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Comment

Interactive comment on “Carbon Monitoring Satellite (CarbonSat): assessment of scattering related atmospheric CO₂ and CH₄ retrieval errors and first results on implications for inferring city CO₂ emissions” by M. Buchwitz et al.

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First of all, we would like to thank "Anonymous Referee #1" for the careful review and for providing useful interactive comments on our manuscript “Carbon Monitoring Satellite (CarbonSat): assessment of scattering related atmospheric CO₂ and CH₄ retrieval errors and first results on implications for inferring city CO₂ emissions” by M. Buchwitz et al. All comments will be carefully considered for the revised version of the manuscript. Below we give point by point answers to each of the referee’s comments.

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Both referees recommend to significantly shorten the manuscript, e.g., by removing parts (e.g., referee #1 suggests to remove the part on plant fluorescence) or by splitting the paper in two or more separate paper (e.g., referee #2 recommends to publish the part on the Berlin CO₂ emissions in a separate paper). Both referees also ask for more explanations on various items. To consider these comments we plan the following for the revised version of the paper: As the paper is already quite long - and adding explanations will make it even longer - we will remove the Berlin emission part, which will be published in a separate paper.

1. Referee: "Main question": "What is the origin of the systematic errors derived in section 4 and used furtheron throughout the study? ...".

Answer: The spectra measured by CarbonSat depend on many (atmospheric and surface) parameters. This is illustrated in Fig. 2 showing various derivatives ("Jacobians") of these spectra with respect to parameters such as CO₂ and CH₄ variations in different atmospheric layers, aerosol and cirrus optical depth, cirrus altitude, surface albedo, etc. As can be seen, these derivatives are to some extent correlated. Typically, the Jacobians of scattering related parameters (aerosols, cirrus, but also albedo, which determines the fraction of photons detected by the satellite reflected at the surface relative to the fraction scattered in the atmosphere) show significant spectral variations in those spectral regions, where absorption due to atmospheric gases (including, e.g., CO₂) are strong (the Jacobians also vary if the atmospheric absorption is weak, but this is difficult to see in Fig. 2). Outside of spectral regions with atmospheric absorption, the Jacobians are typically "flat", as the assumed wavelength dependence of scattering and surface parameters is weak compared to the highly structured atmospheric absorption features. What is the reason for this correlation? Imagine, for example, the extreme case of a spectral region, where essentially all photons are absorbed in the atmosphere. In this spectral region, the surface albedo Jacobian would be zero, as the radiance will not change due to a change of albedo. This is because none of the photons hitting the surface will be measured by CarbonSat (as they are all

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absorbed in the (lower layers of the) atmosphere independent of how large the albedo is). For neighboring spectral regions, where the atmospheric absorption is weaker, the albedo Jacobian will differ from zero, i.e., will depend on albedo. As a consequence, the albedo Jacobian will have a spectral structure, which is correlated with atmospheric absorption features, even if this structure is not present in the spectral albedo itself. In principle, similar effects are also present for other parameters such as aerosol and cirrus parameters. As a consequence of these correlations and due to the fact that the radiance dependence on many parameters is non-linear, it is not possible to determine all parameters, which influence the radiance, without any error (even for very high signal to noise ratio). Systematic errors are only zero if the parameters used to generate the simulated observations are exactly identical to the parameters assumed for the retrieval (this has been verified by simulation). If one or several of the parameters differ, it is (depending on parameter) typically possible to retrieve parameters, which are close to the true values (see, e.g., Fig. 5, top panel for cirrus optical depth; note that in this case the retrieval assumes a cirrus optical depth of 0.05, whereas the true optical depth varies between 0-0.4) but typically some difference remains. This difference ("true minus retrieved") is the systematic error (shown for XCO₂ in, e.g., Fig. 6 panel (b)). So the referee is right with the following: "If simulation and retrieval forward models were consistent, there should be no systematic error due to scattering (unless there are "technical" issues such as non-convergence, not finding the true minimum of the cost function, etc.). So, how is the simulation model different from the retrieval model?". We will explain this better in the revised version of the manuscript and will explicitly list key parameters which differ between simulation and retrieval model. For example, for the various combinations of cirrus optical depth and altitude (COD and CTH) and aerosol optical depth (AOD) shown in Fig. 5 as used for the simulated measurements only a single set of a priori and first guess values have been used: COD: 0.05, CTH: 10 km, AOD: 0.12. These are the constant a priori values for these parameters as mentioned on page 4785, lines 3-4, ("Here we utilize the following simple approach: We use constant a priori values for COD, CTH and AOD") and they have been used for all results

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shown in our manuscript. This missing information will be added.

In the following we provide answers to "Further comments":

2. Referee: page 4779, line 27: "Why would one design a full physics retrieval algorithm that retrieves two types of AOD such as AODNIR and AODSW2 which are uncoupled among the retrieval windows?"

Answer: We retrieve four scattering related parameters: Two for aerosols (AOD in the NIR and SWIR-2 bands) and two for cirrus (optical depth and altitude). Several other "full physics" algorithms exist (see references listed and discussed in our paper) and each one deals with scattering related errors by retrieving (a small number of) scattering related parameters. Which parameters are used differs among the different algorithms. These parameters are typically interpreted as "effective parameters". Their purpose is to minimize scattering related errors for XCO₂ (and/or XCH₄) retrieval. Their purpose is not (necessarily) to generate additional geophysical data products providing quantitative information on, e.g., aerosols. Aerosols are complicated as their altitude dependent scattering and absorption characteristics depend on many parameters - much more than can be retrieved using "full physics" XCO₂ retrieval schemes (the spectra do not permit to retrieve all parameters). Which (few) parameters are the best to minimize XCO₂ retrieval errors is a priori not clear. In our approach we vary aerosol optical depth in the NIR and SWIR-2 bands independently and use the retrieved AOD values to constrain the AOD in the SWIR-1 band. It is an open question if this approach is better or worse than any of the other "full physics" retrieval approaches for XCO₂ and/or XCH₄ retrieval. The two spectral windows NIR and SWIR-2 are spectrally located far from each other, i.e., their AODs are only correlated if one assumes a certain wavelength dependence or certain aerosols types (in the various atmospheric layers). We treat these two spectral regions essentially independent of each other whereas other algorithms use other parameterizations (e.g., a wavelength dependence, which can be described with one or a few parameters). At the end it only matters which method is the best to reduce scattering related XCO₂ and/or XCH₄ er-

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rors. This is a difficult question, which at present cannot be answered with confidence. More work is needed to find out if our approach can be significantly improved or not. In Sect. 8, "Limitations and outlook to future work", we have highlighted this aspect. In any case we do not claim that our approach is the best to minimize XCO₂ errors nor do we claim that our approach gives the best scattering related parameters in terms of absolute values of the individual retrieved scattering parameters. We understand our parameters as effective parameters needed to deal with the variability of the radiance due to aerosols and cirrus to the extent needed to model their impact on the radiance and with the only purpose to minimize XCO₂ and XCH₄ retrieval errors. Note that our approach in principle permits one to obtain information on aerosol type from the AOD ratio at NIR and SWIR-2 wavelength. This shows that we consider aerosol type dependence, at least to some extent, in terms of AOD dependence on wavelengths.

3. Referee: page 4780, section 3.2: "Section 3.2 seems unnecessary to me. Please consider removing it since the manuscript is lengthy anyway. ..."

Answer: We think that this is an important aspect which should at least be shortly mentioned and discussed as it has been identified in recent peer-reviewed publications that this is a potentially important error source for XCO₂ retrieval. We therefore would like to explain at least shortly how we deal with this. However, we agree that this does not necessarily have to be included in the main text. We therefore plan to only shortly mention this in the main text referring to a short separate Annex, where details are given.

4. Referee: page 4783, section 4: "Section 4 describes how retrieval simulations are used to setup an error parameterization. The following points remain unclear to me. - See main question: What are the error terms evaluated here? For each retrieval simulation, an overall error e_T can be derived via "retrieved minus true" (p4785, l22). The systematic one is a forward model error e_F which is due to the fact that the retrieval forward model (for scattering) is physically different from the simulation model, i.e. the retrieval cannot converge to the truth. Is this correct? The second error contribution

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is the noise error e_M which comes from instrument performance parameters (table 1). How do you disentangle e_M from e_F in the total error e_T ? Do you use the gain matrix and the individual instrument noise error (known from the simulations) or do you run an ensemble of noise realizations"

Answer: For the first questions, please see our answer to your main question given above: Yes, typically the retrieval is not converging to the truth and this is the origin of the systematic error. How do we disentangle the noise error e_M from e_F in the total error e_T ? First of all, we do not compute e_T as we do not add noise to the spectra. The retrieval algorithm is applied to noise free observations (which have "systematic errors" as the simulation differs from the retrieval model as explained above). We directly compute e_F from "retrieved minus true". Using this approach we can avoid running "an ensemble of noise realizations". We will explain this better in the revised version.

4b. Referee: Scattering particle type (size, chemical composition) has been identified as one of the critical parameters since it is the particle type together with spectral variation of surface albedo that drives the spectral dependence of light path modification. All state-of-the-art full-physics algorithms aim at estimating the particle type with some sort of approach [eg. O'Dell et al., 2012, Butz et al., 2012, Yoshida et al., 2013]. If I understand correctly, the study includes no estimate on how the particle type affects performance. I would consider this a serious shortcoming. The authors comment on this shortcoming in section 8.

Answer: For the first part of the questions please see our detailed answer to item 2 (Referee: page 4779, line 27) given above. In short: Implicitly, our retrieval method considers particle type dependence (at least to some extent) by retrieving AOD in the NIR and SWIR-2 spectral regions independently. If this approach can be improved or not and if it is better or worse than other approaches, remains to be investigated – this is not clear a priori (see above). It is true that particle type effects are not considered for the error parameterization. This is a limitation as explained in Section 8. Note that

in section 8 we also report errors when particle type errors (or other error sources, e.g., altitude variations) are considered.

4c. Referee: In my opinion, the error parameterization derived in section 4.3 gives a very poor fit to the actually observed errors although the fit is based on most parameters relevant for scattering effects. Are you sure that there is no “hidden” source of error other than scattering (eg. non-convergence, too tight prior constraints) that affects performance?

Answer: It is true that the error parameterization fit results are far from perfect. We tried several approaches but failed to get better fits. This is clearly an aspect which needs further study, e.g., by using other (not yet investigated) fitting methods. The main reason for this is the complex dependence of the systematic errors on the parameters investigated. There are some cases where convergence is not achieved but this is only true for a very small fraction of the retrievals. The number of iterations however depends significantly on the scenario. We also tried various a priori constraints and have not been able to improve the situation. However, we investigated only a very small number of cases and therefore all this aspect needs further study and may result in a better performance in the future. For the results shown in our manuscript one can see that especially the systematic errors are not underestimated using the error parameterization. The opposite is true: Typically the error parameterization gives larger systematic errors. This clearly indicates that there is room for improvement.

5. Referee: p4789, section 5: The case study (for Germany) discussed in section 5 seems very benign to me. The cirrus and aerosol optical depths sum up to 0.1 for most of the scene, which is at the lower end of simulations conducted in section 4 and which for cirrus is close to the a priori value (COD = 0.05). Further, the albedo is on the order of 0.2 for most of the scene, the range for which light path enhancing and shortening effects tend to cancel anyway (at SWIR wavelengths). Did you check on performance if scattering is simply neglected which could be used as a contrasting case to quantify the “benefit of the method”?

Answer: We have checked the “benefit of the method” several times when further developing / improving the retrieval method. Concerning cancelation of errors at SWIR wavelength: Our method is based on a three band retrieval similar as the algorithms used for GOSAT and planned for OCO-2. If under certain conditions errors would be smaller using a SWIR only retrieval this would be nice but will be only of marginal help for an algorithm which is designed to work with global satellite data.

6. Referee: page 4792, line 15: "In the view of shortening the paper, one could remove the section on the proxy retrieval. Maybe I misunderstood the rationale here, but the formula for propagating CO₂ and CH₄ errors into a proxy error (p4792, l29) seems wrong to me. For a ratio quantity, it should be the relative errors that add up quadratically not the absolute errors."

Answer: We think that the proxy aspect is an important aspect, which should at least be shortly mentioned and discussed. However, we agree that this does not necessarily have to be included in the main text. We therefore plan to only shortly mention this in the main text referring to a short separate Annex, where details are given. Concerning the error formulas: You are right for the general case. The “simple” formulas given in our manuscript are valid for small errors only, i.e., if the ratio of the errors (e.g., 1 ppm for XCO₂ or a few ppb for XCH₄) to the absolute values (e.g., 390 ppm for XCO₂ or 1694 ppb for XCH₄) is much smaller than 1.0, which is true for all cases discussed here. We will mention this in the revised version.

7. Referee: page 4794, section 6: "If I understand correctly, the inverse modelling study assumes that the spatial pattern of anthropogenic emissions and the atmospheric transport are perfectly known. How would errors in these assumptions propagate into the emission estimates?"

Answer: Yes, the understanding is correct. The main purpose of the assessment was to quantify to what extent the CO₂ emission estimates are influenced by the random and systematic errors of the CarbonSat observations taking into account the spatio-

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temporal sampling of CarbonSat. Errors due to imperfect atmospheric transport modelling and imperfect knowledge of the spatial pattern of the anthropogenic emissions have not been quantified. These additional errors, which arise from error sources not directly related to CarbonSat, still need to be quantified. This is not trivial as it requires assumptions on transport modelling errors and likely errors of the spatial (and temporal) pattern of the emissions. To consider this we will follow the advice of referee number 2 to publish the results on the Berlin CO₂ emissions in a separate paper (see above). As a consequence, the entire Section 6 will be removed when generating the revised manuscript.

8. Referee: page 4802, section 7: "The errors on the global scale seem extremely low in comparison to what other teams (e.g., working on GOSAT/OCO retrievals and simulations) find. So, it is critical to discuss what systematic error means in the context of this study and in comparison to other studies (see main question)."

Answer: Concerning the definition of and reason for systematic errors: Please see our answer to your main point given above. Concerning comparisons with other studies: As described in our paper, our error parameterization scheme is more advanced than those described in other publications on other satellite instruments which measure or plan to measure XCO₂ such as Hungershoefer et al., 2010 (primarily because we consider more parameters) but still quite simple compared to the complexity of the task, as we neglect, for example, aerosol type variations in the error parameterization. This is a likely reason, why our errors are smaller than those reported in, e.g., O'Dell et al., 2012, for GOSAT XCO₂ retrieval. This will explicitly be mentioned in the revised version of the paper. To improve on this will be a focus of our future activities, as highlighted in Sect. 8, "Limitations and outlook to future work". This limitation is also mentioned in the abstract.

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