Responses to interactive comments on manuscript ACP-2019-874

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February 13, 2020

This document presents a point-by-point reply to the reviewers comments on manuscript ACP-2019-874 (entitled 'The potential of OCO-2 data to reduce the uncertainties in $\rm CO_2$ surface fluxes over Australia using a variational assimilation scheme'). Author Comment on behalf of all Co-Authors.

We would like to thank the reviewers for their comments and efforts towards improving our manuscript. The reviewer's comments are given in Roman type, and my replies are shown in blue.

1 Response to referee #1

1.1 General comments

Authors apply a regional grid-based inversion system built around CMAQ model and its adjoint to conduct OSSE simulations of the $\rm CO_2$ flux uncertainty reduction for Australia using actual OCO-2 retrievals. The work has high methodological value as authors give sufficient detail on the design and operation of the inverse modeling system, so that is can become valuable learning material for those interested in using surface and satellite observation data in the regional inverse modeling studies with the variational optimization approach. Useful results include the impact of increasing prior flux uncertainties versus changing the spatial correlation length for fluxes. The manuscript is well written and appears to be suitable for publications after technical corrections

1.2 Detailed comments

1. Page 2 Line 29 Authors wrote, "Liang et al. (2017) found that GOSAT had a mean bias of -0.62". Different GOSAT retrievals have their own biases, so it would be fair to give more detail, mentioning which product was used and the version number.

We have restructured the paragraph that start in line 29 on page 2

Initial text: A recent study Liang et al. (2017) found that GOSAT had a mean bias of -0.62 ppm and a precision of 2.3 ppm over 2014-2016, while the bias and precision of OCO-2 were 0.27 ppm and 1.56 ppm, respectively;moreover, OCO-2 offers a denser spatial coverage compared to GOSAT, both in space and time

Modified text: "A recent validation experiment, which compares GOSAT and OCO-2 against the Total Carbon Column Observing Network (TCCON) data (Liang et al., 2017) shows that in general OCO-2 has better accuracy in measuring the atmospheric CO₂ column concentration over 2014-2016. Liang et al. (2017) findings show that the mean biases of GOSAT (FTS Level 2-3 data products) were larger than OCO-2. Over 2014-2016, the GOSAT mean bias was of -0.62 ppm with a precision of 2.3 ppm compared to bias of OCO-2 (OCO-2 Lite File Product version 7), which was of 0.27 ppm with a precision 1.56 ppm. Because a wider detection coverage and higher spatial resolution, OCO-2 realize more accurate estimates of carbon dioxide. However, and despite these differences, both satellites on-orbit have atmospheric CO₂ detection capabilities to be used in regional atmospheric inversions to infer CO₂ surface fluxes"

2. Page 19 Line 3 Sentence "The differences are only partly explained by the combination of prior uncertainty and total number of soundings." Authors may need to mention that due to prevailing winds, surface flux footprints for many OCO-2 soundings made over Australia lay over arid land thus contributing little to uncertainty reduction

We have restructured the paragraph that start in line 3 on page 19

Initial text: The differences are only partly explained by the combination of prior uncertainty and total number of soundings. For instance, the number of soundings in September is only 17% greater than 5 in March. The soundings in September are denser over areas with high prior uncertainties such as grasses and cereals, savannah and evergreen broadleaf forest

Modified text: "The differences are only partly explained by the combination of prior uncertainty and total number of soundings. Another possible reason why we obtained a small percentage reduction in March compared to September is that in the northern region of Australia (the area where we assumed large uncertainties) winds come primarily from the north-west. Prevailing winds in this zone limit the ability of OCO-2 to constraint surface fluxes, mainly because we did not include OCO-2 soundings over the ocean. Second, the number of OCO-2 nadir soundings in September is 17% higher than March. Besides most of these soundings are located over land areas where we assumed that uncertainties were high such as grasses and cereals land, savannah and evergreen broadleaf forest.

3. Page 25 Lines 15-18 Removing more observations on the edges of the grid cell in case of finer resolution does not seem to be the only possible way of mapping observations

to the model grid. This limitation can be omitted from discussion.

1.3 Technical corrections

1. Page 7 Line 11 In a sentence which is related to Eq 7 it is written "J is the number of those 1-second values", while in the Eq. 7 the sum runs from 1 to n, so it is likely that n should be in place of J. On the contrary J appears as a number of elements in the next Eq. 8.

Equation 7 has been corrected.

2. Page 7 Line 14 Omit "be" in "uncertainty of about be 0.5 ppm"

Word "be" has been eliminated

- 3. Figure 3 caption: suggest writing as "prior CO2 flux uncertainty" rather than "prior CO2 uncertainty.
- 4. Page 16 Figure 5 caption: The statement on "The fractional error reduction is defined as..." looks somewhat out of place as figure shows percentage error reduction. In Figure 5 caption has been modified, we replaced "The fractional error reduction" with "The percentage of error reduction"

2 Response to referee #2

2.1 General comments

This manuscript is much improved over the previous submission. I think this is an important contribution, as it addresses many important questions about regional-scale inversions with satellite data, which to my knowledge has not been handled previously. Other than a few minor revisions, I recommend publication.

2.2 Detailed comments

1. Page 2, Line 15: "More uniform sensitivity" - More uniform than what? This is probably a reference to TES and AIRS, but need to be clear.

We have restructured the paragraph that start in line 15 on page 2

Initial text: The Scanning Imaging Absorption Spectrometer for Atmospheric Cartography (SCIAMACHY; Burrows et al., 1995; Buchwitz et al., 2015), which operated aboard ENVISAT during 2002-2012, was one of the first instruments with a more uniform sensitivity to CO₂ throughout the atmospheric column (including the boundary layer) compared to earliest satellite instruments (Chédin, 2003; Crevoisier et al., 2009; Kulawik et al., 2010)

Modified text: "The Scanning Imaging Absorption Spectrometer for Atmospheric Cartography (SCIAMACHY; Burrows et al., 1995; Buchwitz et al., 2015), which operated aboard ENVISAT during 2002-2012, was one of the first instruments with a more uniform sensitivity to CO₂ throughout the atmospheric column (including the boundary layer) compared to earliest satellite instruments such as the Operational Vertical Sounder (TOVS) (Chédin, 2003), the Infrared Atmospheric Sounding Interferometer (IASI) (Crevoisier et al., 2009) and the Tropospheric Emissions Spectrometer (TES) (Kulawik et al., 2010)"

- 2. Page 6, line 4: Kiel et al (2019) is the best reference for the v9 data product We have included the reference (Kiel et al., 2019)
- 3. Page 9, Line 2: Missing reference "(Author, b).

 We have updated the reference to (Harverd, 2018)
- 4. Section 5: This is a bit unsatisfying, as the fluxes aren't reported. Is there a reason not to report the fluxes?

The assessment of posterior fluxes from assimilation of real data will be the subject of an upcoming paper.

5. Page 25, Line 14: More accurately "simulate" concentrations?

We have restructured the paragraph that start in line 14 on page 19. We have added: "Another important consideration in future work is that these flux inversions should be run with a finer temporal and horizontal resolution. Model simulations at higher temporal and spatial resolution are always in better alignment with observation (fewer biases), mostly because they can sample closer to the measurement site location.

3 Response to referee #3

3.1 General comments

This paper describes a regional flux inversion system to estimate fluxes over Australia with column CO_2 observations from OCO-2. The authors test the performance and sensitivity of the system with a series of Observing system simulation experiments (OSSE). The performance of the system is primarily presented with the metric of uncertainty reduction assuming unbiased prior fluxes and pseudo observations. With increasing of satellite observations and the need to understand regional fluxes, the regional flux inversion is highly desirable. Therefore, the topic is important. The overall testing of the regional system roughly follows the traditional global inversion system, which I find is not sufficient. Though uncertainty reduction is a useful quantity to show the performance of the system, which highly depends on experimental setup as also discussed in this paper. In the following, I

suggest a few more experiments and other metric to test the sensitivity and performance of the regional inversions

3.2 Detailed comments

1. Different from global flux inversions, the regional flux inversions are sensitive to boundary conditions. I would suggest adding one experiment to show the sensitivity of the system to prescribed boundary conditions. For example, if the boundary conditions has random error of 1ppm, what does the result look like? Better yet is to assess the uncertainty of the boundary condition from CAMS, and then add that uncertainty in the OSSE.

We agree that regional flux inversions are sensitive to lateral boundary conditions (BCs). The strength of the sensitivity depends on details such as domain size and distance from the boundaries to our region of interest. Ziehn et al. (2014, 2016), using a set-up rather like ours, found little sensitivity. We agree however that some sensitivity cases are warranted and are testing the impact of biased BCs on derived fluxes.

2. Since the inversion assimilation window is short, the regional inversion must be sensitive to initial conditions as well. Therefore, testing the sensitivity of the system to initial condition and whether including the initial condition as part of state vector improve the performance would be very useful

This is probably not the case for two reasons. Firstly, Peylin et al. (2005) found little sensitivity for their European inversion to the initial condition. Sensitivity lasted about five days, comparable to the transit time for a concentration signal. Secondly, we are aiming to understand the uncertainty that will occur in real, much longer inversions. These last many months or even years. They are consequently not sensitive to initial conditions. However, we have decided to include this experiment in the paper (we will include the initial conditions as part of the state vector)

3. Satellites provide much denser observation coverage compared to surface CO₂ observations, especially over tropics and the Southern Hemisphere. But at the same time, it is prone to bias in observations. The OSSEs are perfect to test the sensitivity of the inversion to potential bias in the observations. I suggest adding one experiment that assimilate biased pseudo observations. The bias could be based on the bias correction algorithm used in the OCO-2 retrieval products.

This is an excellent idea. We are running experiments using the differences between raw and bias-corrected XCO_2 as a bias term in our OSSE.

4. Unbiased prior fluxes certainly satisfy the theoretical assumptions in the variational optimization, but it is rarely the case in estimating land fluxes in atmospheric CO₂ flux inversion. Scientifically, it is more useful to estimate a mean offset between the true

fluxes and the prior fluxes. So I suggest to have a prior fluxes that have different mean values from the truth, and then test how the inversion could recover the mean fluxes.

This is also an excellent idea. We will run a biased prior case where we use the prior uncertainty not as a random perturbation (different for each realisation) but as a bias.

3.3 Some minor comments

1. I don't see the necessity to have section 5, since no real fluxes are presented. Also, the numbers on figure 10 are not consistent with the text.

We disagree with this point. A common critique of OSSEs is that we have no way of assessing the input uncertainties. Comparing simulations and observations is one such check so we think it is important support to the results.

Number in the figure 10 has been corrected.

2. The observation operator is different from several previous studies(e.g., Basu et al., 2013 cited in your paper). In equation (12), you interpret the averaging kernel to model levels. In a lot studies, the model vertical profiles are interpolated to the vertical levels of the retrievals, and pressure weighting function from retrievals is used in calculating model equivalent column CO₂. I think if the observation operator is done in this way, you will not have the problem having to remove 1-second averaging observations if they span several grids

We agree that this approach would solve that problem. However CMAQ data is at higher vertical resolution than the 20 levels of the OCO2 retrieval. Running at least a simple interpolation from CMAQ to OCO-2 risks neglecting high resolution features in the CMAQ profiles. The averaging kernel is fairly smooth so the problem is less severe in this direction. It is a judgement call either way.

3.4 Technical corrections

1. Line 6 on page 11, seems missing a word.

We have restructured the paragraph that start in line 6 on page 11. We have added: "We solve the minimization with a change of variable \vec{x}^b . Given that our control vector \vec{x} depends on the size of the multipliers of the principal eigenvectors of **B**. Our vector \vec{x}^b was reconstructed (as is given in Eq.11). This reconstruction includes a new vector \vec{q} , which is normalized the by the square-root of the eigenvalues of **B**; this transformation involves minimization with respect to \vec{q} , rather than $\vec{x_p}$."

 $2.\ \, {\rm Line}\ 3$ on page 17, remove "uncertainty".

corrected

3. Line 3 on page 19, what could be other reasons? You used "partly" in the sentence..

This comment also was made by referee #1. We have restructured the paragraph that start in line 3 on page 19. We have added: "Another reason for a lower reduction in March compared to September is that in the northern region of Australia (the region where we assumed large uncertainties in March see Fig.3a) winds come from primarily from the west (active monsoon). Prevailing winds in this zone restrict the ability of OCO-2 to constraint surface fluxes (primarily because we did not include OCO-2 soundings over the ocean). Taking into account only the number of soundings in September, we can see that the increase of the OCO-2 data (17%) has a significant impact on the percentage of uncertainty reduction of the prior flux"

4. Line 14 on page 25, double check the sentence. "the potential to more accurately observations"

This comment also was made by referee 2. We have restructured the paragraph that start in line 14 on page 19. We have added: "Another important consideration in future work is that these flux inversions should be run with a finer temporal and horizontal resolution. Model simulations at higher temporal and spatial resolution are always in better alignment with observation (fewer biases), mostly because they can sample closer to the measurement site location".

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