that a possible constant contribution (global offset) has been subtracted. Also listed is the overall uncertainty computed "root-sum-square" (RSS) from the random and systematic error components. Most of the errors (but not all, see below) have been established by performing retrievals applied to simulated CarbonSat spectra including and excluding a given error source. Details on the simulation framework are given in [8]. As can be seen, the required XCO<sub>2</sub> and XCH<sub>4</sub> threshold

performance (bottom right) can be met for the assumed instrument threshold performance used here.

The error budget has been established iteratively, starting with an initial error budget, initial instrument requirements and an initial retrieval algorithm. If instrument requirements were considered too demanding it had been identified via simulated retrievals to what extent requirements can be relaxed. In parallel, also the retrieval algorithm has been improved to better deal with specific instrument errors (e.g., zero-level-offsets) and geophysical error sources (e.g., errors due to clouds and aerosols). For most of the error sources comprehensive simulations have been carried out (e.g., for clouds and aerosols and various instrument-related errors) but for some error sources the values listed in Tab. 2 have to be interpreted as a requirement (e.g., for spectroscopy). In the following, specific aspects are presented in some detail.

Error source	Error source Overall uncertainty				Required maximum error			
	XCO <sub>2</sub> [ppm]	XCH4 [ppb]	Random error per sounding "Precision"		Systematic error (monthly regional-scale, non-constant part only) "Relative accuracy"			
Algorithm			XCO <sub>2</sub>	XCH <sub>4</sub>	XCO <sub>2</sub>	XCH <sub>4</sub>		
Clouds & zerosols	0.50	4.24	[ <b>ppm</b> ]	[ <b>ppb</b> ]	[ <b>ppm</b> ]	<b>[ppb]</b>		
Meteorology (n T H-O)	0.30	1 13	0.40	0.80	0.30	0.80		
Spectroscopy	0.14	1.13	0.10	0.80	0.10	0.80		
Other	0.14	1.13	0.10	0.80	0.10	0.80		
Instrument (Threshold)	0.11	1.10	0.10	0.00	0.10	0.00		
Signal-to-Noise Ratio (SNR)	1.20	9.00	1.20	9.00	0.00	0.00		
Radiometric:								
Multiplicative / absolute	0.20	1.97	0.17	1.80	0.10	0.80		
Multiplicative / relative	0.45	4.47	0.40	4.00	0.20	2.00		
Additive (zero level offset)	0.20	1.97	0.17	1.80	0.10	0.80		
Instrument Spectral Response Function (ISRF)	0.20	1.97	0.17	1.80	0.10	0.80		
Spectral calibration	0.20	1.97	0.17	1.80	0.10	0.80		
Spatio-temporal co-registration	0.48	3.00	0.48	3.00	0.00	0.00		
Heteogeneous scenes / Pseudo	0.32	2.62	0.30	2.50	0.10	0.80		
Noise (PN)								
Other	0.14	1.13	0.10	0.80	0.10	0.80		
Total (roo	1.50	11.69	0.47	4.33				
<b>Required</b> (MR	Dv1.2, thre	shold (T)):	3.00	12.00	0.50	5.00		

# CarbonSat XCO<sub>2</sub> and XCH<sub>4</sub> Error Budget Nadir/Land (v5)

Table 2: CarbonSat error budget for the  $XCO_2$  and  $XCH_4$  data products over land. The estimated total random and systematic errors are listed in the orange cells (bottom right). These values are compared with the required performance as listed in the cells below. The estimated total errors have been computed by adding the errors from various error sources in a root-sum-square (RSS) manner. Note that this table is valid for threshold (i.e., minimum) instrument performance and that the resulting performance is compared with the required  $XCO_2$  and  $XCH_4$  threshold performance as specified in ESA's Mission Requirements Document (MRD) version 1.2.

#### 3.1 Clouds and aerosols

As can be seen from Tab. 2, scattering related errors due to clouds and aerosols are expected to be a major error source for XCO<sub>2</sub> and XCH<sub>4</sub> retrievals, which is in agreement with the analysis of real SCIAMACHY and GOSAT satellite data (e.g., [5]). Detailed assessments related to this error source have already been presented elsewhere [2, 6] but here we present an update (see below). Figure 4 shows a typical example for cloud and aerosol related errors. Here the latest version of the CarbonSat BESD/C retrieval algorithm [2, 6] has been used. BESD/C is based on "Optimal Estimation" CarbonSat 3-band retrieval, i.e., extracts the desired XCO<sub>2</sub> and XCH<sub>4</sub> information from all three CarbonSat bands [2, 6]. To have good first guess and a priori values for surface albedo, vegetation chlorophyll Solar-Induced Fluorescence (SIF) and Cirrus Optical Depth (COD) a pre-processing step is used exploiting appropriate small spectral regions. For example, initial values for SIF are retrieved from a small fitting window located at 755 nm [6] and COD is retrieved from the saturated water vapour band at 1939 nm [15]. As can be seen in Fig. 4, in particular XCO<sub>2</sub>, XCH<sub>4</sub> and cirrus parameters can be very well retrieved.

We have also updated a one year data set of simulated CarbonSat observations as described in [6]. We now also consider aerosol type related errors (Fig. 5). As can be seen in Fig. 5, this results in a positive bias of the  $XCO_2$  retrievals (as the *a priori* value for aerosol type has a quite large Angström exponent). We therefore have used a bias correction (BC) scheme to reduce biases (Fig. 6). Updates of the corresponding figures shown in [6] are shown here in Figs. 7-9.

CarbonSat BESD	D/C: 1.09	GHG (FF StdDev:	<b>P) pro</b> 0.04	duct quality XCO <sub>2</sub> (FP) precision	Scen QF: COD	ario: VEG5	DCA <0.3	
o [bbm] Erro	Mean:	0.20	StdDev:	0.19	XCO <sub>2</sub> (FP) bias		N <sub>ALL</sub> : 45	N <sub>QF</sub> : 24 ( 53.3%
-4 [qdd]	Mean:	9.24	StdDev:	0.18	XCH <sub>4</sub> (FP) precision			
or [ppb] Error	Mean:	0.71	StdDev:	1.22	XCH₄(FP) bias		<u></u>	•••
ы -12 L 0			10		20 Scenario number [-]	30		40
,	A priori	i Tru	e Retrie	eved	Cloud (cirrus) Optical Depth	(COD)		
· 0.50 0.25 0.00				•				
-					Cloud (cirrus) Top Height (	CTH)		
Wy 14 HLC 6	***	***	╤╤╲╻╴	<u></u>		****		
_				A	erosol Optical Depth (AOD+W	/OD, NIR	R)	
-] 0.4 0.2 0.0				<b>A</b> .,		<u></u>		

Fig. 4: Assessment of the capability of CarbonSat to retrieve  $XCO_2$  and  $XCH_4$  for various scenarios defined by different values of cirrus optical depth (COD), cirrus altitude (CTH) and aerosol optical depth (AOD). The grey curves and symbols show the results for all 45  $XCO_2$  and  $XCH_4$  retrievals and the black symbols only the 53% "good" ones as automatically determined via the quality filtering procedure, which is based on retrieved COD and AOD. See [6] for details.



Fig. 5: Left: Aerosol-related  $XCO_2$  biases for the different aerosol types Continental Average (CA), Continental Polluted (CP), Desert (DE) and Maritime (MA). Right: Same as left side but ordered by Angström Exponent and including error parameterization (blue line) via Angström Exponent (ANG), solar zenith angle (SZA) and surface albedo (ALB).



Fig. 6: XCO<sub>2</sub> bias at and around Beijing. Light red: Error parameterization from [6]; grey: as in [6] but including aerosol-type related errors; black: as for grey but with bias correction (BC) using the TCCON [28] ground-based XCO<sub>2</sub> retrievals at Lamont, USA, to obtain regression coefficients used for bias correction of the global data.



Fig. 7:  $XCO_2$  random error for two CarbonSat orbit overpasses over Germany. The assumed swath width is 200 km. Gaps are due to clouds and the limited swath width. This is an update of the figure shown in [6].



Fig. 8: Estimated CarbonSat random and systematic  $XCO_2$  and  $XCH_4$  BESD/C Full Physics (FP) retrieval errors for July at 5°x5° spatial resolution for nadir-mode observations over land. Update of figures shown in [6].



Fig. 9: Error statistics for various regions for  $CH_4$  (left) and  $CO_2$  (right). Update of [6], where more details are given.

#### 3.2 Radiometric errors

Several radiometric error sources are listed in Tab. 2. "Multiplicative / absolute" are errors related to Absolute Radiometric Accuracy (ARA). ARA is important, for example, to retrieve a sufficiently accurate first guess value for surface albedo / reflectivity from the continuum radiance level in each band. Additive offsets (zero level offsets) are critical for accurate XCO<sub>2</sub> and XCH<sub>4</sub> retrieval and need to be sufficiently small. Therefore many simulations have been carried out to establish the acceptable radiance levels such that the error values listed in Tab. 2 are not exceeded. Error source "Multiplicative / relative" consists of various subcomponents. There are components which are assumed not to generate "spectral features", which adversely interfere with the absorption features of CO<sub>2</sub> and CH<sub>4</sub>, and components which likely do interfere. An example for the first category are "multiplicative gain" related reflectance errors (Fig. 10).



Fig. 10:  $XCO_2$  errors resulting from multiplicative gain errors. Shown are results for different retrieval algorithms and different CarbonSat bands. As can be seen, the  $XCO_2$  errors are typically below 0.1 ppm.

Most critical are radiance / reflectance errors with spectral features which correlate with the spectral signals of interest. This aspect is addressed via the so-called Effective Spectral Radiometric Accuracy (ESRA) requirement, which covers errors due to polarization, non-linearity, straylight and diffuser speckles. The requirement to be met by industry is formulated in terms of maximum  $XCO_2$  and  $XCH_4$  errors, which can be computed for a given error spectrum using provided socalled retrieval "gain matrices" (provided as three appropriate vectors obtained from the full gain matrix, see Fig. 11). In addition, errors have been quantified independently in the context of this study. Fig. 11 shows a typical example for polarization related errors. Another potentially important error source is related to inhomogeneous scenes, which are expected to result in errors of the Instrument Spectral Response Function (ISRF) (Fig. 12). Here it has been identified that mitigation methods need to be implemented such as a "Slit homogenizer".



Fig. 11: Example of the assessment of polarization related retrieval errors using the gain matrix/vector approach. Top row: Retrieval gain vectors for  $CO_2$  column (red),  $CH_4$  column (green) and the dry air column (blue).  $2^{nd}$  row: Degree of linear polarization for the scenario investigated.  $3^{rd}$  row: Spectra of Instrument Mueller Matrix element ratios (as provided by one of the CarbonSat industrial consortia). Bottom row: Relative spectral radiance or reflectance error due to residual polarization-related errors. The  $XCO_2$  and  $XCH_4$  biases (bottom right; blue text) have been computed from scalar products of the gain vectors (top row) and the relative measurement error (bottom row). As can be seen, the biases are ~0.01 ppm for  $XCO_2$  and ~0.03 ppb for  $XCH_4$ .



Fig. 12: Example result for the assessment of errors due to inhomogeneous scenes (top row: radiance at high spatial resolution;  $2^{nd}$  row: the same scene as seen by CarbonSat (considering, e.g., along-track smear due to spacecraft motion) resulting in inhomogeneous spectrometer entrance slit illumination ( $2^{nd}$  row) and Instrument Spectral Response Functions (ISRFs, rows 3-5, which differ from homogeneous ones (red curves in row 4). As can be seen, the ISRF errors can be quite large (here for SWIR-2 7.2% of the maximum value of the unperturbed ISRF). As this would result in quite large XCO<sub>2</sub> and XCH<sub>4</sub> errors mitigation measures are foreseen ("slit homogenizer") to reduce the ISRF error to below 2% as (implicitly) required by the error budget.

## 4. SUMMARY AND CONCLUSIONS

We presented an error budget for CarbonSat atmospheric  $XCO_2$  and  $XCH_4$  retrievals for nadir-mode observations over land covering error sources such as cloud and aerosol related errors as well as various instrument related errors. We focus on threshold (minimum) instrument performance and show that the corresponding threshold requirements for  $XCO_2$  and  $XCH_4$  in terms of precision and accuracy can be met.

The error analysis has been carried out by applying a retrieval algorithm (BESD/C [2, 6]) to simulated CarbonSat radiance and reflectance spectra. To estimate cloud and aerosol related errors full iterative retrievals have been carried out focusing on a relative small amount of data but also using an improved error parameterization scheme developed to analyze one year of data. The previously developed and used error parameterization scheme - used to compute errors for each single CarbonSat observation in a one year time period - is described in [6] and was based on six input parameters: solar zenith angle, surface albedo in two bands, aerosol and cirrus optical depth, and cirrus altitude variations. This scheme has been extended for the results shown here to also consider aerosol type variations. As this results in somewhat larger errors as those shown in [6], we have developed and used a simple bias correction scheme (similar as currently also used for real satellite data, see algorithm descriptions in ATBDs on http://www.esa-ghg-cci.org/). Overall it has been found that the scattering related errors are very similar (or even smaller) than the errors presented and discussed in [6]. The number of quality filtered observations over land surfaces is on the order of 10 million per month. We also performed detailed retrieval simulations to address a number of instrument related errors such as radiometric errors. As typical examples, we presented results for polarization related errors and errors related to inhomogeneous scenes, which result in errors of the Instrument Spectral Response Function (ISRF). As already explained earlier, we also retrieve vegetation chlorophyll Solar-Induced Fluorescence (SIF) from clear solar Fraunhofer lines located at 755 nm during a pre-processing retrieval step. The SIF single measurement precision is expected to be typically better than 0.3 mW/m<sup>2</sup>/nm/sr (1-sigma) [6], which indicates that CarbonSat will also provide highly valuable information on SIF collocated with XCO<sub>2</sub> as currently also delivered by GOSAT (see [14, 20] and references given therein).

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used the USGS GTOPO30 digital elevation model and the USGS land use/land cover information (<u>http://edc2.usgs.gov/glcc/tabgoode\_globe.php</u>). We also thank NASA/JPL for providing AVIRIS radiances. We thank ECMWF for ERA Interim meteorological data and ECMWF and the European MACC-II/MACC-III projects for global aerosol data sets (obtained from http://data-portal.ecmwf.int/data/d/macc\_reanalysis).

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