I thank the referees for their helpful comments. I have addressed all the issues they have raised in the following. The full reviews are copied hereafter and my responses are inserted where appropriate.

Referee #1

> This work presents essentially two different, though related, pieces of research.

There is indeed a theoretical part and a practical one, but they are not two different pieces of research: they are not more different than a conclusion is from an introduction. This misunderstanding may actually originate from the way the asbtract was built (the two parts were just linked by "More generally") and I have made it reflect the structure of the paper better in the revised version by putting the arguments in the same order than in the core of the text (theory first, then practice).

> The first argues that the current pipeline used to derive optimal flux estimates from satellite measurements of column CO2 (XCO2) are fundamentally flawed. They are flawed because different prior assumptions are used in the retrieval as compared to the inversion, and the author argues that this inconsistency could bias inversion results. The author then argues that using a strong prior constraint (as most inverse models would suggest) in the GOSAT retrieval algorithm seems to yield better agreement between the XCO2 in his MACC (v13.1) model, than do comparisons with the standard ACOS (v3.5) XCO2 retrievals. He also states that ACOS - MACC XCO2 differences appear to be correlated with surface albedo, though only upon visual inspection of difference maps.
>
> This paper, while certainly thought-provoking, suffers from a severe logical deficiency that must be addressed before publication.

The reviewer's remarks have given me the opportunity to clarify a few points, but not to change the paper logic, as I will explain below.

> Regarding the first point, of the basic inconsistency between the GOSAT retrieval's prior CO2 covariance assumption and that of the model, it is worth stating that retrieval groups use a loose prior primarily because they want to be maximally consistent with any model prior covariance. A sufficiently loose covariance is always consistent with a tighter one, but not necessarily the other way around.

This statement is actually a misconception that this paper tries to correct. The requirement of statistical consistency expressed by Eq. (7) in the paper indicates that a loose covariance is *never* consistent with a tighter one within an assimilation system that uses averaging kernels. Actually, we can find the same requirement in the alternative (and heavier) approach of Migliorini (2012, doi:10.1175/MWR-D-10-05047.1, bottom right of p. 263), a paper that I found after the present one was published in ACPD. I have added a paragraph in Section 3 to summarise his findings.

> Therefore, it is not clear to me that using a tighter covariance is required to yield formal mathematical consistency upon assimilation of the satellite-retrieved XCO2, assuming the averaging kernels are fairly applied.

The way the averaging kernels are applied makes the retrieval prior disappear from the equation, but not the retrieval prior error statistics. Intuitively, we can understand that retrieval prior error statistics that are different from what the inversion system assumes, prevent the inversion equation from looking like radiance assimilation and therefore corrupt the optimality of the system.

> My strongest concern, however, regards the author's evaluation of the GOSAT XCO2 retrieval quality via the comparison to a single model. Disagreement does not necessarily mean the GOSAT retrievals are biased. Models have many sources of error: transport model error, imperfect prior fluxes, and the assimilation of datasets that are sparse in many regions of the world.

This remark has been anticipated and is actually written in many places of the original paper (e.g., abstract, l. 7-8; p. 11, l. 24-25; conclusion, p. 17, l. 12-13).

> The author's only serious argument

The reviewer dismisses the other parts of the discussion in Section 4.1, but it would have been helpful to substantiate this opinion.

> is that the difference map between the model-predicted and satelliteretrieved XCO2 should not have sharp spatial gradients because these should be smoothed out by transport effects (page 1900, line 8). But this argument problematic for at least two reasons:
>
> - He does not specifically demonstrate that there is no way such a spatial gradient can be supported by transport, even if the underlying flux was large and itself contained a strong spatial boundary, as of course happens in some ecotones as well as at land/ocean interfaces; and

We are discussing here column-integrated CO_2 concentrations, not surface concentrations. For instance, a megacity like Los Angeles forms an emission hotspot that enhances χ_{CO2} by 3.2 ppm on average only (Kort et al. 2012, doi:10.1029/2012GL052738). Land/ocean interfaces cannot have a comparable effect in magnitude. For ecotones, the paper already discusses the impact of the Corn Belt on χ_{CO2}, which is found indeed very small.

- One certainly cannot make this argument on maps that contain variable spatio-temporal sampling all plotted on the same map. For example, in the seasonally dry African Sahel region, the satellite has strong seasonality in its ability to monitor this region (namely due to wet vs. dry seasons), and this in and of itself could cause apparent spatial gradients because, in fact different times are plotted on the same map.

This is exactly why monthly maps are also shown in Fig. 3. The reviewer can see that the patterns are indeed robust.

> Secondly, the author states that in certain regions of large (1-2 ppm) model-satellite disagreement, the fault likely lies in the satellite data. While this is certainly possible, the reverse is of course also possible in the lack of additional information.

The former sentence is correct, but not the latter. The regions where the fault is attributed to the satellite data are the regions where models are very unlikely wrong that way, as discussed in the paper. The discussion clearly states that the models can be wrong for other patterns.

> Even though the author admits a few times in the text that the model may be imperfect, he does not comment about the general agreement (or disagreement) between the XCO2 of different carbon inverse model systems.

Indeed this is not the purpose of the paper. The maps of Figs. 1-3 aim at showing and discussing some regional suspicious patterns of the retrievals before the misfits are binned by more abstract retrieval increment size.

> These differences exist and they have been shown to be notable especially in regions where the models are not well constrained by in-itu data. For example, Kulawik et al. (AMTD, 2015) and Lindqvist et al. (ACPD, 2015) have recently shown that inversion models can have major differences in the seasonal magnitude of their optimized XCO2 values both latitudinally and longitudinally. Most of the regions with large retrieval-to-model differences in Fig. 2a are, interestingly, the same regions where also model-to-model differences in XCO2 can be notable: for example, in the African savannas, in seasonally dry forest/grassland regions in South America, in India, and in the high northern latitudes there can be up to 1-3 ppm differences in monthly averages between different inverse models constrained by in-situ measurements.

Kulawik et al. and Lindqvist et al. indeed show large differences between models but they do not show that models can reproduce some of the gradients that are discussed as unphysical in my paper. Incidently, I note that

MACCv13r1 has the best latitudinal fit to ACOS-GOSAT in the Tropics and in the high latitudes (Lindqvist et al., Fig. 7, which they comment with "ACOS is in excellent agreement to MACC from 0 to 50°N"): I interpret this feature as a likely low noise level of this product in these latitudes, that should help isolating local retrieval errors.

> Ultimately, of course, we would like to know what is driving these persistent model differences. Nevertheless, the author's conclusions would be on much more solid ground if independent model data sets were shown to support the author's arguments both about the surface albedo effect on retrievals and over-fitting of the radiances.

The reviewer's recommendation would be on much more solid ground if it came after a discussion of the detailed arguments of Sections 4. Analysing one model is already challenging. Suggesting analysing two or more models without further motivation may be a side step.

> The author argues that the differences between the model and the retrieval over land at high latitudes are likely due to retrieval errors over dark surfaces. While this argument might have some truth to it (as retrieved XCO2 is indeed sensitive to the surface albedo in all three bands, and to its changes within each band), it is not entirely supported by the figures shown: the map of the mean surface albedo (Fig. 4) shows that the darkest land regions are in Scandinavia and the westernmost Russia while the largest positive differences are most continuous and consistent in central and eastern Russia.

The paper does not claim that the bias is a monotoneous function of the surface albedo, at least because surface albedo is not the only variable that interferes with the retrieval of χ_{CO2}.

> Moreover, the author says that the regions with the largest positive differences correspond to the evergreen needle leaf forest biome type, which is not true especially for central Russia where differences in June vary from -1.5 to 1.5 ppm inconsistently (Fig. 3b) and parts of Alaska.

I am referring to the classification of `http://www.esa-landcover-cci.org/`, but do not claim that the correspondance is systematic. The pattern is just strikingly similar (see the land cover map viewer at `http://maps.elie.ucl.ac.be/CCI/viewer/index.php`).

> The author finds substantial model-to-retrieval differences in the African savanna/Sahel region, and attributes these differences to "systematic errors in the retrievals", speculating about averaging kernels not peaking low enough in the atmosphere due to too loose

> retrieval prior error variances. However, the author does not speculate more about the reason for such regionally constrained errors: why would the prior error variances have more impact in that particular region compared to elsewhere?

My statement was not rigorous enough and I apologize for it. Rather than loose retrieval prior error variances, some of the fault should lie in inappropriate prior error correlations. The sentence has been corrected.

> He suggests that CO2 from fires inaccurately represented in the MACC model might be another cause for the differences but considers this unlikely.

Indeed, "if the model was underestimating the intensity of the fire, we would expect the mean difference to take the shape of a plume, i.e. to spread downstream the source region, but this is not the case." (p. 12, l. 20-25, of the original paper).

> However, a look at this particular region's optimized, natural CO2 fluxes inverted by different models reveals extremely large differences in the fluxes, and also that similar differences are reflected in that region's XCO2. As long as the model differences in this region are unexplainably large, one of the models cannot be fairly used to speculate about biases in the satellite retrievals in that region without some kind of additional information.

The reviewer does not explain how any model would have so high values of χ_{CO2} over this specific land region. Actually the same difference pattern between ACOS-OCO-2 and the GEOS-5 model was shown at the first OCO-2 Science Team Meeting (Pasadena, CA, USA, February 2015) by Baker et al.

> Page 11901 line 21. It is mentioned that "boreal forests are covered with needle-leaved trees". It is safer to say "are largely covered". Apart from the widespread light coniferous larch and pine forests, dark coniferous needle-leaved trees can not dominate the landscape and often appear in mosaic patches with broad-leaved trees mostly due to post-fire successional dynamics (eg Shvidenko and Nilsson, Tellus, 2003).

I have made the change.

> The author presents in Figs. 5-8 an interesting metric for evaluating overfitting in the retrievals (i.e., too tight a prior), and shows that increasing the weight of the prior XCO2 could make the retrievals statistically more consistent with the model. However, he does not show any spatial patterns of this metric; therefore it remains unclear if the suggested change in the retrieval prior errors would lead to worse misfits in some currently well-matched regions in addition to the likely improvements in the model-retrieval misfits in the regions where the differences are large.

The reviewer seems to suggest re-drawing the mean difference map of Fig. 2 with $\breve{\mathbf{x}}^{a,r}$. However, $\breve{\mathbf{x}}^{a,r}$ is not bias-corrected and this map could not be interpreted in terms of better or worse misfits. The argument made with Fig. 6 relies on the standard deviation of the misfit distribution, not on its mean. For this reason, the original conclusion states that "the optimal-estimation retrieval process and, *consequently, its posterior bias correction* need retuning".

> And even if he did, it would still suffer from the problem of comparing to a single model,

As explained in p. 14 l. 17-19, of the original version, what matters here, while discussing about random differences (standard deviations) is that the model errors are uncorrelated with the retrieval errors and with the retrieval-prior errors. This hypothesis is further discussed in p. 15 l. 10-13 of the original version. I have completed the discussion by excluding the possibility that subgrid scale variability plays a role in the results: "at the sub-grid scale, the variability of χ_{CO2} is usually well below the ppm (Alkhaled et al. 2008, Corbin et al. 2008), i.e. one order of magnitude smaller than the prior-to-retrieval degradation". I have also added a sentence about the relevant results from Kulawik et al.: "Some, but not all, of the degradation is purely random and disappears after enough averaging (see Fig. 6 of Kulawik et al. 2015)".

> and the fact that it couldn't be accounted for by faithfully using the column averaging kernel in the assimilation.

This fact just comes from the maths (Eq. (7) of Section 3).

> Overall, by counting too much on the results obtained by this metric, we risk the possibility of both the model and the prior XCO2 being wrong

Again, what matters is that they are not similarly wrong (correlated errors), which is the case.

> and the satellite observations the truth. The satellite retrievals are certainly not (yet) completely free of retrieval biases, but it is fruitful to remind oneself why they are being carried out: because neither our prior knowledge nor our models are perfect.

This question actually forms the first sentence of the introduction: "CO_2 surface fluxes at the Earth's surface can be inferred from accurate surface measurements of CO_2 concentrations, but the sparseness of the current global network still leaves the flux horizontal and temporal gradients, and even their latitudinal distribution, very uncertain (Peylin et al. 2013)".

> Even if similar results were obtained based on comparisons to other models, this philosophical dilemma would still remain in the background but the reasons that support to change the current retrieval procedure would be stronger.

Adding models would not change the maths (Section 3). Our study with a single model, in particular Figs. 5-8, is just an illustration of this theoretical section.

Detailed comments:

> - Page 11893, line 21. The author should state that the use of a rather loose prior CO2 covariance is not specific to ACOS, with some examples. For instance: 1) The RemoTeC retrieval has a formally unconstrained XCO2 (Butz et al., Applied Optics, 2009), and 2) the BESD retrieval uses a prior error on XCO2 of 15.6 ppm (Reuter et al, AMT, 2010). etc.

This section is about ACOS and the two references would not fit there, but I have added them in Section 2 after "This condition is not achieved by current satellite retrieval algorithms, at least because they artificially maximize the measurement contribution in the retrievals through the use of very large prior error variances".

> - Page 11896, line 3: "H a linearized" $\longrightarrow$ H is a linearized

I have corrected it.

> - Page 11896, line 12: "inversion window for the inversion" $\longrightarrow$ inversion window

I have replaced the first "inversion" by "assimilation".

> - Page 11897, Eq. (4): might be more informative to simply show the derivation of Eq. (4) instead of describing it in the previous paragraph.

I agree with the reviewer and have revised the demonstration in the following way. I have redefined $\widehat{\mathbf{y}}'$ in order to express the elimination of $\breve{\mathbf{x}}^b$ directly at this level rather than in Eq. (4). To help the reader, I have also put the formula of $\widehat{\mathbf{H}}'$ rather than defining it with words. That was made possible by stating that, without loss of generality in our linear framework, we consider the assimilation of a single sounding using its averaging kernel.

I have noticed a misplaced prime in Eq. (4), that induced missing primes in Eq. (6-7). Additionally, I have also noticed that, when we make Eqs. (5-6) consistent, the requirement of Equation (7) can be relaxed to $\breve{\mathbf{H}}\breve{\mathbf{B}}\breve{\mathbf{H}}^{\mathrm{T}} = \breve{\mathbf{H}}\widehat{\mathbf{H}}\widehat{\mathbf{B}}\widehat{\mathbf{H}}^{\mathrm{T}}\breve{\mathbf{H}}^{\mathrm{T}}$, which means that consistency needs only to be satisfied at the resolution (information content) of the retrieval. I have corrected these equations and updated the text accordingly.

> - Page 11899, line 16: "long-tern" $\longrightarrow$ long-term

I have corrected this.

> - Page 11899, lines 17-18: variability in the XCO2 field is ~ 8 ppm in Fig. 1, retrieval-to-model differences are most typically less than 1 ppm (Fig. 2a). Therefore, the retrieval-model difference is "much less" than the variability within the modeled or retrieved XCO2 field.

I have removed this statement.

> - Page 11900, lines 10-11: it is incorrect to say that the local spatial gradients mostly reflect the retrieval gradients. For example, the gradients in Fig. 3a for South Africa, South America, and the latitudinal gradients in the oceans are not obviously wrong in the retrievals (Fig. 1a).

The text does not say that the retrieval gradients are wrong there, but that they explain the gradients of the differences there. Wether they are right or wrong is the topic of the rest of the section.

> - Page 11900, lines 23-25: The surprising discontinuity in XCO2 on the NW coast of the U.S. compared to the adjacent ocean data is more clearly seen in the model (Fig. 1b) than in the retrieval.

I have removed the statement.

> - The benefits of showing Tables 1 & 2 are not clear. Because the paper otherwise concentrates on the GOSAT data years 2009-2013, it might be more helpful to the reader to see a map of where the in-situ data were collected during these years.

The tables follow a request from a station PI to have the name of his station appear publicly. It takes 1.5 pages on the "printer-friendly" version, which seems reasonable to me, but adding a map may be too much. I leave this question to the editor.

> - Figures 5-8 need a more informative y-axis label. For example "XCO2ˆ a - XCO2ˆ model (ppm), mean(—) or sigma (___)", or something similar.

I have replaced the label by "mean or σ of the χ_{CO2} misfits (ppm)".

> - Figure 6: the two blue shades look very similar in the printed version. Consider colors with a larger contrast.

I have replaced the light blue by gold.

Referee #2

Author provides arguments on desirable improvements in overall consistency in a two-step process of estimating CO_2 fluxes using firstly the atmospheric χ_{CO2} retrievals from satellite observations, and secondly CO_2 flux inversions. The discussion points at an inflated prior uncertainty for retrievals as a factor contributing to retrieval product deficiencies. It was found that tightening retrieval uncertainties can reduce posterior misfit between concentrations optimized with inversion and retrieved χ_{CO2} values. It is also mentioned that possible posterior adjustments to uncertainties are making empirical bias correction inconsistent. The methods and materials applied in the analysis appear valid, and the discussion and conclusions are valuable for those working on concentration retrievals and inverse modeling of the surface fluxes. Several minor changes are recommended before publication.

Suggestions on the text

Page 11896 line 19. The derivation of Eq. (4), with elimination of $\breve{\mathbf{x}}^b$ should be included, to convince the reader that there is no omission or use of simplifying assumptions on the way.

I have developed the demonstration as suggested. In practice, I have redefined $\widehat{\mathbf{y}}'$ in order to express the elimination of $\breve{\mathbf{x}}^b$ directly at this level rather than in Eq. (4). To help the reader, I have also put the formula of $\widehat{\mathbf{H}}'$ rather than defining it with words. That was made possible by stating that, without loss of generality in our linear framework, we consider the assimilation of a single sounding using its averaging kernel.

I have noticed a misplaced prime in Eq. (4), that induced missing primes in Eq. (6-7). Additionally, I have also noticed that, when we make Eqs. (5-6) consistent, the requirement of Equation (7) can be relaxed to $\breve{\mathbf{H}}\breve{\mathbf{B}}\breve{\mathbf{H}}^{\mathrm{T}} = \breve{\mathbf{H}}\widehat{\mathbf{H}}\widehat{\mathbf{B}}\widehat{\mathbf{H}}^{\mathrm{T}}\breve{\mathbf{H}}^{\mathrm{T}}$, which means that consistency needs only to be satisfied at the resolution (information content) of the retrieval. I have corrected these equations and updated the text accordingly.

Page 11898 line 3. It is mentioned "if enough intermediate variables were saved by the retrieval schemes, it would be possible to reconstruct the retrievals with a different prior". Reader may get impression that Level 2 products do not carry "enough intermediate variables", while the reality is that a number of products include prior and posterior matrixes, as well as column averaging kernel and prior profile $\breve{\mathbf{x}}^b$. As author wrote, the information is not sufficient to reconstruct the retrievals with a different prior error covariance matrix $\breve{\mathbf{B}}$, but it is sufficient for a) getting approximation to $\breve{\mathbf{x}}^a$ for $\breve{\mathbf{B}}$ modified by multiplying it by scaling factor,

The gain matrix $\breve{\mathbf{K}}$ depends on both $\breve{\mathbf{B}}$ and $\breve{\mathbf{R}}$. Scaling $\breve{\mathbf{x}}^a$ from a scaled $\breve{\mathbf{B}}$ would not be a good approximation. Further, $\breve{\mathbf{B}}$ is made of both variances, that indeed can be scaled, and correlations that cannot be changed with a scaling factor.

b) replacing the prior profile $\breve{\mathbf{x}}^b$ with any other.

Atmospheric inversions are insensitive to $\breve{\mathbf{x}}^b$ provided that $\breve{\mathbf{x}}^a$ is assimilated with its averaging kernel (Eq. (4)). Therefore, we are not interested in changing $\breve{\mathbf{x}}^b$.

> Thus if one wants to have the retrieval with deflated prior uncertainty as suggested in the manuscript, it can be done. For the sake of clarity it is better to mention that although we can not get retrieval result for different prior error covariance $\breve{\mathbf{B}}$, simple scaling should work.

This proposition is similar to what is done in the paper with $\breve{\mathbf{x}}^{a,r}$, but I do not recommend it because it does not improve the correlations in $\breve{\mathbf{B}}$.

I have made it clearer that we need to change both variances and correlations by replacing "matrix" by "variances and correlations".

> Page 11898 line 19. The comment that with large prior uncertainties for retrievals, "the retrieval averaging kernel would not peak low enough in the vertical" is not supported by discussion or reference.

I have made the sentence more general by changing it to "In particular, the sub-optimality of $\breve{\mathbf{K}}$ affects the retrieval averaging kernel, that may not peak at the right height."

> Page 11901 line 21. It is mentioned that "boreal forests are covered with needle-leaved trees". It is safer to say "are largely covered". Apart from the widespread light coniferous larch and pine forests, dark coniferous needle-leaved trees can not dominate the landscape and often appear in mosaic patches with broad-leaved trees mostly due to post-fire successional dynamics (eg Shvidenko and Nilsson, Tellus, 2003).

I have removed this mistake. The text a few lines later ("dominated by") was more cautious.

> Page 11903 line 15. The test results introduced on Fig. 6 are most impressive, and show advantage of mixing retrieval with prior χ_{CO2}. Here it is worth mentioning that making weighted average of

> prior and posterior has similar effect with reducing prior uncertainty for retrieval. The result needs more discussion, as long as a) mixing proportion of 1/2 is chosen arbitrarily; b) the prior performed worse than retrievals on Fig.5 so it is not clear why mixing with it would improve the mismatch.

The interpretation is that the retrieval scheme overshoots the truth, i.e. that the increments are in the right direction but are too large. I have added this clarification in the paragraph.

On the statistical optimality of CO_2 atmospheric inversions assimilating CO_2 column retrievals

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~~9~~ 9 July~~April~~ 2015

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Abstract

The extending archive of the Greenhouse Gases Observing SATellite (GOSAT) measurements (now covering about six years) allows increasingly robust statistics to be computed, that document the performance of the corresponding retrievals of the column-average dry air-mole fraction of CO_2 (XCO_2). Here, we demonstrate that atmospheric inversions cannot be rigorously optimal when assimilating current XCO_2 retrievals, even with averaging kernels, in particular because retrievals and inversions use different assumption about prior uncertainty. W~~w~~e look for some practical evidence of this sub-optimality from the view point of atmospheric inversion by comparing~~e~~ a model simulation constrained by surface air-sample measurements with one of the GOSAT retrieval products (NASA's ACOS). The retrieval-minus-model differences result from various error sources, both in the retrievals and in the simulation: we discuss the plausibility of the origin of the major patterns. We find systematic retrieval errors over the dark surfaces of high-latitude lands and over African savannahs. More importantly, we also find a systematic over-fit of the GOSAT radiances by the retrievals over land for the high-gain detector mode, which is the usual observation mode. The over-fit is partially compensated by the retrieval bias-correction. These issues are likely common to other retrieval products and may explain some of the surprising and inconsistent CO_2 atmospheric inversion results obtained with the existing GOSAT retrieval products. We suggest that reducing the observation weight in the retrieval schemes (for instance so that retrieval increments to the retrieval prior values are halved for the studied retrieval product) would significantly improve the retrieval quality and reduce the need for (or at least reduce the complexity of) ad-hoc retrieval bias correction~~. More generally, we demonstrate that atmospheric inversions cannot be rigorously optimal when assimilating XCO_2 retrievals, even with averaging kernels~~.

1. Introduction

CO_2 surface fluxes at the Earth's surface can be inferred from accurate surface measurements of CO_2 concentrations, but the sparseness of the current global network still leaves the flux horizontal and temporal gradients, and even their latitudinal distribution, very uncertain (Peylin et al. 2013). This limitation has provided a major incentive to develop the monitoring of CO_2 concentrations from space. First retrievals were obtained from existing instruments measuring either the thermal infrared radiation emitted by the atmosphere (Chédin et al. 2003) or the reflected sunlight in the near-infrared (NIR)/ shortwave infrared (SWIR) spectral regions (Buchwitz et al. 2005). The latter technique allows retrieving XCO_2 while the former is not sensitive to CO_2 in the lower atmosphere, near the CO_2 sources and sinks. Since active (lidar) measurement techniques for XCO_2 from space are still in development (e.g., Ingmann et al. 2009), NIR/SWIR measurements currently offer the best prospect to provide "retrievals of CO_2 of sufficient quality to estimate regional sources and sinks", as phrased by objective A.8.1 of the Global Climate Observing System programme (GCOS, 2010), in the short term. However, they are hampered by uncertain knowledge about scatterers in the atmosphere at the corresponding wavelengths (aerosols and cirrus clouds) with an effect that varies with surface albedo, which is itself uncertain (e.g., Aben et al. 2007). Such interference in the XCO_2 signal seen in the NIR/SWIR measurements is of concern because even sub-ppm systematic errors (corresponding to less than 0.25% of the signal) can severely flaw the inversion of CO_2 surface fluxes (Chevallier et al. 2007, Miller et al. 2007). This risk motivated dedicated developments of the retrieval algorithms in order to de-convolve the spectral signatures of the involved compounds as much as possible (e.g., Reuter et al. 2010, Guerlet et al. 2013b).

The Japanese GOSAT, launched in January 2009, and the USA second Orbiting Carbon Observatory (OCO-2), launched in July 2014, observe the NIR/SWIR radiation with unprecedented spectral resolution in order to specifically address this remote sensing challenge. The GOSAT archive already covers ~~nearly~~ six years and can provide good insight into the adequacy of NIR/SWIR retrievals for CO_2 source-sink inversion. In terms of random errors, raw GOSAT retrievals now reach single shot precision better than 2 ppm (one sigma) in ~~favourable~~ fair measurement conditions (e.g., Nguyen et al. 2014). This performance is better than what pre-launch studies suggested: for instance Maksuytov et al. (2008) expected 2.5-10 ppm single shot precision only. Systematic errors are difficult to quantify or else they would be removed. They are likely state-dependent with absolute values varying in time and space about the ppm before any bias correction (Nguyen et al. 2014). They also depend on the retrieval algorithm (e.g., Oshchepkov et al. 2013). As expected, the remaining uncertainty has profound impact on CO_2 source-sink inversions (Basu et al. 2013, Chevallier et al. 2014), but XCO_2 retrievals have already served as a basis to study the carbon budgets of some regions (Guerlet et al. 2013a, Basu et al. 2014, Reuter et al. 2014). For instance, 25 scientists analysed several XCO_2 retrievals over continental Europe and concluded that the current understanding of the European carbon sink brought by bottom-up inventories had to be revisited (Reuter et al. 2014).

This paper aims at contributing to the debate about the relevance of current GOSAT retrievals for atmospheric inversions. Our starting point is a critical review of the basic principles behind the current processing chains that go in successive steps from GOSAT measured radiance spectra to surface flux estimates (Section 3). We then focus on the GOSAT retrievals provided by NASA's Atmospheric CO_2 Observations from Space project (ACOS, build 3.4, described in Section 2) for the period between June 2009 and May 2013. They are of particular interest because they have been processed in a way that prefigures the official OCO-2 retrievals in terms of spectral bands and available simultaneous observations (O'Dell et al. 2012). In Section 4, we analyse the residuals between the ACOS-GOSAT retrievals and the simulated CO_2 concentration fields of the Monitoring Atmospheric Chemistry and Climate atmospheric inversion product (MACC, version 13r1, also described in Section 2) that assimilated surface air sample measurements from various networks. Concluding discussion follows in Section 5.

2. Retrievals and model simulation

2.1. ACOS-GOSAT retrievals

GOSAT is a joint venture by the Japan Aerospace Exploration Agency (JAXA), the National Institute for Environmental Studies (NIES) and the Ministry of the Environment (MOE) in Japan. This spacecraft is operated in a sun-synchronous polar orbit that crosses the Equator at about 13:00 local time during daytime and that repeats every 3 days. As described by O'Dell et al. (2012) and Osterman et al. (2013), the ACOS algorithm retrieves XCO_2 from a selection of GOSAT measurements of reflected sunlight made in the same spectral bands than OCO-2. Over land, such measurements are made by pointing the instrument to the Earth on both sides of the satellite track. Given the low reflectivity of water surfaces, ocean measurements are only possible when the instrument is pointed to the sun-glint spot, which is only done within 40° from the Equator in the summer hemisphere. GOSAT also carries a cloud and aerosol imager that can help filtering difficult scenes out, but unlike other GOSAT retrieval algorithms, ACOS does not use it since OCO-2 does not contain a similar instrument.

Following Boesch et al. (2006) and Connor et al. (2008), the ACOS algorithm relies on optimal estimation (i.e. Bayesian methods) to retrieve the vertical profile of the CO_2 dry air mole fraction together with variables interfering in the measurements: the surface pressure and the surface albedo, some variables describing temperature, water vapour, clouds and aerosols in the atmosphere, and channel offsets for the instrument. The retrieved XCO_2 is simply obtained by integrating the retrieved CO_2 profile. In this Bayesian formulation of the retrieval, prior information about CO_2 is given an artificially small weight in order to maximize the observation contribution to the result: for instance, the standard deviation of the uncertainty assigned to the prior XCO_2 is larger than 10 ppm (O'Dell et al., 2012), i.e. larger than typical variations of XCO_2 at the continental scale (e.g., Keppel-Aleks et al. 2011). We will discuss the impact of this choice later and for simplicity, we will call XCO_2^b and XCO_2^a the prior (*background*) and the retrieved (*analysed*) XCO_2, respectively. XCO_2^a can be compared with model simulations, as will be done here, or with other measurements via the associated CO_2 averaging kernel profiles and prior profiles (e.g., Connor et al., 1994). For nadir viewing, XCO_2^a is representative of a volume that has a circular footprint at the Earth's surface of diameter about 10 km.

Previous comparisons between XCO_2^a and model simulations or reference ground-based XCO_2 measurements from Total Carbon Column Observing Network (TCCON) highlighted some systematic dependency of the error of XCO_2^a as a function of a series of internal variables of the algorithm (Wunch et al. 2011b). This feature reveals some limitations of the algorithm but also allows correcting them empirically, for instance before they are assimilated in atmospheric inversion systems (Crisp et al. 2012). We will call $XCO_2^{a,c}$ the bias-corrected retrievals.

2.2. MACC CO_2 inversion

Since year 2011, the MACC pre-operational service (www.copernicus-atmosphere.eu) has been delivering a CO_2 inversion product with biannual updates. Release 13r1 primarily describes

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the CO_2 surface fluxes over more than three decades, from 1979 to 2013, at resolution 3.75° × 1.9° (longitude-latitude) and 3-hourly, based on 131 CO_2 dry air mole fraction station records from three large databases:

- the NOAA Earth System Research Laboratory archive (NOAA CCGG, http://www.esrl.noaa.gov/gmd/ccgg/index.html),
- the World Data Centre for Greenhouse Gases archive (WDCGG, http://ds.data.jma.go.jp/gmd/wdcgg/),
- the Réseau Atmosphérique de Mesure des Composés à Effet de Serre database (RAMCES, https://www.~~ramces.~~lsce.ipsl.fr/).

The three databases include both in situ measurements made by automated quasi-continuous analysers and irregular air samples collected in flasks and later analyzed in central facilities. The detailed list of sites is provided in Tables 1 and 2.

The MACC Bayesian inversion method is formulated in a variational way in order to estimate the CO_2 surface fluxes at the above-described relatively high resolution over the globe (Chevallier et al. 2005, 2010). For v13r1, the system used a single 35-year inversion window, therefore enforcing physical and statistical consistency in the inverted fluxes. Fluxes and mole fractions are linked in the system by the global atmospheric transport model of the Laboratoire de Météorologie Dynamique (LMDZ, Hourdin et al. 2006) with 39 layers in the vertical and with the same horizontal resolution than the inverted fluxes. LMDZ is nudged to ECMWF-analysed winds for flux inversion.

The MACC inversion product also contains the 4D CO_2 field that is associated to the inverted surface fluxes through the LMDZ transport model. Simulating the GOSAT retrievals from this field is nearly straight-forward. The only difficulty lies in the interpolation from the LMDZ 39-level vertical grid to the 20-level vertical grid of the retrievals, before the retrieval averaging kernels are applied. Indeed, the model orography at resolution 3.75° × 1.9° significantly differs from the high-resolution orography seen by the retrievals. For the interpolation, we assume that CO_2 concentrations vary linearly with the pressure in the vertical. When the model surface pressure is smaller than the retrieved surface pressure, the profile is artificially extended at constant value below the model surface. In the opposite case, model levels below the sounding surface are ignored. We compensate this artificial change of mass in the profile by systematically adjusting the interpolated profile so that its pressure-weighted mean equals that of the profile before the interpolation.

3. Theoretical aspects

Like the other retrieval and inversion systems (see, e.g., Oshchepkov et al., 2013, and Peylin et al., 2013), ACOS-GOSAT and MACC both follow the Bayesian paradigm in its Gaussian linear form (e.g., Rodgers, 2000) in order to estimate the most likely state, in a statistical sense, of the CO_2 profile and of the CO_2 surface fluxes, respectively. In mathematical terms, given $\mathbf{x}$ the vector that gathers the variables to be inferred (either a 1D CO_2 profile or 2D+1D CO_2 surface fluxes), given $\mathbf{x}^b$ an a priori value of $\mathbf{x}$ (coming from a climatology or from a model), and given $\mathbf{y}$ the vector that gathers all relevant observations (either radiances or retrievals), the most likely state of $\mathbf{x}$ is written:

$$\mathbf{x}^a = \mathbf{x}^b + \mathbf{K}(\mathbf{y} - \mathbf{H}\,\mathbf{x}^b) \qquad (1)$$

$\mathbf{H}$ is a linearized observation operator that links variables $\mathbf{x}$ and $\mathbf{y}$ (i.e. essentially a radiative transfer model or a transport model). $\mathbf{K}$ is the following “Kalman gain” matrix:

$$\mathbf{K} = \mathbf{B}\,\mathbf{H}^T(\mathbf{HBH}^T + \mathbf{R})^{-1} \qquad (2)$$

$\mathbf{B}$ and $\mathbf{R}$ are the error covariance matrices of $\mathbf{x}^b$ and $\mathbf{y}$, respectively.

The error covariance matrix of $\mathbf{x}^a$ is obtained by:

$$\mathbf{A} = (\mathbf{I} - \mathbf{KH})\,\mathbf{B} \tag{3}$$

with $\mathbf{I}$ the identity matrix with appropriate dimension.

For simplicity, Eq. (1) does not make other variables that are simultaneously inferred appear, like clouds, aerosols or surface variables for the retrievals, or the 3D state of CO_2 at the start of the ~~inversion~~ assimilation window for the inversion.

The current processing chains that go from radiances to surface fluxes are two-step processes (let aside some attempts to introduce an additional intermediate step in the form of a short-window analysis of the 3D concentrations; Engelen et al. 2009). We now distinguish the retrieval process and the inversion process by putting breves ˘ on all symbols related to the former and hats ˆ on all symbols related to the latter. In a first step, the CO_2 profiles and their uncertainty $\{\breve{\mathbf{x}}^{\boldsymbol{a}}\cancel{\breve{\mathbf{x}}}, \breve{\mathbf{A}}\}$ are retrieved for each sounding $\{\breve{\mathbf{y}}, \breve{\mathbf{R}}\}$ separately. The resulting ensemble forms the observations to be simultaneously assimilated $\{\hat{\mathbf{y}}, \widehat{\mathbf{R}}\}$ for the second step. The presence of prior information $\mathbf{x}^b$ in both steps complicates the transition between the two. Following Connor et al. (1994) and the current practice, we can technically eliminate the influence of $\breve{\mathbf{x}}^{\boldsymbol{b}}$ (but not of its uncertainty) by the following adaptation of Eq. (1) in the second step: we assimilate $\hat{\mathbf{y}}' = \breve{\mathbf{x}}^{\boldsymbol{a}} - (\mathbf{I} - \breve{\mathbf{K}}\breve{\mathbf{H}})\breve{\mathbf{x}}^{\boldsymbol{b}} = \breve{\mathbf{K}}\,\breve{\mathbf{y}}$ rather than $\hat{\mathbf{y}}$ and change the observation operator from $\widehat{\mathbf{H}}$ to $\widehat{\mathbf{H}}' = \breve{\mathbf{K}}\breve{\mathbf{H}}\widehat{\mathbf{H}}$. $\breve{\mathbf{K}}\breve{\mathbf{H}}$ is called ~~subtract the retrieval prior $\breve{\mathbf{x}}^{\boldsymbol{b}}$ from each CO_2 profile simulated by the transport model at the sounding location $\widehat{\mathbf{H}}\,\hat{\mathbf{x}}^{\boldsymbol{b}}$, we multiply the result by~~ the retrieval *averaging kernel* ~~matrix $\breve{\mathbf{K}}\breve{\mathbf{H}}$ and finally add $\breve{\mathbf{x}}^{\boldsymbol{b}}$~~. The retrieval error covariance matrix should consistently be diminished (e.g., Connor et al., 2008, paragraph 37) and is then~~. We~~ called ~~$\widehat{\mathbf{H}}'$ the convolution of the transport model operator with the individual retrieval averaging kernels and~~ $\widehat{\mathbf{R}}'$ hereafter.

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For simplicity, and without loss of generality in our linear framework, let us consider the assimilation of a single sounding $\{\breve{\mathbf{y}}, \breve{\mathbf{R}}\}$ using its averaging kernel. By definition, given the changes made to $\hat{\mathbf{H}}$ and $\hat{\mathbf{R}}$, the gain matrix changes as well and we call ~~adjusted retrieval error covariance matrix~~$\hat{\mathbf{K}}'$ the new one. By applying Eq. (1) ~~twice~~in this configuration, the analysed surface fluxes can be directly expressed ~~and after accounting for the above adaptation, the processing chain can be written~~ in a concise form:

$$\hat{\mathbf{x}}^{a} = \hat{\mathbf{x}}^{b} + \hat{\mathbf{K}}' \, \breve{\mathbf{K}} \, (\breve{\mathbf{y}} - \breve{\mathbf{H}} \, \hat{\mathbf{H}}\cancel{'} \hat{\mathbf{x}}^{b}) \tag{4}$$

~~If we neglect the influence of the averaging kernel, t~~This equation has the desired shape of Eq. (1), i.e. the sum of the prior value and of a linear function of model-minus-measurement misfits. By construction, it does not depend on the retrieval prior $\breve{\mathbf{x}}^{b}$. However, to follow the optimal estimation framework, we still need to be able to develop the product of the gain matrices consistently with Eq. (2), i.e. like (neglecting errors in the observation operators):

$$\mathbf{K} = \hat{\mathbf{B}} \, \hat{\mathbf{H}}^{T} \breve{\mathbf{H}}^{T} (\breve{\mathbf{H}} \, \hat{\mathbf{H}} \, \hat{\mathbf{B}} \, \hat{\mathbf{H}}^{T} \breve{\mathbf{H}}^{T} + \breve{\mathbf{R}})^{-1} \tag{5}$$

In practice, we see that:

$$\hat{\mathbf{K}}' \, \breve{\mathbf{K}} = \hat{\mathbf{B}} \, \hat{\mathbf{H}}'^{T} (\hat{\mathbf{H}}' \, \hat{\mathbf{B}} \, \hat{\mathbf{H}}'^{T} + \hat{\mathbf{R}}')^{-1} \, \breve{\mathbf{B}} \, \breve{\mathbf{H}}^{T} (\breve{\mathbf{H}} \, \breve{\mathbf{B}} \, \breve{\mathbf{H}}^{T} + \breve{\mathbf{R}})^{-1} \tag{6}$$

Eqs. (5-6) can be made consistent in general provided

$$\breve{\mathbf{H}} \, \breve{\mathbf{B}} \, \breve{\mathbf{H}}^{T} = \breve{\mathbf{H}} \, \hat{\mathbf{H}} \, \hat{\mathbf{B}} \, \hat{\mathbf{H}}^{T} \breve{\mathbf{H}}^{T} \tag{7}$$

and (by developing $\hat{\mathbf{H}}'$ and using Eq. (7))

$$\breve{\mathbf{H}}^{T} \breve{\mathbf{K}}^{T} (\breve{\mathbf{K}} \, \breve{\mathbf{H}} \, \breve{\mathbf{B}} \, \breve{\mathbf{H}}^{T} \, \breve{\mathbf{K}}^{T} \cancel{\hat{\mathbf{H}} \, \hat{\mathbf{B}} \, \hat{\mathbf{H}}^{T}} + \hat{\mathbf{R}}')^{-1} \, \breve{\mathbf{B}} \cancel{\hat{\mathbf{H}} \, \hat{\mathbf{B}} \, \hat{\mathbf{H}}^{T}} = \mathbf{I} \tag{8}$$

Equation (7) simply expresses consistency between the prior error statistics within the information content of the retrievals: the uncertainty of the retrieval prior and of the flux prior should ~~correspond~~ be the same ~~to the uncertainty of the flux prior projected~~ in ~~the profile space~~radiance space. This condition is not achieved by current satellite retrieval algorithms, at least because they artificially maximize the measurement contribution in the retrievals through the use of very large prior error variances (see Section 2.1 or Butz et al. 2009, Reuter et al. 2010). However, if enough intermediate variables were saved by the retrieval schemes, it would be possible to reconstruct the retrievals with ~~a different~~ appropriate prior error ~~covariance matrix $\breve{\mathbf{B}}$.~~variances and correlations.

Equation (8) can ~~obviously only~~ be satisfied in general if the retrieval ~~error variances are negligible compared to the flux prior error variances projected in the same space (which would actually relax the previous requirement as well)~~averaging kernel $\breve{\mathbf{K}}\breve{\mathbf{H}}$ is close to unity. ~~Typically, the standard deviation of the uncertainty (1 σ) in the de-trended columns simulated by free models is not larger than a couple of ppm, at least for broad scale statistics (Chevallier and O'Dell 2013; Peng et al. 2015), i.e. about the current GOSAT retrieval uncertainty (Oshchepkov et al., 2013). Note that the situation is more favourable when considering TCCON retrievals, because of their better precision~~. In practice, the retrieval averaging kernel for profiles is far from unity because current radiance measurements do not provide any vertical resolution for CO_2. The situation is better if the state vector $\breve{\mathbf{x}}$ is the integrated column (in that case $\breve{\mathbf{H}}$ includes an operator to distribute the column in the vertical).

As a consequence of deviations from Eqs (7-8), the effective gain matrix $\widehat{\mathbf{K}}'\,\breve{\mathbf{K}}$ significantly differs from the optimal one for GOSAT, resulting in a wrong balance between prior flux information and measured radiances. Overall, $\breve{\mathbf{K}}$ pulls too much towards the measured radiances and $\widehat{\mathbf{K}}'$ pulls too much towards the prior. This suboptimality very likely flaws the 4D information flow from the radiance measurements to the surface flux estimates. ~~Further~~In particular, the sub-optimality of $\breve{\mathbf{K}}$ ~~also~~ affects the retrieval averaging kernel ~~that is part of $\hat{\mathbf{H}}'$~~, ~~meaning~~ that ~~the model-data misfits in Eq. (4) are not computed correctly, for instance because the retrieval averaging kernel would~~may not peak ~~low enough in the vertical~~at the right height.

Migliorini (2012) proposed a sophisticated alternative to the averaging kernel assimilation of Connor et al. (1994), where the retrievals are assimilated after a linear transformation of both the retrievals and the observation operator. The transformation is heavier to implement than the above approach because it involves the retrieval signal-to-noise matrix $\breve{\mathbf{R}}^{-1/2}\breve{\mathbf{H}}\,\breve{\mathbf{B}}^{1/2}$. It avoids the requirement of Eq. (8), but still requires consistent prior error statistics (Eq. (7)).

The situation complicates even further if we account for the facts that inversion systems assimilate ~~the retrieved profiles as vertical integrals (because XCO_2 is less sensitive to vertical transport model errors than the CO_2 profile), that these vertical integrals are empirically~~ bias-corrected retrievals (thereby implicitly re-introducing $\breve{\mathbf{x}}^{\boldsymbol{b}}$ that had been neutralised by the use of averaging kernels, in the equations), ~~and~~ that $\breve{\mathbf{H}}$ and $\hat{\mathbf{H}}$ are imperfect operators, the uncertainty of which should be reported in $\breve{\mathbf{R}}$, following Eq. (5), and that $\breve{\mathbf{H}}$ is usually non-linear. The need to report all observation operator uncertainties in $\breve{\mathbf{R}}$ means that retrieval configuration should in principle be tailored to the retrieval end-application, i.e. to the precision of the observation operator that is used in this end-application. For flux inversion, the transport model uncertainty in XCO_2 space is about 0.5 ppm (1 σ, Houweling et al. 2010). When optimizing parameters of a flux model rather than for the flux themselves (in Carbon Cycle Data Assimilation Systems, Rayner et al. 2005), the uncertainty of the flux model equations has also to be reported in $\breve{\mathbf{R}}$: when projected in the space of XCO_2, they are comparable to transport model uncertainties (Kuppel et al. 2013).

4. Practical aspects

Given the particular concerns raised about the optimality of XCO_2 retrievals ~~themselves~~ and of their averaging kernels in the previous section, we now focus on one specific retrieval product, ACOS-GOSAT, in order to look for some practical evidence of this sub-optimality.

4.1. Mean differences

Fig. 1 shows the mean bias-corrected retrievals $XCO_2^{a,c}$ and the mean corresponding posterior XCO_2 field of the MACC inversion over the June 2009 – May 2013 period per 3.75° × 1.9° grid cell. All retrievals are used, provided they are found good by the ACOS standard quality control. The data density (Fig. 2b) follows the frequency of favourable retrieval conditions: more sunlight in the Tropics, less cloud over desert areas or over subsidence ocean regions. The long-~~tern~~ term mean of the retrieval-minus-model differences (Fig. 2a) is usually about the ppm~~, i.e. not much less than the variability of the mean XCO_2 field (Fig. 1)~~. Interestingly, it appears to be organized spatially. Over land, large positive values (> 0.5 ppm, ACOS-GOSAT being larger) are seen over boreal forests, over most of South America, over grassland/cropland regions in Central Africa and over the West coast of the USA. Negative values occur over most of the other lands, with smaller values (up to ~ -1 ppm) mostly over South and East Asia. Over the oceans, values are mostly positive north of 30°N and south of 10°S, and negative in between. Both errors in ACOS-GOSAT and errors in the model simulations contribute to these differences, which complicates the interpretation of Fig. 2a. For instance, the zonal structure of the differences over the oceans could well be caused by the model, either because of too few surface air-sample sites in the Tropics or because the LMDZ transport model would not represent the inter-hemispheric exchange well enough (Patra et al. 2011). Alternatively, misrepresented clouds around the convergence zones could also induce them in the retrievals. Some of the patterns of Fig. 2a are similar to the surface cover, like the gradient between the Sahel and the African savannahs, or the one between the equatorial Atlantic and the African savannahs, while we expect the true XCO_2 fields to be first driven by large-scale horizontal advection (Keppel-Aleks et al. 2011). The main local spatial gradients in the mean differences are also seen on monthly means despite less data density (Fig, 3). They mostly reflect the retrieval gradients (Fig. 1a), because the model XCO_2 simulation is spatially smoother (Fig. 1b), even though it uses the retrieval averaging kernels (that change from scene to scene as a function, among other factors, of surface conditions) and even though it is sampled like the retrievals (i.e. with a spatially heterogeneous data density, also varying as a function, among other things, of surface conditions).

The jump of the long-term mean difference from the African savannahs to Sahel or equatorial Atlantic (while there is no jump between subtropical Atlantic and Western Sahara for instance) mostly corresponds to data from March (Fig. 3a), at the end of the savannah burning season (e.g. van der Werf et al. 2010). The model shows elevated values (Fig. 1b), but much less than the retrievals (Fig. 1a). If the model was underestimating the intensity of the fire, we would expect the mean difference to take the shape of a plume, i.e. to spread downstream the source region, but this is not the case. This suggests that the retrievals are affected by systematic errors over this region.~~ Similarly, we note a surprising discontinuity of the mean difference on the north-western coast of the US in Fig. 2a.~~

The positive differences of Fig. 2a in Eurasia notably follow the boreal forests, while negative values are found over the neighbouring regions of sparse tundra vegetation north of Siberia, or those of grassland/cropland south of them. The same remark applies to North America. The link with boreal forests is less obvious when looking at one isolated year because of the relatively small number of retrievals in these regions (not shown). The misfit pattern in Siberia and in North

America contains many values larger than 1 ppm corresponding to relatively large retrieved XCO_2 (Fig. 1a). These large values are all the more surprising that retrievals in these high latitudes are obtained during the growing season and that boreal forests in Eurasia are identified as large carbon sinks by bottom-up inventories (Pan et al. 2011, Dolman et al. 2012). By comparison, we can look at agricultural regions, where the model could miss gradients during crop growth, both because the MACC inversion prior fluxes do not explicitly represent agricultural practices and because the location of the assimilated surface air-sample measurements only provides rough information about crop fluxes: the differences are marginal (-0.1 ppm on average, whether we compute the mean at the global scale or only for latitudes above 40°N) for retrievals located in crop regions, as identified by the high-resolution land cover map of ESA's Land Cover Climate Change Initiative project (http://www.esa-landcover-cci.org/). In the Corn Belt, the intensively agricultural region in the Midwest of the USA, differences are negative, but they are much smaller in absolute value (the differences are larger than -0.4 ppm) than over the boreal forests, and the Corn Belt boundaries do not sharply appear, in particular on its eastern side. The Corn Belt does not particularly appear in monthly means either (e.g., Fig. 3b). These elements suggest that the long-term mean differences over boreal forests come from a retrieval artifact rather than from the MACC inversion product.

From a radiative transfer point of view, boreal forests are largely covered with needle-leaved trees with low albedo in the strong CO_2 spectral band of GOSAT near 2.1 μm (Fig. 4): these low values hamper the XCO_2 retrieval. O'Dell et al. (2012) already showed that large positive biases can occur for needle-leaved evergreen forests, with the retrieval exchanging surface albedo for very thin cloud or aerosol. Extreme cases are filtered out by the ACOS-GOSAT quality control, but Fig. 2a suggests that the remaining retrievals over boreal forests, including the region in Siberia East of 100°E which is dominated by deciduous needle-leaved trees with slightly larger

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albedos, are still biased. In temperate regions, south of 50^{o}N, the differences for needle-leaf cover (mainly in Southeast USA and Southeast China) have the opposite sign, but they do not show up distinctly in the difference map like the boreal forests. Tropical forests in South America and in Africa also have low albedo and correspond to negative differences. They are more identifiable in Fig. 2a, but could be explained by an insufficient carbon sink in the model as well as by a retrieval artifact.

4.2. Link to the retrieval increment

We now look at the XCO_2 misfit statistics over land and for the high-gain mode as a function of the size of the retrieval increment to its prior information (XCO_2^a - XCO_2^b) in Fig. 5. We look at the misfits of the model to XCO_2^a, to $XCO_2^{a,c}$ and to XCO_2^b, in order to visualize the added value brought by the retrieval process and by the bias correction, successively, on top of the prior estimate. This prior estimate about atmospheric CO_2 has been provided to the retrieval scheme by a data-driven empirical model (Wunch et al. 2011a). In Fig. 5, each bin along the abscissa encompasses a large diversity of times during the four years and a large diversity of locations over the globe, over which the model simulation should be overall more accurate (smaller root mean square error) than XCO_2^b, XCO_2^a and even $XCO_2^{a,c}$ (Chevallier and O'Dell 2013). Further, we expect the model error to be uncorrelated with the error of XCO_2^b, XCO_2^a and $XCO_2^{a,c}$ so that a smaller standard deviation of the misfits (e.g., using XCO_2^a rather than XCO_2^b) can be interpreted in terms of better precision of the corresponding retrieval quantity.

The mean difference significantly varies with the increment size: starting at 0.7 ppm for the smallest increments it reaches about 2 ppm and -1 ppm, for XCO_2^b and XCO_2^a respectively. As expected, the mean difference is systematically better with XCO_2^a than with XCO_2^b. The bias correction ($XCO_2^{a,c}$) further reduces the mean difference to a small extent.

The standard deviation for XCO_2^b is 1.1 ppm for small increments and smoothly increases to 2 ppm for retrieval increments of size 6 ppm. This trend demonstrates some skill of the retrieval algorithm to characterize the error of XCO_2^b from the GOSAT radiances and to generate a sizeable increment accordingly. By comparison, the model variability for a given increment size over the four years ranges between 3 and 4 ppm (1 σ), the prior variability is about 3 ppm and the retrieval variability ranges between 3 and 7 ppm. The standard deviation that uses XCO_2^a is 1.1 ppm for small increments. It smoothly increases to 4 ppm for retrieval increments of size 6 ppm: it is systematically larger than the standard deviation that uses XCO_2^b (despite a smaller mean difference). The standard deviation that uses $XCO_2^{a,c}$ is also 1.1 ppm for small increments and is also systematically larger than the standard deviation that uses XCO_2^b, but it performs better than XCO_2^a. The worse standard deviation of the misfit of XCO_2^a and $XCO_2^{a,c}$ to the model compared to XCO_2^b cannot be explained by a common lack of variability in the model and in XCO_2^b~~,~~ (that would correlate the model error with the that of XCO_2^b), because (i) at the large scale, thinning the retrievals (for instance by keeping only one retrieval every nine model grid boxes for a given day) only marginally changes the figure (not shown), and (ii) at the sub-grid scale, the variability of XCO_2 is usually well below the ppm (Alkhaled et al. 2008, Corbin et al. 2008), i.e. one order of magnitude smaller than the prior-to-retrieval degradation. Some, but not all, of the degradation is purely random and disappears after enough averaging (see Fig. 6 of Kulawik et al. 2015).

The fact that the standard deviation smoothly increases with increment size suggests that the increment size is systematically overestimated. Fig. 6 presents a~~n~~ simple~~empirical~~ test where we halve the retrieval increments, without any bias correction: we call $XCO_2^{a,r} = XCO_2^b + (XCO_2^a - XCO_2^b)/2$ the result. The reduction is seen to cancel most of the dependency of the statistics of the observation-minus-model misfits to the increment size: the standard deviation and the mean are then stable around 1.1 ppm and -0.3 ppm, respectively for increments up to 4 ppm without any bias correction. The standard deviation is systematically better than for XCO_2^b, which shows added value brought by the radiance measurements, in contrast to the previous results. This result also empirically confirms that the initial increments are in the right direction but are too large.

For the medium-gain retrievals (Fig. 7) and for the ocean glint retrievals (Fig. 8), the standard deviation of the misfits using $XCO_2^{a,c}$ is not significantly larger than that using XCO_2^b.

5. Discussion and conclusions

Small uncertainties in aerosols, cirrus cloud or surface albedo are known to heavily affect the quality of the XCO_2 satellite retrievals and to propagate into biases in the fluxes inverted from them, even when the parasite signal in XCO_2 is sub-ppm. This weakness lead the science team of NASA's OCO, a satellite that failed at launch in February 2009, to conclude that the space-based NIR/SWIR measurements of XCO_2 could not be used alone for CO_2 source-sink inversions and that they had to be combined with observations from a reasonable number of surface stations (Miller et al. 2007). However, so much improvement has been obtained in these issues by various institutes during the last few years, that it is sometimes thought that the space-borne XCO_2 retrievals have reached sufficient quality for source-sink inversion. The present paper discusses where we stand in this respect both from general theoretical considerations and from one of the most advanced GOSAT retrieval products.

From the theory, we have shown that a two-step approach to infer the surface fluxes from the GOSAT measured radiances, with CO_2 retrievals as an intermediate product, cannot be optimal. This suboptimality corrupts the 4D information flow from the radiance measurements to the surface flux estimates. It is amplified by the current retrieval strategy where prior errors are much larger (by an order of magnitude in terms of variances) than the performance of prior CO_2 simulations used in atmospheric inversions. Indeed, the use of averaging kernels makes atmospheric inversion insensitive to the choice of a particular retrieval prior CO_2 profile (Connor et al. 1994) if retrievals are assimilated without any bias correction, but it does not make the retrieval prior error statistics disappear from the inverse modelling equations. The current strategy likely generates retrieval averaging kernels that are inappropriate for atmospheric inversions in their default configurations, with a wrong vertical distribution and an excessive weight towards the measured radiances. Paradoxically, empirical bias correction of the retrievals (e.g., Wunch et al., 2011b) also contributes to the degradation of the 4D information flow, because it carries the imprint of the retrieval prior and of the retrieval prior error statistics. Direct assimilation of the measured radiances would solve the inconsistency, but would increase the computational burden of atmospheric inversions by several orders of magnitude. Alternatively, we could adapt the inversion systems to the current retrieval configuration by using minimal prior information about the surface fluxes, typically a flat prior flux field, but the result would still over-fit the measured radiances due to the absence of other (compensating) information. ~~We note that the situation is more favourable when assimilating TCCON retrievals, as has been done by Chevallier et al. (2011), or possibly future OCO-2 retrievals, due to better measurement precision than for GOSAT.~~

We have compared the ACOS-GOSAT retrievals with a transport model simulation constrained by surface air-sample measurements in order to find some evidence of retrieval sub-optimality. Flaws in this transport model and in these inverted surface fluxes necessarily flaw the simulation in many places over the globe and at various times of the year. We therefore carefully selected some of the relatively large discontinuities in the XCO_2 fields that the simulation unlikely generated. We found some evidence of retrieval systematic errors over the dark surfaces of the high-latitude lands and over African savannahs. We note that the mean differences over the African savannahs during the burning season could be explained by retrieval averaging kernels not peaking low enough in the atmosphere further to the assignment of ~~loose retrieval~~inappropriate prior error correlation~~variance~~s. Biomass burning aerosols that would not be well identified by the retrieval scheme could also play a role. We also found some evidence that the high-gain retrievals over land systematically over-fit the measured radiances, as a consequence of the prior uncertainty overestimation and of an underestimation of the observation uncertainty (as seen by the underlying radiative transfer model). This over-fit is partially compensated by the bias correction. An empirical test indicates that halving the retrieval increments without any posterior bias correction actually cancels the dependency of the statistics of the observation-minus-model misfits to the increment size and makes the standard deviation systematically better than for the retrieval prior XCO_2^b, which shows added value brought by the radiance measurements, in contrast to the previous results. We argue here that the optimal-estimation retrieval process and, consequently, its posterior bias correction need retuning.

Given the diversity of existing satellite retrieval algorithms, our conclusions cannot be easily extrapolated to other GOSAT retrieval products and even less to XCO_2 retrievals from other instruments, but we note that such mistuning like the one highlighted here is common practice, both because the errors of the retrieval forward model are difficult to characterize and because satellite retrievals are usually explicitly designed to maximize the observation contribution, at the risk of over-fitting radiance and forward model noise. A primary consequence of this mistuning is the usual underestimation of retrieval errors: for instance, O'Dell et al. (2012) recommended inflating this error by a twofold factor for ACOS-GOSAT b2.8. More importantly, our results show that the mistuning generates excessive (unphysical) space-time variations of the retrievals up to ~1%. This noise level would not matter for short-lived species, but for CO_2 it is enough to significantly degrade the assimilation of the retrievals for flux inversion and may explain some of the inconsistency seen between GOSAT-based top-down results and bottom-up results for CO_2 (Chevallier et al. 2014, Reuter et al. 2014). Therefore, with the current mistuning, we reiterate previous recommendations to take GOSAT-based CO_2 inversion results particularly cautiously. But we also suggest that this situation may dramatically improve by simply retuning the retrieval schemes. Ultimately, internal statistical consistency of the retrievals and of the inversion schemes is needed to establish the credibility of their end product.

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References

Aben, I., Hasekamp, O., and Hartmann, W.: Uncertainties in the space-based measurements of CO_2 columns due to scattering in the Earth's atmosphere, J. Quant. Spectrosc. Radiat. Trans., 104(3), 450–459, 2007

Alkhaled, A. A., Michalak, A. M., and Kawa, S. R.: Using CO_2 spatial variability to quantify representation errors of satellite CO_2 retrievals, Geophys. Res. Lett., 35, L16813, doi:10.1029/2008GL034528, 2008.

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Basu, S., Guerlet, S., Butz, A., Houweling, S., Hasekamp, O., Aben, I., Krummel, P., Steele, P., Langenfelds, R., Torn, M., Biraud, S., Stephens, B., Andrews, A., and Worthy, D.: Global CO_2 fluxes estimated from GOSAT retrievals of total column CO_2, Atmos. Chem. Phys., 13, 8695-8717, doi:10.5194/acp-13-8695-2013, 2013.

Basu, S., M. Krol, A. Butz, C. Clerbaux, Y. Sawa, T. Machida, H. Matsueda, C. Frankenberg, O. P. Hasekamp, and I. Aben, The seasonal variation of the CO_2 flux over Tropical Asia estimated from GOSAT, CONTRAIL, and IASI, Geophys. Res. Lett., 41, 1809–1815, doi:10.1002/2013GL059105, 2014.

Boesch, H., Toon, G. C., Sen, B., Washenfelder, R. A., Wennberg, P. O., Buchwitz, M., de Beek, R., Burrows, J. P., Crisp, D., Christi, M., Connor, B. J., Natraj, V., and Yung, Y. L.: Space-based near-infrared CO_2 measurements: Testing the Orbiting Carbon Observatory retrieval algorithm and validation concept using SCIAMACHY observations over Park Falls, Wisconsin, J. Geophys. Res. Atmos., 111, D23302, doi:10.1029/2006JD007080, 2006.

Buchwitz, M., de Beek, R., Burrows, J. P., Bovensmann, H., Warneke, T., Notholt, J., Meirink, J. F., Goede, A. P. H., Bergamaschi, P., Körner, S., Heimann, M., and Schulz, A.: Atmospheric methane and carbon dioxide from SCIAMACHY satellite data: initial comparison with chemistry and transport models, Atmos. Chem. Phys., 5, 941-962, doi:10.5194/acp-5-941-2005, 2005.

Butz, A., Hasekamp, O. P., Frankenberg, C., and Aben, I.: Retrievals of atmospheric CO_2 from simulated space-borne measurements of backscattered near-infrared sunlight: accounting for aerosol effects, Appl. Opt., 48, 3322–3336, doi:10.1364/AO.48.003322, 2009

Chédin, A., Serrar, S., Scott, N. A., Crevoisier, C., and Armante, R.: First global measurement of midtropospheric CO_2 from NOAA polar satellites: Tropical zone, J. Geophys. Res., 108(D18), 4581, doi:10.1029/2003JD003439, 2003..

Chevallier, F., Fisher, M., Peylin, P., Serrar, S., Bousquet, P., Bréon, F.-M., Chédin, A., and Ciais, P.: Inferring CO_2 sources and sinks from satellite observations: method and application to TOVS data, J. Geophys. Res., 110, D24309, doi:10.1029/2005JD006390, 2005.

Chevallier, F.: Impact of correlated observation errors on inverted CO_2 surface fluxes from OCO measurements, Geophys. Res. Lett., 34, L24804, doi:10.1029/2007GL030463, 2007.

Chevallier, F., Bréon, F.-M., and Rayner, P. J.: The contribution of the Orbiting Carbon Observatory to the estimation of CO_2 sources and sinks: Theoretical study in a variational data assimilation framework. J. Geophys. Res., 112, D09307, doi:10.1029/2006JD007375, 2007.

Chevallier, F., Ciais, P., Conway, T. J., Aalto, T., Anderson, B. E., Bousquet, P., Brunke, E. G., Ciattaglia, L., Esaki, Y., Fröhlich, M., Gomez, A., Gomez-Pelaez, A. J., Haszpra, L., Krummel, P. B., Langenfelds, R. L., Leuenberger, M., Machida, T., Maignan, F., Matsueda, H., Morgui, J.

Mis en forme : Indice

A., Mukai, H., Nakazawa, T., Peylin, P., Ramonet, M., Rivier, L., Sawa, Y., Schmidt, M., Steele, L. P., Vay, S. A., Vermeulen, A. T., Wofsy, S., and Worthy, D.: CO_2 surface fluxes at grid point scale estimated from a global 21-year reanalysis of atmospheric measurements. *J. Geophys. Res.*, 115, D21307, doi:10.1029/2010JD013887, 2010.

~~Chevallier, F., N. Deutscher, T.J. Conway, P. Ciais, L. Ciattaglia, S. Dohe, M. Fröhlich, A.J. Gomez-Pelaez, D. Griffith, F. Hase, L. Haszpra, P. Krummel, E. Kyrö, C. Labuschagne, R. Langenfelds, T. Machida, F. Maignan, H. Matsueda, I. Morino, J. Notholt, M. Ramonet, Y. Sawa, M. Schmidt, V. Sherlock, P. Steele, K. Strong, R. Sussmann, P. Wennberg, S. Wofsy, D. Worthy, D. Wunch, M. Zimnoch, 2011: Global~~ $\cancel{CO_2}$ ~~fluxes inferred from surface air-sample measurements and from TCCON retrievals of the~~ $\cancel{CO_2}$ ~~total column. Geophys. Res. Lett., 38, L24810, doi:10.1029/2011GL049899.~~

Chevallier, F., and O'Dell, C. W., Error statistics of Bayesian CO_2 flux inversion schemes as seen from GOSAT. Geophys. Res. Lett., 40, 1252–1256, doi:10.1002/grl.50228, 2013.

Chevallier, F., Palmer, P. I., Feng, L., Boesch, H., O'Dell, C. W., and Bousquet, P.: Towards robust and consistent regional CO_2 flux estimates from in situ and space-borne measurements of atmospheric CO_2, Geophys. Res. Lett., 41, 1065–1070, doi:10.1002/2013GL058772, 2014.

Connor, B. J., Siskind, D. E., Tsou, J. J., Parrish, A., and Remsberg, E. E.: Ground-based microwave observations of ozone in the upper stratosphere and mesosphere, J. Geophys. Res., 99, 16,757–16,770, 1994.

Connor, B. J., Boesch, H., Toon, G., Sen, B., Miller, C., and Crisp, D.: Orbiting Carbon Observatory: Inverse method and prospective error analysis, J. Geophys. Res. Atmos., 113, D05305, doi:10.1029/2006JD008336, 2008.

Corbin, K., Denning, A. S., Wang, J.-W., Lu, L., and Baker, I. T.: Possible representation errors in inversions of satellite CO_2 retrievals, J. Geophys. Res., 113, D02301, doi:10.1029/2007JD008716, 2008.

Mis en forme : Indice

Crisp, D., Fisher, B. M., O'Dell, C., Frankenberg, C., Basilio, R., Bösch, H., Brown, L. R., Castano, R., Connor, B., Deutscher, N. M., Eldering, A., Griffith, D., Gunson, M., Kuze, A., Mandrake, L., McDuffie, J., Messerschmidt, J., Miller, C. E., Morino, I., Natraj, V., Notholt, J., O'Brien, D. M., Oyafuso, F., Polonsky, I., Robinson, J., Salawitch, R., Sherlock, V., Smyth, M., Suto, H., Taylor, T. E., Thompson, D. R., Wennberg, P. O., Wunch, D., and Yung, Y. L.: The ACOS CO₂ retrieval algorithm – Part II: Global XCO_2 data characterization, Atmos. Meas. Tech., 5, 687–707, doi:10.5194/amt-5-687-2012, 2012.

Dolman, A. J., Shvidenko, A., Schepaschenko, D., Ciais, P., Tchebakova, N., Chen, T., van der Molen, M. K., Belelli Marchesini, L., Maximov, T. C., Maksyutov, S., and Schulze, E.-D.: An estimate of the terrestrial carbon budget of Russia using inventory-based, eddy covariance and inversion methods, Biogeosciences, 9, 5323-5340, doi:10.5194/bg-9-5323-2012, 2012.

Engelen, R. J., Serrar, S., and Chevallier, F.: Four-dimensional data assimilation of atmospheric CO_2 using AIRS observations, J. Geophys. Res., 114, D03303, doi:10.1029/2008JD010739, 2009.

Mis en forme : Indice

Global Climate Observing System (GCOS), Systematic observation requirements for satellite-based products for climate, Supplemental details to the satellite-based component of the "Implementation Plan for the Global Observing System for Climate in Support of the UNFCCC (2010 update)", Prepared by World Meteorological Organization (WMO), Intergovernmental

Oceanographic Commission, United Nations Environment Programme (UNEP), International Council for Science, Doc.: GCOS 154, 2010.

Guerlet, S., S. Basu, A. Butz, M. C. Krol, P. Hahne, S. Houweling, O. P. Hasekamp, and I. Aben, Reduced carbon uptake during the 2010 Northern Hemisphere summer as observed from GOSAT, Geophys. Res. Lett., 40, 2378–2383, doi:10.1002/grl.50402, 2013a.

Guerlet, S., Butz, A., Schepers, D., Basu, S., Hasekamp, O. P., Kuze, A., Yokota, T., Blavier, J.-F., Deutscher, N. M., Griffith, D. W. T., Hase, F., Kyrö, E., Morino, I., Sherlock, V., Sussmann, R., Galli, A., and Aben, I.: Impact of aerosol and thin cirrus on retrieving and validating XCO_2 from GOSAT shortwave infrared measurements, J. Geophys. Res. Atmos., 118, 4887–4905, doi:10.1002/jgrd.50332, 2013b.

Hourdin, F., Musat, I., Bony, S., Braconnot, P., Codron, F., Dufresne, J. L., Fairhead, L., Filiberti, M. A., Friedlingstein, P., Grandpeix, J. Y., Krinner, G., Levan, P., Li, Z. X., and Lott, F.: The LMDZ4 general circulation model: climate performance and sensitivity to parametrized physics with emphasis on tropical convection, *Climate Dynamics*, 27, 787-813, doi:10.1007/s00382-006-0158-0, 2006.

Houweling, S., Aben, I., Breon, F.-M., Chevallier, F., Deutscher, N., Engelen, R., Gerbig, C., Griffith, D., Hungershoefer, K., Macatangay, R., Marshall, J., Notholt, J., Peters, W., and Serrar, S.: The importance of transport model uncertainties for the estimation of CO_2 sources and sinks using satellite measurements, Atmos. Chem. Phys., 10, 9981-9992, doi:10.5194/acp-10-9981-2010, 2010.

Ingmann, P.: A-SCOPE, Advanced Space Carbon and Climate Observation of Planet Earth, Report of Assessment, SP-1313/1, ESA Communication Product Office, Noordwijk, The Netherlands, 2009.

Keppel-Aleks, G., Wennberg, P. O., and Schneider, T.: Sources of variations in total column carbon dioxide, Atmos. Chem. Phys., 11, 3581–3593, doi:10.5194/acp-11-3581-2011, 2011.

Kulawik, S. S., Wunch, D., O'Dell, C., Frankenberg, C., Reuter, M., Oda, T., Chevallier, F., Sherlock, V., Buchwitz, M., Osterman, G., Miller, C., Wennberg, P., Griffith, D. W. T., Morino, I., Dubey, M., Deutscher, N. M., Notholt, J., Hase, F., Warneke, T., Sussmann, R., Robinson, J., Strong, K., Schneider, M., and Wolf, J.: Consistent evaluation of GOSAT, SCIAMACHY, CarbonTracker, and MACC through comparisons to TCCON, Atmos. Meas. Tech. Discuss., 8, 6217-6277, doi:10.5194/amtd-8-6217-2015, 2015.

Kuppel, S., Chevallier, F. and Peylin, P.: Quantifying the model structural error in Carbon Cycle Data Assimilation Systems. Geosci. Model Dev., 6, 45-55, doi:10.5194/gmd-6-45-2013, 2013.

Maksyutov, S., Kadygrov, N., Nakatsuka, Y., Patra, P. K., Nakazawa, T., Yokota, T. and Inoue, G~~., ~~.: Projected impact of the GOSAT observations on regional CO_2 flux estimations as a function of total retrieval error, J. Remote Sens. Soc. Jpn., 28, 190–197, 2008.

Migliorini, S.: On the equivalence between radiance and retrieval assimilation. Mon. Wea. Rev., 140, 258-265. doi:10.1175/MWR-D-10-05047.1, 2012.

Miller, C. E., Crisp, D., DeCola, P. L., Olsen, S. C., Randerson, J. T., Michalak, A. M., Alkhaled, A., Rayner, P., Jacob, D. J., Suntharalingam, P., Jones, D. B. A., Denning, A. S., Nicholls, M. E., Doney, S. C., Pawson, S., Boesch, H., Connor, B. J., Fung, I. Y., O'Brien, D., Salawitch, R. J., Sander, S. P., Sen, B., Tans, P., Toon, G. C., Wennberg, P. O., Wofsy, S. C., Yung, Y. L., and Law, R. M~~et al~~.: Precision requirements for space-based XCO_2 data, J. Geophys. Res., 112, D10314, doi:10.1029/2006JD007659, 2007.

Nguyen, H., Osterman, G., Wunch, D., O'Dell, C., Mandrake, L., Wennberg, P., Fisher, B., and Castano, R.: A method for colocating satellite XCO_2 data to ground-based data and its

Mis en forme : Anglais (États Unis)

Code de champ modifié

Mis en forme : Anglais (États Unis)

application to ACOS-GOSAT and TCCON, Atmos. Meas. Tech., 7, 2631-2644, doi:10.5194/amt-7-2631-2014, 2014.

O'Dell, C. W., Connor, B., Bösch, H., O'Brien, D., Frankenberg, C., Castano, R., Christi, M., Eldering, D., Fisher, B., Gunson, M., McDuffie, J., Miller, C. E., Natraj, V., Oyafuso, F., Polonsky, I., Smyth, M., Taylor, T., Toon, G. C., Wennberg, P. O., and Wunch, D.: The ACOS CO_2 retrieval algorithm – Part 1: Description and validation against synthetic observations, Atmos. Meas. Tech., 5, 99–121, doi:10.5194/amt-5-99-2012, 2012.

Oshchepkov, S., Bril, A., Yokota, T., Wennberg, P. O., Deutscher, N. M., Wunch, D., Toon, G. C., Yoshida, Y., O'Dell, C. W., Crisp, D., Miller, C. E., Frankenberg, C., Butz, A., Aben, I., Guerlet, S., Hasekamp, O., Boesch, H., Cogan, A., Parker, R., Griffith, D., Macatangay, R., Notholt, J., Sussmann, R., Rettinger, M., Sherlock, V., Robinson, J., Kyrö, E., Heikkinen, P., Feist, D. G., Morino, I., Kadygrov, N., Belikov, D., Maksyutov, S., Matsunaga, T., Uchino, O., and Watanabe, H.: Effects of atmospheric light scattering on spectroscopic observations of greenhouse gases from space. Part 2: Algorithm intercomparison in the GOSAT data processing for CO_2 retrievals over TCCON sites, J. Geophys. Res., 118, 1493-1512, doi:10.1002/jgrd.50146, 2013.

Osterman, G., Eldering, A., Avis, C., O'Dell, C., Martinez, E., Crisp, D., Frankenberg, C., and Frankenberg, B., ACOS Level 2 Standard Product Data User's Guide v3.4, Revision Date: Revision B, 3 October 2013, available at: https://co2.jpl.nasa.gov/static/docs/v3.4_DataUsersGuide-RevB_131028.pdf (last access: 20 April 2015), 2013.

Pan, Y., Birdsey, R. A., Fang, J., Houghton, R., Kauppi, P. E., Kurz, W. A., Phillips, O. L., Shvidenko, A., Lewis, S. L., Canadell, J. G., Ciais, P., Jackson, J. B., Pacala, S., McGuire, A.

Mis en forme : Anglais (États Unis)

D., Piao, S., Rautiainen, A., Sitch, S., and Hayes, D.: A large and persistent carbon sink in the world's forests, Science, 333, 988–993, 2011.

Patra, P. K., Houweling, S., Krol, M., Bousquet, P., Belikov, D., Bergmann, D., Bian, H., Cameron-Smith, P., Chipperfield, M. P., Corbin, K., Fortems-Cheiney, A., Fraser, A., Gloor, E., Hess, P., Ito, A., Kawa, S. R., Law, R. M., Loh, Z., Maksyutov, S., Meng, L., Palmer, P. I., Prinn, R. G., Rigby, M., Saito, R., and Wilson, C.: TransCom model simulations of CH_4 and related species: linking transport, surface flux and chemical loss with CH_4 variability in the troposphere and lower stratosphere, Atmos. Chem. Phys., 11, 12813-12837, doi:10.5194/acp-11-12813-2011, 2011..

Peng, S., Ciais, P., Chevallier, F., Peylin, P., Cadule, P., Sitch, S., Piao, S., Ahlström, A., Huntingford, C., Levy, P., Li, X., Liu, Y., Lomas, M., Poulter, B., Viovy, N., Wang, T., Wang, X., Zaehle, S., Zeng, N., Zhao, F., and Zhao, H.:~~et al.,~~ Benchmarking the seasonal cycle of CO_2 fluxes simulated by terrestrial ecosystem models, Global Biogeochem. Cycles, 29, 46–64, doi:10.1002/2014GB004931, 2015.

Peylin, P., Law, R. M., Gurney, K. R., Chevallier, F., Jacobson, A. R., Maki, T., Niwa, Y., Patra, P. K., Peters, W., Rayner, P. J., Rödenbeck, C., van der Laan-Luijkx, I. T., and Zhang, X.: Global atmospheric carbon budget: results from an ensemble of atmospheric CO_2 inversions, Biogeosciences, 10, 6699-6720, doi:10.5194/bg-10-6699-2013, 2013.

Rayner, P., Scholze, M., Knorr, W., Kaminski, T., Giering, R., and Widmann, H.: Two decades of terrestrial Carbon fluxes from a Carbon Cycle Data Assimilation System (CCDAS), Global Biogeochem. Cy., 19, GB2026, doi:10.1029/2004GB002254, 2005

Reuter, M., Buchwitz, M., Schneising, O., Heymann, J., Bovensmann, H., and Burrows, J. P.: A method for improved SCIAMACHY CO_2 retrieval in the presence of optically thin clouds, Atmos. Meas. Tech., 3, 209-232, doi:10.5194/amt-3-209-2010, 2010.

Mis en forme : Anglais (Royaume-Uni)

Reuter, M., Buchwitz, M., Hilker, M., Heymann, J., Schneising, O., Pillai, D., Bovensmann, H., Burrows, J. P., Bösch, H., Parker, R., Butz, A., Hasekamp, O., O'Dell, C. W., Yoshida, Y., Gerbig, C., Nehrkorn, T., Deutscher, N. M., Warneke, T., Notholt, J., Hase, F., Kivi, R., Sussmann, R., Machida, T., Matsueda, H., and Sawa, Y.: Satellite-inferred European carbon sink larger than expected, Atmos. Chem. Phys.~~ Discuss.~~, 14, 13739–13753, doi:10.5194/acp-14-13739~~21829–21863, doi:10.5194/acpd-14-21829~~-2014, 2014.

Rodgers, C.D.: Inverse Methods for Atmospheric Sounding: Theory and Practice, World Scientific Publishing Co. Ltd., London, 2000.

van der Werf, G. R., Randerson, J. T., Giglio, L., Collatz, G. J., Mu, M., Kasibhatla, P. S., Morton, D. C., DeFries, R. S., Jin, Y., and van Leeuwen, T. T.: Global fire emissions and the contribution of deforestation, savanna, forest, agricultural, and peat fires (1997–2009), Atmos. Chem. Phys., 10, 11,707–11,735, doi:10.5194/acp-10-11707-2010, 2010.

Wunch, D., Toon, G. C., Blavier, J.-F. L., Washenfelder, R. A., Notholt, J., Connor, B. J., Griffith, D. W. T., Sherlock, V., and Wennberg, P. O., The Total Carbon Column Observing Network, Phil. Trans. R. Soc. A:2011369 2087-2112;DOI: 10.1098/rsta.2010.0240, 2011a.

Wunch, D., Wennberg, P. O., Toon, G. C., Connor, B. J., Fisher, B., Osterman, G. B., Frankenberg, C., Mandrake, L., O'Dell, C., Ahonen, P., Biraud, S. C., Castano, R., Cressie, N., Crisp, D., Deutscher, N. M., Eldering, A., Fisher, M. L., Griffith, D. W. T., Gunson, M., Heikkinen, P., Keppel-Aleks, G., Kyrö, E., Lindenmaier, R., Macatangay, R., Mendonca, J., Messerschmidt, J., Miller, C. E., Morino, I., Notholt, J., Oyafuso, F. A., Rettinger, M., Robinson, J., Roehl, C. M., Salawitch, R. J., Sherlock, V., Strong, K., Sussmann, R., Tanaka, T., Thompson, D. R., Uchino, O., Warneke, T., and Wofsy, S. C.: A method for evaluating bias in global measurements of CO_2 total columns from space, Atmos. Chem. Phys., 11, 12317–12337, doi:10.5194/acp-11-12317-2011, 2011b.

Locality (indentifier)	Period	Source
Alert, Nunavut, CA (ALT)	1988-2012	WDCGG/ EC
Amsterdam Island, FR (AMS)	1981-2011	LSCE
Argyle, Maine, US (AMT)	2003-2011	NOAA/ ESRL
Anmyeon-do, KR (AMY)	1999-2012	WDCGG/ KMA
Barrow, Alaska, US (BRW)	1979-2013	NOAA/ ESRL
Candle Lake, CA (CDL)	2002-2012	WDCGG/ EC
Monte Cimone, IT (CMN)	1996-2010	WDCGG/ IAFMS
Cape Ochi-ishi, JP (COI)	1995-2002	WDCGG/ NIES
Cape Point, SA (CPT)	1993-2013	WDCGG/ SAWS
Egbert, CA (EGB)	2005-2012	WDCGG/ EC
East Trout Lake, CA (ETL)	2005-2012	WDCGG/ EC
Frasedale, CA (FSD)	1990-2012	WDCGG/ EC
Hateruma, JP (HAT)	1993-2002	WDCGG/ NIES
Hegyhatsal tower, 115m level, HU (HUN0115)	1994-2013	WDCGG/ HMS
Tenerife, Canary Islands, ES (IZO)	1984-2013	WDCGG/ AEMET
Jubany, Antartica, AR (JBN)	1994-2009	WDCGG/ ISAC IAA
Jungfraujoch, CH (JFJ)	2004-2013	WDCGG/ Univ. Of Bern
K-puszta, HU (KPS)	1981-1999	WDCGG/ HMS
Park Falls, Wisconsin, US (LEF)	2003-2011	NOAA/ ESRL
Mace Head, County Galway, IE (MHD)	1992-2012	LSCE

Mauna Loa, Hawaii, US (MLO)	1979-2013	NOAA/ ESRL
Minamitorishima, JP (MNM)	1993-2013	WDCGG/ JMA
Pallas-Sammaltunturi, GAW Station, FI (PAL)	1999-2013	WDCGG/ FMI
Plateau Rosa, IT (PRS)	2000-2013	WDCGG/ CESI RICERCA
Puy de Dome, FR (PUY)	2000-2010	LSCE
Ryori, JP (RYO)	1987-2013	WDCGG/ JMA
Tutuila, American Samoa (SMO)	1979-2013	NOAA/ ESRL
Sonnblick, AU (SNB)	1999-2013	WDCGG/ EEA
South Pole, Antarctica, US (SPO)	1979-2013	NOAA/ ESRL
Tsukuba tower, 200m level, JP (TKB)	1986-2000	WDCGG/ MRI
Westerland, DE (WES)	1979-2013	WDCGG/ UBA
Moody, Texas, US (WKT)	2003-2011	NOAAA/ ESRL
Yonagunijima, JP (YON)	1997-2013	WDCGG/ JMA

Table 1: List of the continuous sites used in the MACC CO_2 inversion v13r1 together with the period of coverage (defined as the period between the first sample and the last one), and the data source. Each station is identified by the name of the place, the corresponding country (abbreviated) and the code used in the corresponding database.

Locality (indentifier)	Period	Source
Alert, Nunavut, CA (ALT)	1985-2013	NOAA/ ESRL
Amsterdam Island, FR (AMS)	1979-1990	NOAA/ ESRL
Amsterdam Island, FR (AMS)	2003-2013	LSCE
Ascension Island, GB (ASC)	1979-2013	NOAA/ ESRL
Assekrem, DZ (ASK)	1995-2013	NOAA/ ESRL
St. Croix, Virgin Islands, USA (AVI)	1979-1990	NOAA/ ESRL
Terceira Island, Azores, PT (AZR)	1979-2013	NOAA/ ESRL
Baltic Sea, PL (BAL)	1992-2011	NOAA/ ESRL
Bering Island, RU (BER)	1986-1994	WDCGG/ MGO
Begur, ES (BGU)	2000-2013	LSCE /IC3
Baring Head, NZ (BHD)	1999-2013	NOAA/ESRL
Baring Head, NZ (BHD)	1979-2011	WDCGG/ NIWA
Bukit Kototabang, ID (BKT)	2004-2013	NOAA/ESRL
St. Davids Head, Bermuda, GB (BME)	1989-2009	NOAA/ ESRL
Tudor Hill, Bermuda, GB (BMW)	1989-2013	NOAA/ ESRL
Barrow, Alaska, US (BRW)	1979-2013	NOAA/ ESRL
Portsall, FR (BZH)	1998-2001	CarboEurope/LSCE
Cold Bay, Alaska, US (CBA)	1979-2013	NOAA/ ESRL
Cape Ferguson, AU (CFA)	1991-2013	WDCGG/ CSIRO
Cape Grim, Tasmania, AU (CGO)	1984-2013	NOAA/ ESRL
Christmas Island, Republic of Kiribati (CHR)	1984-2013	NOAA/ ESRL

Cape Meares, Oregon, US (CMO)	1982-1998	NOAA/ ESRL
Crozet Island, FR (CRZ)	1991-2013	NOAA/ ESRL
Cape St. James, CA (CSJ)	1979-1992	WDCGG/ EC
Casey Station, AU (CYA)	1996-2013	WDCGG/ CSIRO
Drake Passage (DRP)	2003-2013	NOAA/ ESRL
Easter Island, CL (EIC)	1994-2013	NOAA/ ESRL
Estevan Point, British Columbia, CA (ESP)	1992-2012	WDCGG/ EC
Estevan Point, British Columbia, CA (ESP)	1993-2001	WDCGG/ CSIRO
Finokalia, Crete, GR (FIK)	1999-2013	LSCE
Mariana Islands, Guam (GMI)	1979-2013	NOAA/ ESRL
Dwejra Point, Gozo, MT (GOZ)	1993-1999	NOAA/ ESRL
Halley Station, Antarctica, GB (HBA)	1983-2013	NOAA/ ESRL
Hohenpeissenberg, DE (HPB)	2006-2013	NOAA/ ESRL
Hegyhatsal, HU (HUN)	1993-2013	NOAA/ ESRL
Storhofdi, Vestmannaeyjar, IS (ICE)	1992-2013	NOAA/ ESRL
Grifton, North Carolina, US (ITN)	1992-1999	WDCGG/ ESRL
Tenerife, Canary Islands, ES (IZO)	1991-2013	NOAA/ ESRL
Key Biscayne, Florida, US (KEY)	1979-2013	NOAA/ ESRL
Kotelny Island, RU (KOT)	1986-1993	WDCGG/ MGO
Cape Kumukahi, Hawaii, US (KUM)	1979-2013	NOAA/ ESRL

Sary Taukum, KZ (KZD)	1997-2009	NOAA/ ESRL
Plateau Assy, KZ (KZM)	1997-2009	NOAA/ ESRL
Lulin, TW (LLN)	2006-2013	NOAA/ ESRL
Lampedusa, IT (LMP)	2006-2013	NOAA/ ESRL
Ile grande, FR (LPO)	2004-2013	LSCE
Mawson, AU (MAA)	1990-2013	WDCGG/ CSIRO
Mould Bay, Nunavut, CA (MBC)	1980-1997	NOAA/ ESRL
Mace Head, County Galway, IE (MHD)	1991-2013	NOAA/ ESRL
Mace Head, County Galway, IE (MHD)	1996-2013	LSCE
Sand Island, Midway, US (MID)	1985-2013	NOAA/ ESRL
Mt. Kenya, KE (MKN)	2003-2011	NOAA/ ESRL
Mauna Loa, Hawaii, US (MLO)	1979-2013	NOAA/ ESRL
Macquarie Island, AU (MQA)	1990-2013	WDCGG/ CSIRO
Gobabeb, NA (NMB)	1997-2013	NOAA/ ESRL
Niwot Ridge, Colorado, US (NWR)	1979-2013	NOAA/ ESRL
Olympic Peninsula, WA, USA (OPW)	1984-1990	NOAA/ ESRL
Ochsenkopf, DE (OXK)	2003-2013	NOAA/ ESRL
Pallas-Sammaltunturi, GAW Station, FI (PAL)	2001-2013	NOAA/ ESRL

Pic du Midi, FR (PDM)	2001-2013	LSCE
Pacific Ocean, 0N (POC000)	1987-2011	NOAA/ ESRL
Pacific Ocean, 5N (POCN05)	1987-2011	NOAA/ ESRL
Pacific Ocean, 10N (POCN10)	1987-2011	NOAA/ ESRL
Pacific Ocean, 15N (POCN15)	1987-2011	NOAA/ ESRL
Pacific Ocean, 20N (POCN20)	1987-2011	NOAA/ ESRL
Pacific Ocean, 25N (POCN25)	1987-2011	NOAA/ ESRL
Pacific Ocean, 30N (POCN30)	1987-2011	NOAA/ ESRL
Pacific Ocean, 5S (POCS05)	1987-2011	NOAA/ ESRL
Pacific Ocean, 10S (POCS10)	1987-2011	NOAA/ ESRL
Pacific Ocean, 15S (POCS15)	1987-2011	NOAA/ ESRL
Pacific Ocean, 20S (POCS20)	1987-2011	NOAA/ ESRL
Pacific Ocean, 25S (POCS25)	1987-2011	NOAA/ ESRL
Pacific Ocean, 30S (POCS30)	1987-2011	NOAA/ ESRL
Pacific Ocean, 35S (POCS35)	1987-2011	NOAA/ ESRL
Palmer Station, Antarctica, US (PSA)	1979-2013	NOAA/ ESRL
Point Arena, California, US (PTA)	1999-2011	NOAA/ ESRL
Puy de Dome, FR (PUY)	2001-2013	LSCE
Ragged Point, BB (RPB)	1987-2013	NOAA/ ESRL
South China Sea, 3N (SCSN03)	1991-1998	NOAA/ ESRL
South China Sea, 6N (SCSN06)	1991-1998	NOAA/ ESRL
South China Sea, 9N (SCSN09)	1991-1998	NOAA/ ESRL
South China Sea, 12N (SCSN12)	1991-1998	NOAA/ ESRL
South China Sea, 15N (SCSN15)	1991-1998	NOAA/ ESRL

South China Sea, 18N (SCSN18)	1991-1998	NOAA/ ESRL
South China Sea, 21N (SCSN21)	1991-1998	NOAA/ ESRL
Mahe Island, SC (SEY)	1980-2013	NOAA/ ESRL
Southern Great Plains, Oklahoma, US (SGP)	2002-2013	NOAA/ ESRL
Shemya Island, Alaska, US (SHM)	1985-2013	NOAA/ ESRL
Ship between Ishigaki Island and Hateruma Island, JP (SIH)	1993-2005	WDCGG/ Tohoku University
Shetland, Scotland, GB (SIS)	1992-2003	WDCGG/ CSIRO
Tutuila, American Samoa (SMO)	1979-2013	NOAA/ ESRL
South Pole, Antarctica, US (SPO)	1979-2013	NOAA/ ESRL
Ocean Station M, NO (STM)	1980-2009	NOAA/ ESRL
Summit, GL (SUM)	1997-2013	NOAA/ ESRL
Syowa Station, Antarctica, JP (SYO)	1986-2013	NOAA/ ESRL
Tae-ahn Peninsula, KR (TAP)	1991-2013	NOAA/ ESRL
Tierra Del Fuego, Ushuaia, AR (TDF)	1994-2013	NOAA/ ESRL
Trinidad Head, California, US (THD)	2002-2013	NOAA/ ESRL
Tromelin Island, F (TRM)	1998-2007	LSCE
Wendover, Utah, US (UTA)	1993-2013	NOAA/ ESRL
Ulaan Uul, MN (UUM)	1992-2013	NOAA/ ESRL

Sede Boker, Negev Desert, IL (WIS)	1995-2013	NOAA/ ESRL
Sable Island, CA (WSA)	1979-2012	WDCGG/ EC
Mt. Waliguan, CN (WLG)	1990-2013	NOAA/ ESRL
Western Pacific Cruise (WPC)	2004-2013	NOAA/ ESRL
Ny-Alesund, Svalbard, Norway and Sweden (ZEP)	1994-2013	NOAA/ ESRL

Table 2: Same as Table 1 but for the flask-sampling sites.

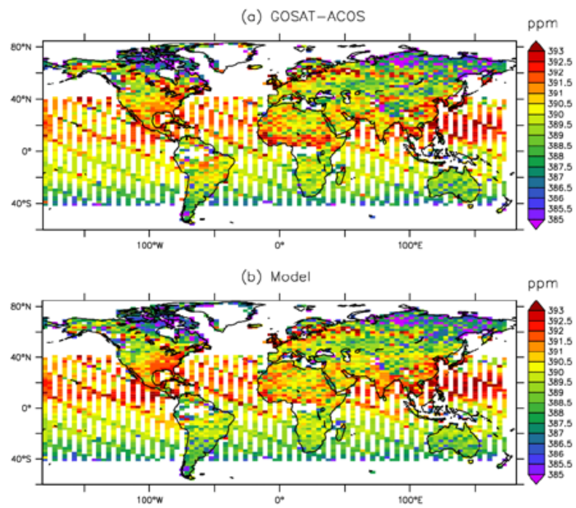


Fig. 1. (a) Mean ACOS-GOSAT bias-corrected retrievals in the model grid over 4 years (June 2009-May 2013). (b) Corresponding mean CO_2 4D field associated to the MACC CO_2 inversion (computed using the averaging kernels and the prior profiles of the retrievals).

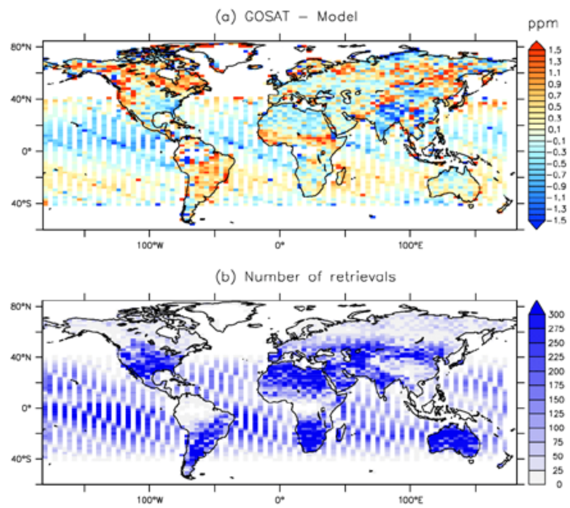


Fig. 2. (a) Mean difference between the maps of Fig. 1 (retrievals minus model). (b) Corresponding number of retrievals.

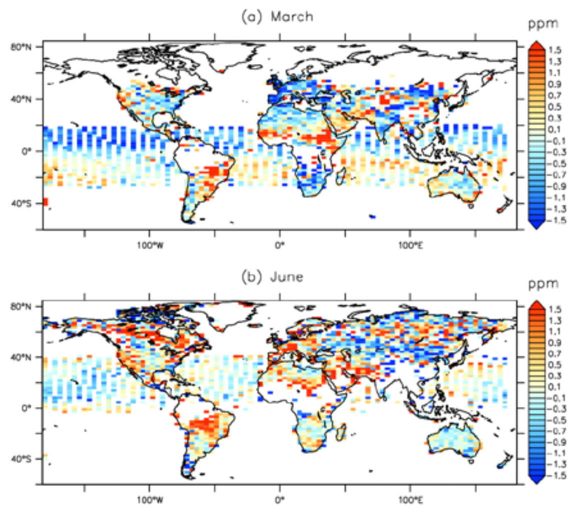


Fig. 3. Same as Fig. 2(a) (retrievals minus model), but focussing on the months of March and June.

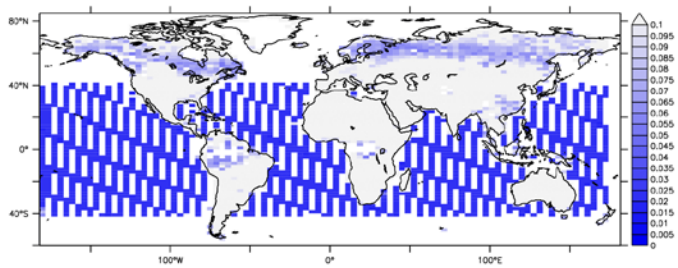
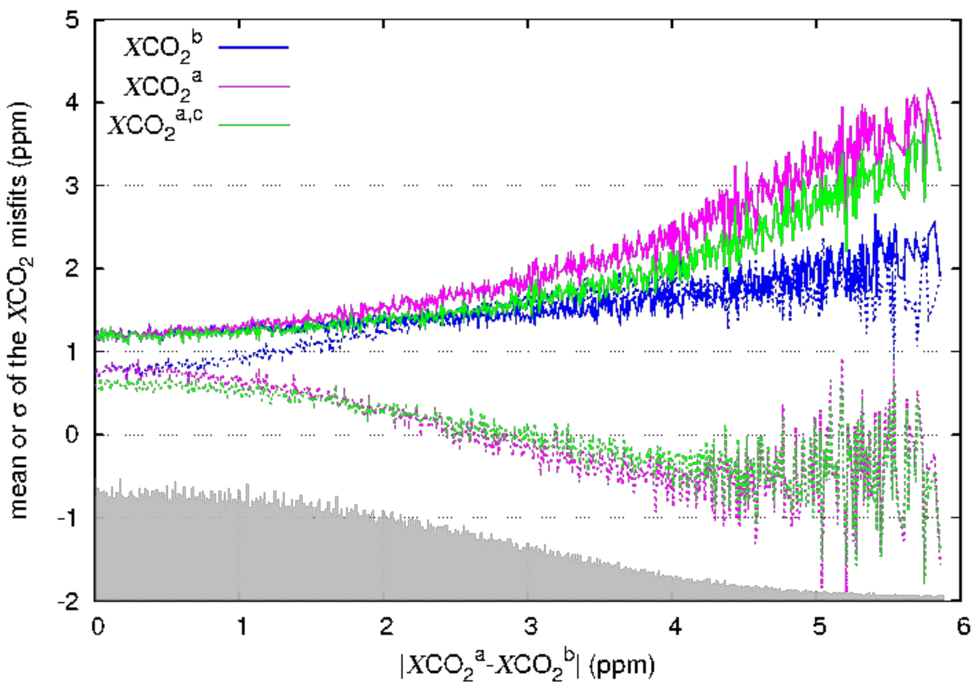


Fig. 4. Mean surface albedo retrieved in the strong CO_2 band by ACOS-GOSAT in the model grid over 4 years (June 2009-May 2013). The blue scale focuses on the values less than 0.1.



XCO2b
XCO2a
XCO2a,c
mean or σ of the XCO2 misfits (ppm)
|XCO2a-XCO2b| (ppm)
5
4
3
2
1
0
-1
-2
0
1
2
3
4
5
6

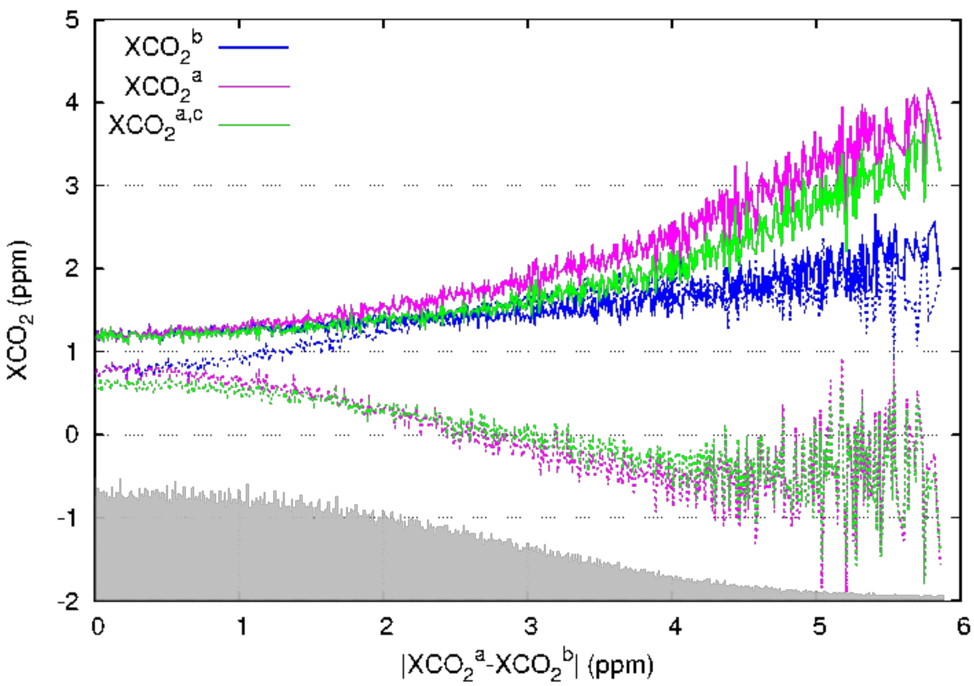
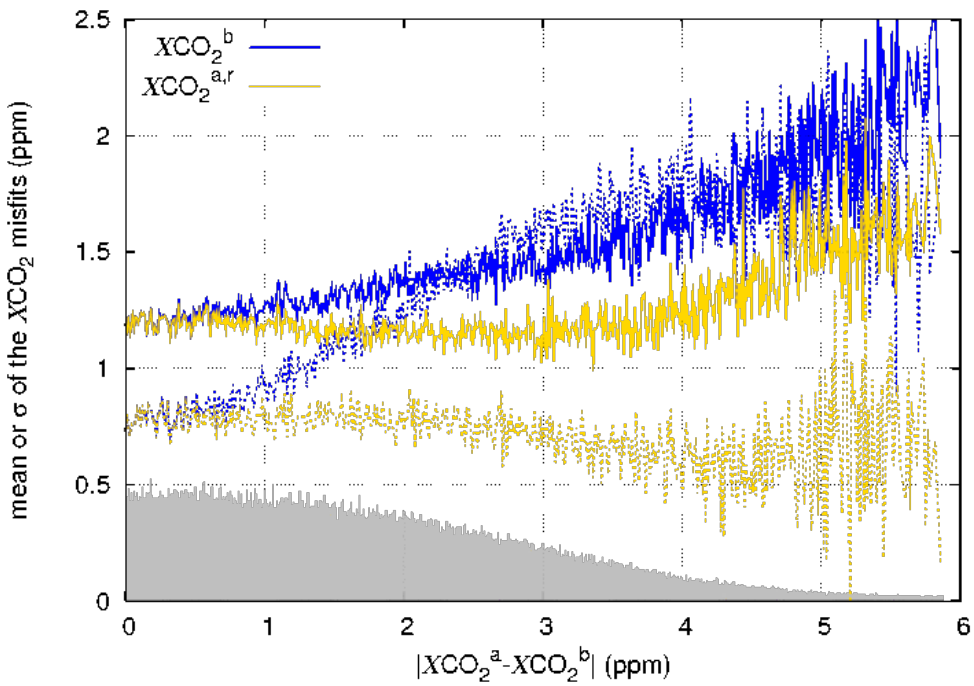


Fig. 5. Mean and standard deviation of the retrieval-minus-model misfits between June 2009 and May 2013 for the high-gain mode retrievals over land as a function of the retrieval increment size. The statistics are also shown for the prior-minus-model misfit. The model values are raw pressure-weighted columns and do not account for the averaging kernels in order not to correlate the two axes (in practice, using the averaging kernels actually does not significantly affect the standard deviations shown). The grey shade shows the distribution of the retrieval density (axis not shown).



XCO_2^b
$XCO_2^{a,r}$
mean or σ of the XCO_2 misfits (ppm)
$|XCO_2^a-XCO_2^b|$ (ppm)
0
0.5
1
1.5
2
2.5
0
1
2
3
4
5
6

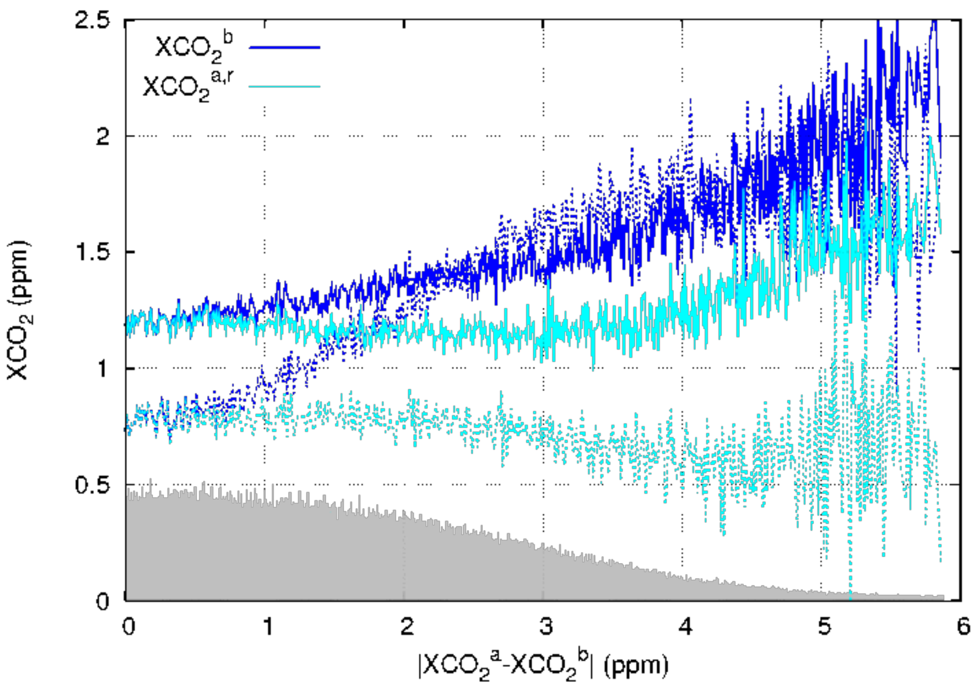
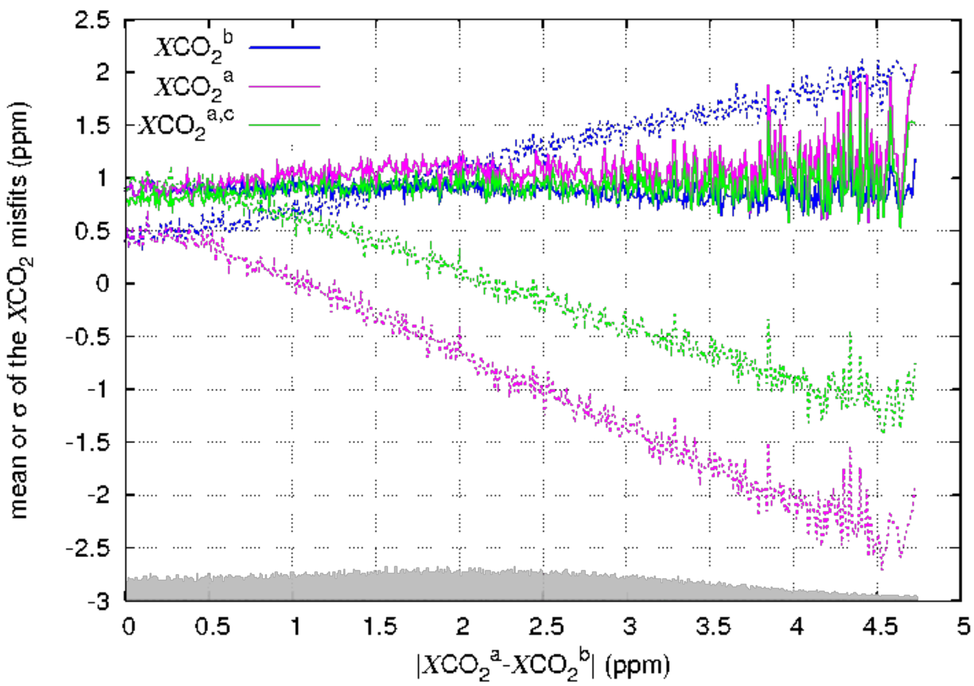


Fig. 6. Same as Fig. 5 (high-gain mode over the lands) but we reduce the retrieval increment size by 50% without any bias correction (we call $XCO_2^{a,r}$ the result). The abscissa shows the unperturbed increment.


XCO2b
XCO2a
XCO2a,c
mean or σ of the XCO2 misfits (ppm)
|XCO2a-XCO2b| (ppm)
2.5
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-2.5
-3
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5

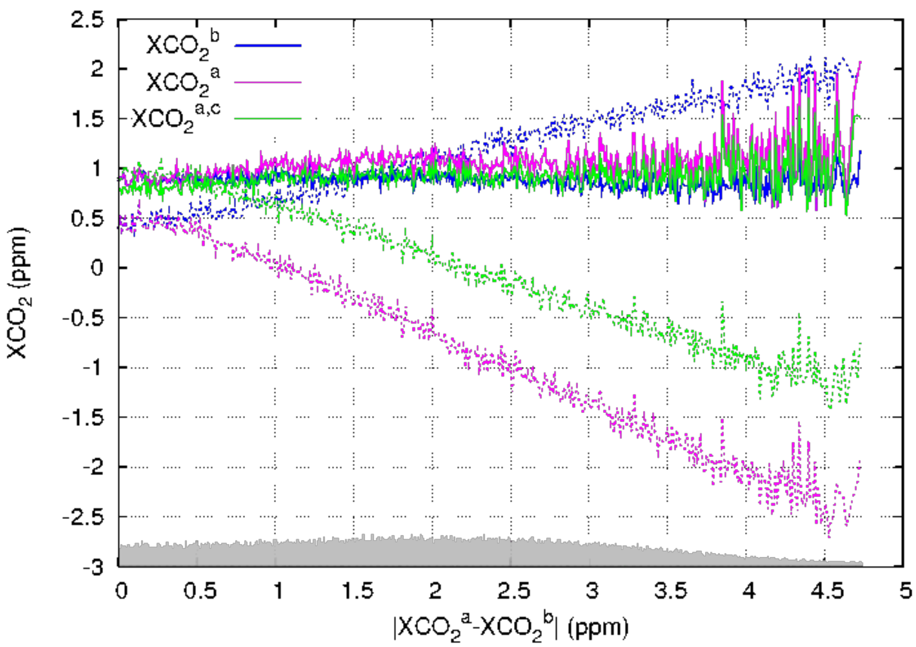

XCO2b
XCO2a
XCO2a,c
XCO2 (ppm)
|XCO2a-XCO2b| (ppm)
2.5
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-2.5
-3
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5

Fig. 7. Same as Fig. 5 for the medium-gain mode.

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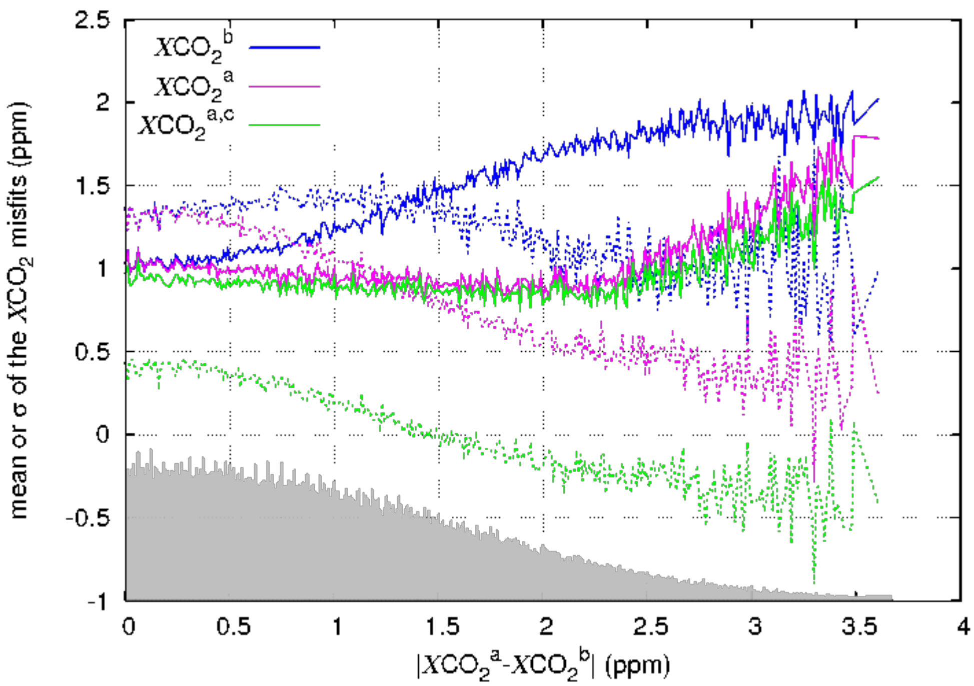

mean or σ of the XCO2 misfits (ppm)
|XCO2a-XCO2b| (ppm)
XCO2b
XCO2a
XCO2a,c
2.5
2
1.5
1
0.5
0
-0.5
-1
0
0.5
1
1.5
2
2.5
3
3.5
4

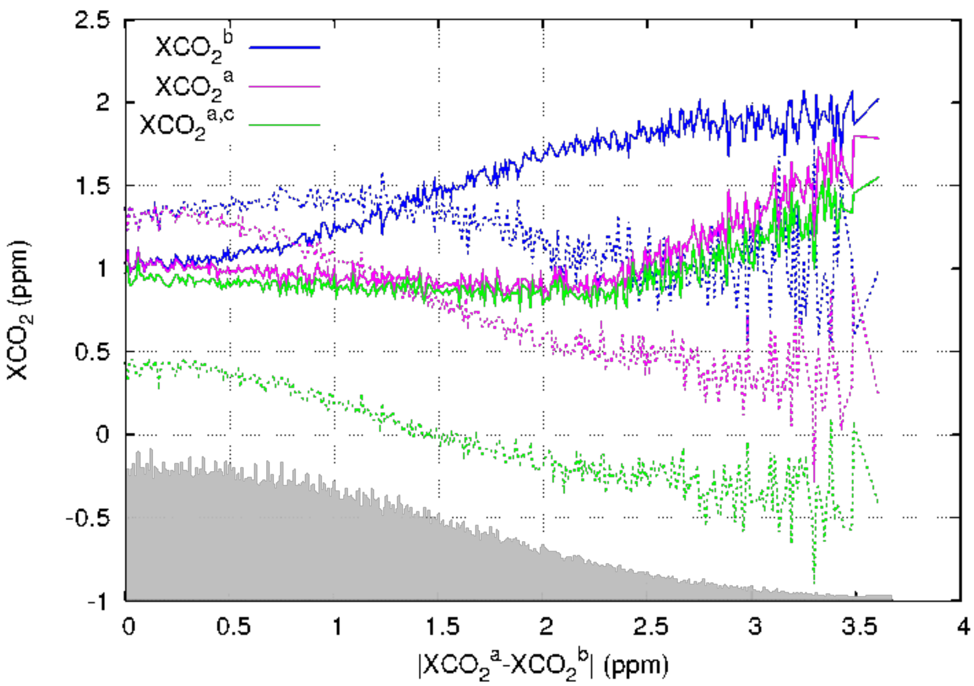

Fig. 8. Same as Fig. 5 for the glint mode over the ocean.