CARBONSAT: ERROR ANALYSIS FOR PRIMARY LEVEL 2 PRODUCTS XCO_2 AND XCH_4 AND SECONDARY PRODUCT VEGETATION CHLOROPHYLL FLUORESCENCE FOR NADIR OBSERVATIONS OVER LAND

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ABSTRACT

Carbon Monitoring Satellite (CarbonSat, http://www.iup.uni-bremen.de/carbonsat/) is one of two candidate missions for ESA's Earth Explorer 8 (EE8) satellite - one of them will be selected in ~2014/15 for a launch around 2020. Using the most recent instrument and mission specification, an error analysis has been performed for the primary data products, which are the column-averaged mixing ratios of CO_2, denoted XCO_2 (in ppm), and CH_4, denoted XCH_4 (in ppb), and also for the secondary product Vegetation Chlorophyll Fluorescence (VCF) retrieved from clear Fraunhofer lines located around 755 nm. The estimated VCF single measurement retrieval precision is 0.3 mW/m^2/nm/sr. To quantify XCO_2 and XCH_4 errors, we have computed random and systematic errors for each sufficiently cloud-free single CarbonSat observation during a one year time period. This has been achieved by developing an error parameterization scheme. The method permits to reliably compute random errors (retrieval precisions) as they primarily depend on the instrument's signal-to-noise performance. We found that the precision is typically 1.2 ppm for XCO_2 and 7 ppb for XCH_4. Systematic retrieval errors, especially their spatio-temporal pattern, also depend critically on other items, e.g., on the retrieval algorithm and on the assumed spatio-temporal distributions of aerosols and cirrus. Therefore, systematic error estimates are preliminary and have to be interpreted with care. Within this study we focus on scattering related errors due to aerosols and cirrus clouds as this error source is expected to dominate the error budget especially for XCO_2 systematic errors. We show that systematic errors, as estimated with our approach, are typically a few 0.1 ppm for XCO_2 and a few ppb for XCH_4. In this manuscript we only present a short overview. For details we refer to Buchwitz et al., AMTD, 2013. We focus on nadir observations over land. Results for sun-glint observations over water are reported elsewhere (Boesch et al., this issue).

1. CARBONSAT MISSION AND INSTRUMENT CONCEPT

The objective of the CarbonSat mission [1,3] is to improve our understanding of the natural and anthropogenic sources and sinks of the two most important anthropogenic greenhouse gases (GHG), carbon dioxide (CO_2) and methane (CH_4). See, e.g., also [1,3,5] and references given therein, for background information on this topic.

The unique feature of CarbonSat is its "GHG imaging capability", which is achieved via a combination of high spatial resolution (~2 km × 2 km) and good spatial coverage (wide swath and gap-free across- and along-track ground sampling). This capability enables global imaging of localized strong emission source such as cities, power plants, methane seeps, landfills and volcanos and thereby permits better disentangling of natural and anthropogenic GHG sources and sinks. CarbonSat will also measure Vegetation Chlorophyll Fluorescence (VCF) emission as secondary product - a parameter strongly correlating with Gross Primary Productivity (GPP) [6]. GHG source/sink information can be derived from the retrieved atmospheric column-averaged mole fractions of CO_2 and CH_4, i.e. XCO_2 (in ppm) and XCH_4 (in ppb), via inverse modeling. More details on the CarbonSat mission goals are reported elsewhere ([4] but also, Bovensmann et al., this issue).

CarbonSat's main mode is the nadir mode. CarbonSat will also obtain solar spectra and perform observations under sun-glint conditions, especially to improve the quality of the observations over water and 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 (no-glint) observations over snow and ice free land surfaces. The orbit is assumed to be sun-synchronous with an equator crossing time around local noon (here we assume 11:30 a.m.).

The CarbonSat imaging spectrometer will cover three spectral bands (Tab. 1, Fig. 1). 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^{-1}). This band permits one to obtain information on aerosols, clouds, surface pressure and Vegetation Chlorophyll Fluorescence (VCF). The first SWIR band (SWIR-1) covers the 1590–1675 nm spectral region at 0.3 nm spectral resolution (~1.2 cm^{-1}). This spectral region contains important absorption bands of CO_2 and CH_4 but is otherwise quite transparent and therefore permits one to retrieve information on CO_2 and CH_4 vertical columns with high near-surface sensitivity. The "strong CO_2 band" SWIR-2 covers the 1925–2095 nm region with a spectral resolution of 0.55 nm (~1.4 cm^{-1}). It provides additional information on CO_2 but also on water vapor and cirrus clouds - the latter in particular from the saturated water band located at 1940 nm. The basic idea is to retrieve CO_2 and CH_4 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 at 0.76 µm (NIR) and 2 µm (SWIR-2) to constrain the CO_2 and CH_4 retrieval at 1.6 µm (SWIR-1). In practice, all the information will essentially be retrieved simultaneously by applying an appropriate retrieval algorithm to all three bands.

For this study we use the latest specification of the CarbonSat imaging spectrometer currently available [4]. The instrument parameters (Tab. 1) are used by a CarbonSat instrument model, which converts high spectral resolution spectra – as computed with the radiative transfer model SCIATRAN [7] – to simulated CarbonSat observations taking into account the relevant instrument characteristics as listed in Tab. 1. As an example, Fig. 1 shows a simulated CarbonSat nadir radiance spectrum for a scene with a typical vegetation albedo (NIR: 0.2, SWIR-1: 0.1, SWIR-2: 0.05) and a solar zenith angle (SZA) of 50^{o}.

A preliminary error budget for XCO_2 and XCH_4 retrievals over land is shown in Tab. 2. As can be seen, scattering related errors due to aerosols and clouds dominate the error budget for systematic errors (biases). It is therefore important to develop appropriate retrievals algorithms to minimize scattering related errors and to reliably estimate scattering related errors for all relevant scenarios. The current status of this activity is presented in the following section.

CarbonSat instrument spectral parameters

Parameter	Spectral band			Comment
	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	-
Approx. single observation continuum Signal-to-Noise Ratio (SNR) for SZA 50^{o}, vegetation albedo (NIR: 0.2, SWIR-1: 0.1, SWIR-2: 0.05)	330	320	200	See [3] for a description of how the SNR as a function of the radiance has been computed.
Reference radiance for listed SNR in photons/s/nm/cm^2/steradiant	2×10^{13}	4×10^{12}	1×10^{12}	-

Table 1: CarbonSat instrument parameters as used for this study. 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. 1.

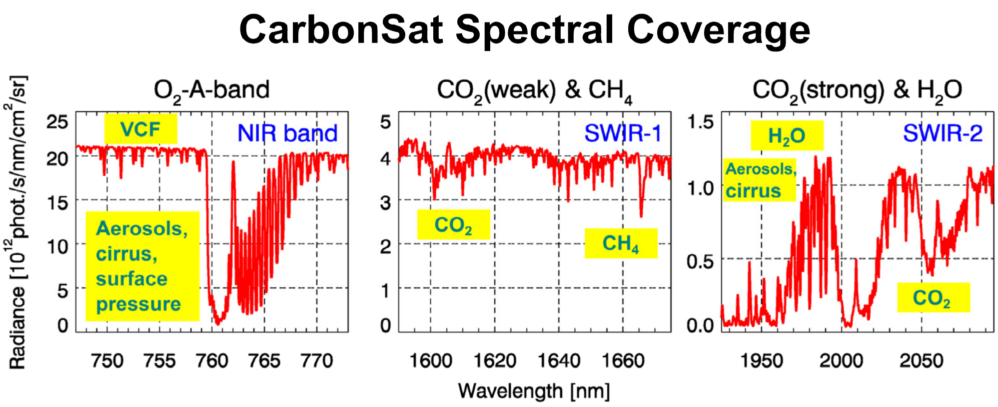

Fig. 1: Typical CarbonSat radiance spectrum as measured in the three spectral bands NIR, SWIR-1 and SWIR-2 (see also Tab. 1).

CarbonSat Preliminary Error Budget for XCO_2 and XCH_4								
Error source	**Total error**		**Assumed error characteristics** (monthly regional-scale, ~500 km x 500 km)		**Required maximum error**			
	XCO_2 [ppm]	**XCH_4 [ppb]**			**Random error** per sounding "Precision"		**Systematic error** (monthly regional-scale, non-constant part only) "Relative accuracy"	
Algorithm			Fraction random	Fraction systemat.	XCO_2 [ppm]	XCH_4 [ppb]	XCO_2 [ppm]	XCH_4 [ppb]
Clouds & aerosols	0.70	5.00	0.5	0.5	0.35	2.50	0.35	2.50
Meteorology (p_o, T, H_2O)	0.20	0.90	0.5	0.5	0.10	0.45	0.10	0.45
Spectroscopy	0.20	2.00	0.5	0.5	0.10	1.00	0.10	1.00
Other	0.40	1.80	0.5	0.5	0.20	0.90	0.20	0.90
Instrument								
Signal-to-Noise Ratio (SNR)	1.20	8.00	1.0	0.0	1.20	8.00	0.00	0.00
Radiometric:								
Multiplicative / absolute	0.20	0.90	0.5	0.5	0.10	0.45	0.10	0.45
Multiplicative / relative	0.20	0.90	0.5	0.5	0.10	0.45	0.10	0.45
Additive (zero level offset)	0.20	0.90	0.5	0.5	0.10	0.45	0.10	0.45
Non-linearity	0.20	0.90	0.5	0.5	0.10	0.45	0.10	0.45
Instrument Spectral Response Function (ISRF)	0.20	0.90	0.5	0.5	0.10	0.45	0.10	0.45
Spectral calibration	0.20	0.90	0.5	0.5	0.10	0.45	0.10	0.45
Spatio-temporal co-registration	0.50	2.25	1.0	0.0	0.50	2.25	0.00	0.00
Pseudo Noise (PN)	0.40	1.80	1.0	0.0	0.40	1.80	0.00	0.00
Other	0.20	0.90	0.5	0.5	0.10	0.45	0.10	0.45
Other								
Sampling	0.20	0.90	0.9	0.1	0.18	0.81	0.09	0.09
Other	0.20	0.90	0.5	0.5	0.10	0.45	0.10	0.45
Total (root-sum-square (RSS)):					**1.89**	**12.07**	**0.49**	**2.95**
MRD v1.1 requirements (threshold (T)):					**3.00**	**17.00**	**0.50**	**10.00**
MRD v1.2 requirements (threshold (T)):					**3.00**	**12.00**	**0.50**	**5.00**
Note: All values 1-sigma								

Table 2: CarbonSat preliminary 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 in the bottom right. These values can be compared with the required performance as listed in the cells below. The initial requirements according to the CarbonSat Mission Requirements Documents (MRD) v1.1 are shown but also the revised requirements according to MRDv1.2 [4]. The estimated total error shown in the orange cells has been computed by adding the errors from various error sources in a root-sum-square (RSS) manner. An error characteristic has been specified for each error source by assuming a certain "fraction random" and "fraction systematic". Some error sources are purely random (fraction random = 1.0) but most of the error sources also have a systematic component (at monthly regional-scale). For most error sources we assume a 0.5/0.5 split.

2. ERROR ANALYSIS METHOD AND RESULTS

Figure 2 shows the simulation framework used for computing random and systematic errors. A radiative transfer model (RTM), here SCIATRAN [7], is used to compute high spectral resolution radiance spectra for a given atmosphere and surface conditions, solar zenith angle (SZA), viewing angles, etc. A CarbonSat instrument model is used to convert these spectra into simulated CarbonSat observations. This step comprises convolution of the spectra with the instrument's spectral response function, spectral sampling according to the instrument's wavelength grid and SNR computations. The simulated observations are then inverted using the optimal estimation retrieval method BESD/C [1, 3].

The inversion provides the XCO_2 and XCH_4 random errors via a mapping of the random error of the spectra (i.e., the inverse SNR) to state vector space.

The systematic errors or biases are obtained by computing the difference between the retrieved and the true values, which are known from the model atmosphere.

Note that this framework is also used to compute the random and systematic errors for VCF retrieval. As can be seen from Fig. 3, which shows results for 180 different scenarios for a scene corresponding to vegetation albedo, the CarbonSat VCF single observation retrieval precision is 0.233+/-0.03 $mW/m^2/nm/sr$ (1-sigma).

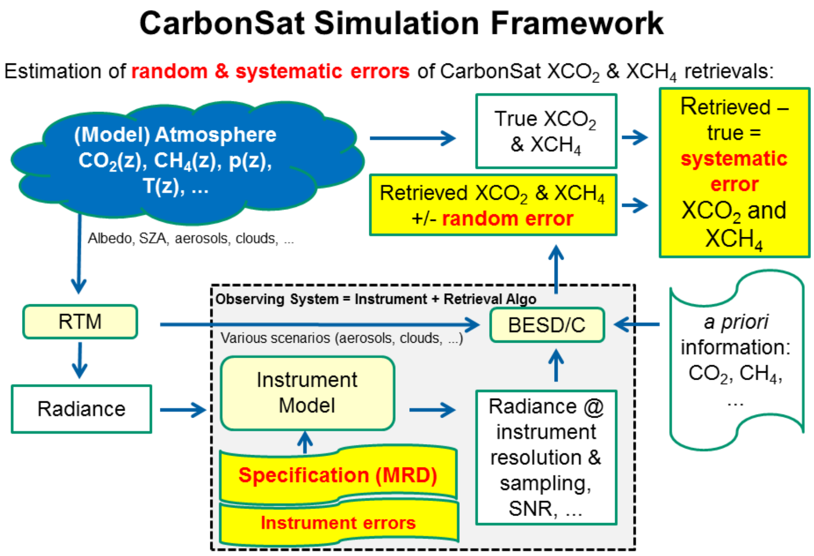

Fig. 2: Framework for the generation of simulated CarbonSat observations with the goal to estimate random and systematic XCO_2 and XCH_4 retrieval errors for different conditions. As radiative transfer model (RTM) SCIATRAN [7] is used. BESD/C is the CarbonSat Level 1 to 2 retrieval algorithm under development at Univ. Bremen.

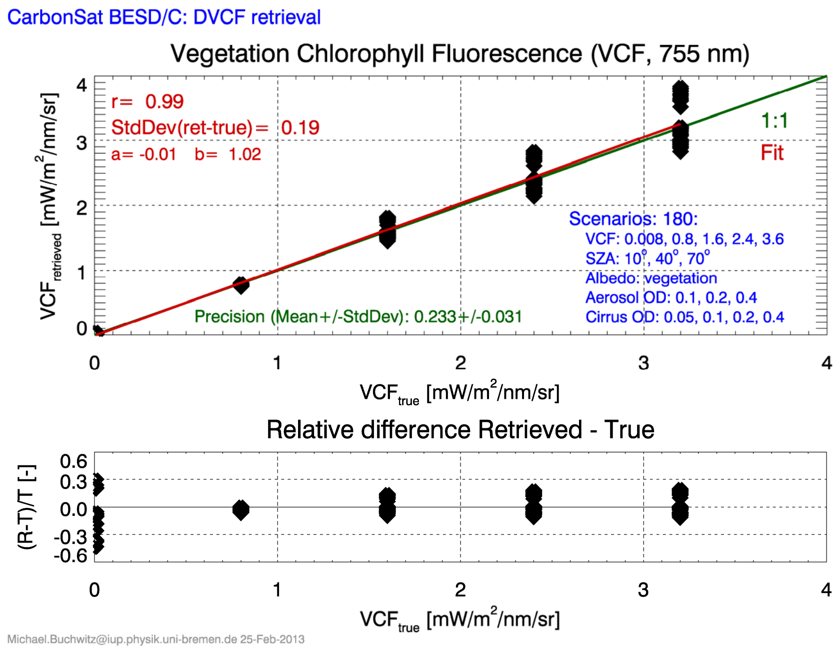

Fig. 3: Initial assessment results for random and systematic errors for the secondary data product Vegetation Chlorophyll Fluorescence (VCF) at 755 nm as retrieved from clear solar Fraunhofer lines. As can be seen, the single observation precision (random error) is 0.233+/-0.03 $mW/m^2/nm/sr$. Source: [3].

This scheme has been used to compute the errors for a number of scenarios depending on solar zenith angle, surface albedos, aerosol amounts and cirrus optical depth and altitude. A regression scheme has been used to model these errors as a function of the scenario input parameters. The regression scheme has been used in combination with various inputs parameters (e.g., the time and location of each CarbonSat observation, global aerosol and cirrus data sets, etc. (see [3] for details)) to compute these errors for each single CarbonSat observation. The resulting “Level 2 error” (L2e) files have been stored in a data base. Figure 4 presents a schematic overview of how these L2e files have been generated.

Figures 5 to 7 show maps generated with the information contained in the L2e files. Figures 5 shows the random errors for each single observation for a CarbonSat overpass over Germany. Figures 6 and 7 show monthly gridded data at 5^ox5^o spatial resolution. Table 4 lists systematic errors for several regions.

For a more detailed description and discussion we refer to [3].

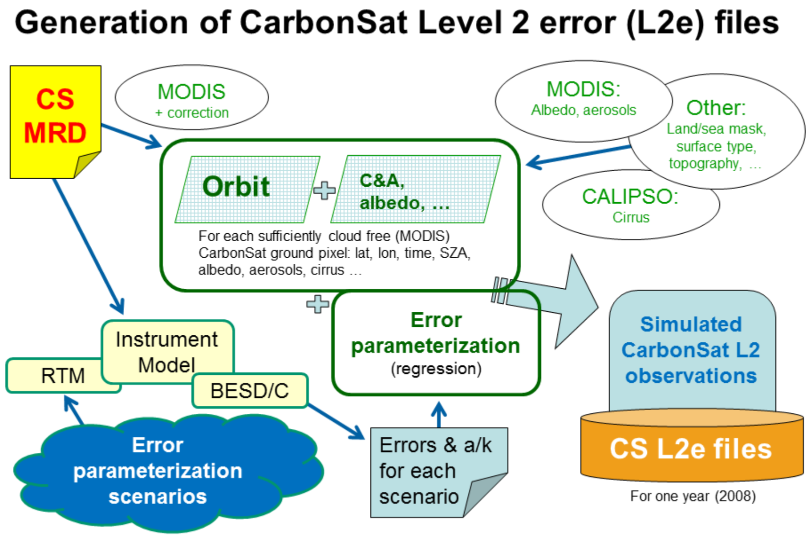

Fig. 4: Framework for the generation of one year of simulated CarbonSat (CS) observations, i.e., for the generation of the CarbonSat Level 2 error (L2e) files. MRD refers to CarbonSat's Mission Requirements Document [4]. a/k stands for averaging kernels, which are also computed and parameterized, and C&A means Clouds & Aerosols.

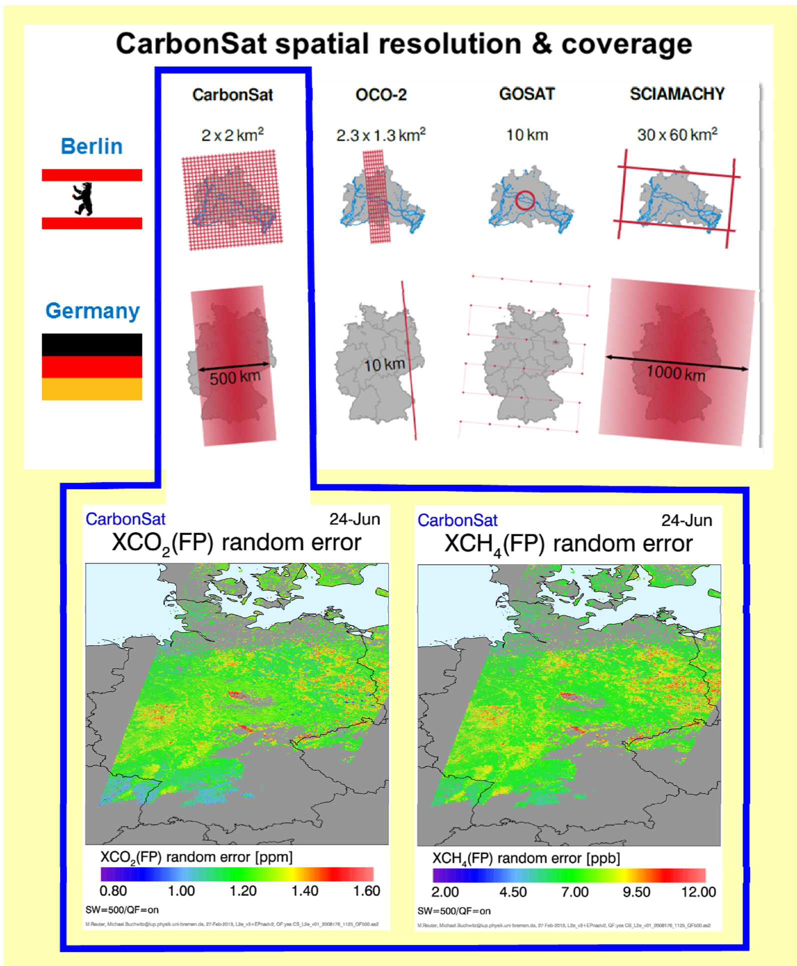

Fig. 5: Top: Comparison of CarbonSat's spatial resolution and coverage (assuming a ground pixels size of 2x2 km^2 and a swath width of 500 km, i.e., CarbonSat's goal swath width) compared to other satellite missions (e.g., SCIAMACHY [2]). Bottom: Simulated CarbonSat observations for one overpass over Germany. Shown are the XCO_2 random error (left) and the XCH_4 random error (right), for all cloud free CarbonSat observations over land (source: [3]). The precision variations are primarily due to variations of surface albedo and are therefore similar for XCO_2 and XCH_4.

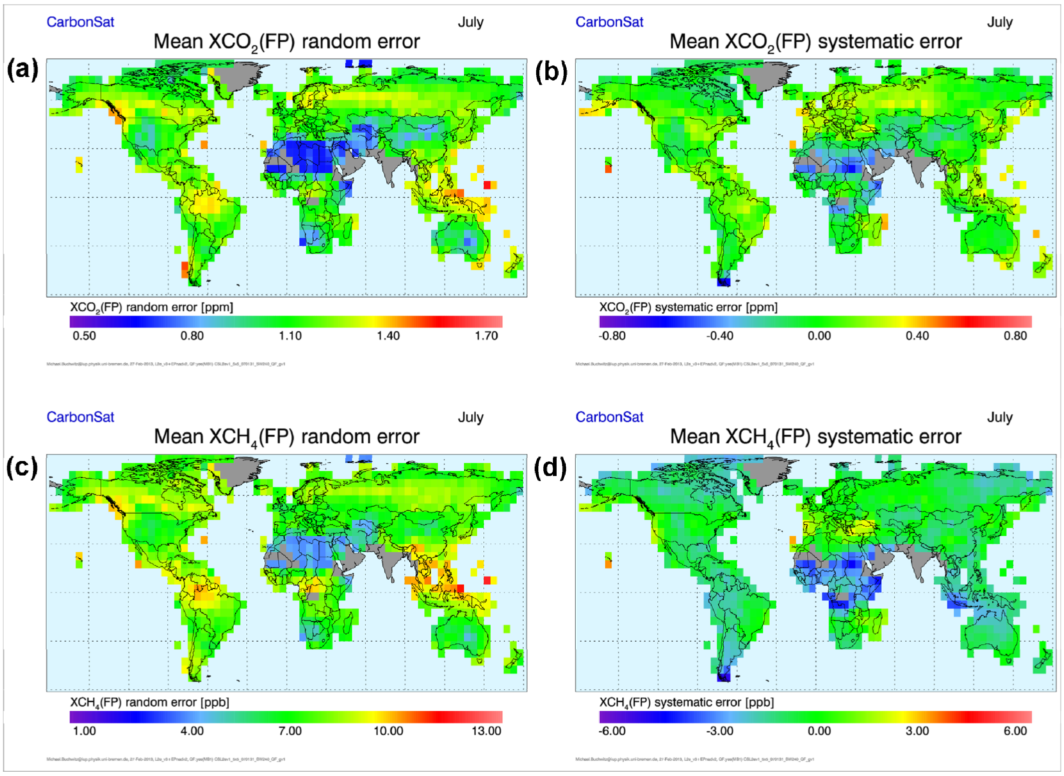

Fig. 6: Mean random and systematic XCO_2 and XCH_4 retrieval errors for July at 5^ox5^o spatial resolution assuming a swath width of 240 km. Source: [3].

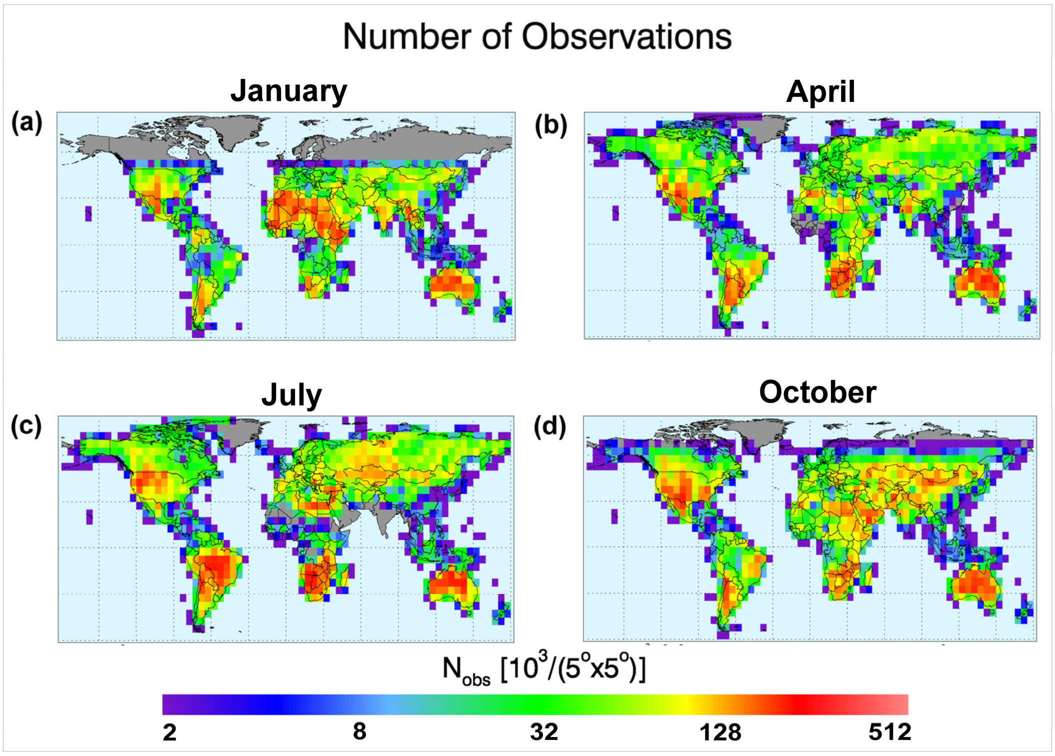

Fig. 7: Number of observations after quality filtering at 5^ox5^o spatial resolution assuming a swath width of 240 km. Note that 32 (green) means 32000 observations per 5^ox5^o grid cell per month. The maximum SZA is 70^o. Source: [3].

Systematic errors for eight regions				
Region	Percentage of XCO_2 retrievals with systematic error		Percentage of XCH_4 retrievals with systematic error	
	< 0.3 ppm	< 0.5 ppm	< 2 ppb	< 4 ppb
USA	69.8	99.5	87.7	99.9
Europe	66.7	97.7	81.1	99.7
China	96.2	99.6	99.5	100.0
Australia	99.7	99.9	65.6	100.0
Canada	97.9	100.0	78.3	100.0
Siberia	88.9	99.8	99.4	100.0
Amazonia	97.1	100.0	89.2	100.0
Central Africa	83.6	99.7	60.2	94.5

Tab. 4: Systematic XCO_2 and XCH_4 errors for eight regions. Source: [3].

3. SUMMARY AND CONCLUSIONS

As shown in this manuscript and explained in detail in *Buchwitz et al., 2013* [3], an error analysis has been performed for CarbonSat using the BESD/C retrieval algorithm using the most recent instrument and mission specification. We focus on systematic errors due to aerosols and thin cirrus clouds, as this is the dominating error source especially with respect to XCO_2 systematic errors. To compute the errors for each single CarbonSat observation in a one year time period, we have developed an error parameterization scheme based on six relevant input parameters: we consider solar zenith angle, surface albedo in two bands, aerosol and cirrus optical depth, and cirrus altitude variations but neglect, for example, aerosol type variations. We have generated and analyzed one year of simulated CarbonSat observations. Using this data set we estimate that scattering related systematic errors are mostly (approx. 85 %) below 0.3 ppm for XCO_2 (<0.5 ppm: 99.5 %) and below 2 ppb for XCH_4 (<4 ppb: 99.3%). We also show that the single measurement precision is typically around 1.2 ppm for XCO_2 and 7 ppb for XCH_4 (1-sigma). The number of quality filtered observations over cloud and ice free land surfaces is in the range 33–47 million per month depending on month. Recently it has been shown that terrestrial Vegetation Chlorophyll Fluorescence (VCF) emission needs to be considered for accurate XCO_2 retrieval [6]. We therefore retrieve VCF from clear solar Fraunhofer lines located around 755 nm and show that CarbonSat will provide valuable information on VCF. The VCF single measurement precision is approximately 0.3 $mW/m^2/nm/sr$ (1-sigma).

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