Reviewer replies

We thank the reviewers for their thoughtful suggestions on the manuscript. Below, we have listed each of the reviewer's comments and have listed replies in blue below each comment.

It's still not clear to me whether or not the authors have correctly applied the observation operator in their inverse modeling. Here in this study, the observation operator should include application of satellite a priori, averaging kernels, pressure weighting function from OCO-2 level2 data files. Please refer to Cogan et al. (2012) for the application of observation operator in comparison between model and satellite XCO2 observations. The application of averaging kernel is very important when comparing model and satellite observations, as this can reduce the impact from satellite a priori. In your synthetic cases, you can also generate synthetic satellite data using model simulation and satellite a priori, averaging kernels, pressure weighting function from OCO-2 level2 data files. Correctly using observation operator or not can impact your top-down CO2 fluxes from both full-data inversion and reduced-data inversion. Thus this can impact the evaluation of your data reduction algorithm.
I recommend publication after the authors clarifying this part and addressing the following questions/comments.

We followed a similar approach to the observation operator as in Cogan et al. (2012). According to Cogan et al. (2012):

$$\mathbf{X}_{\mathbf{CO2}} = \mathbf{h}^T\mathbf{x}_\mathbf{a} + \mathbf{h}^T\mathbf{A}(\mathbf{x} - \mathbf{x}_\mathbf{a}) \qquad (1)$$

where $\mathbf{X}_{\mathbf{CO2}}$ is the retrieved CO_2 observation, $\mathbf{h}$ is the pressure-weighting function, $\mathbf{x}_\mathbf{a}$ is the *a priori* estimate of the CO_2 profile, $\mathbf{A}$ is the averaging kernel, and $\mathbf{x}$ is the true CO_2 profile. Equation 1 can also be re-arranged into two components – information contributed by the prior and by the satellite observation (e.g., Brasseur and Jacob, ch. 11):

$$\mathbf{X}_{\mathbf{CO2}} = \mathbf{X}_{\mathbf{prior}} + \mathbf{X}_{\mathbf{satellite}} \qquad (2)$$

$$\mathbf{X}_{\mathbf{prior}} = \mathbf{h}^T\mathbf{x}_\mathbf{a}(\mathbf{1} - \mathbf{A}) \qquad (3)$$

$$\mathbf{X}_{\mathbf{satellite}} = \mathbf{h}^T\mathbf{A}\mathbf{x} \qquad (4)$$

A common approach in existing satellite-based inverse modeling studies is to either (a) apply Eq. 1 (or Eq. 2) to the atmospheric model outputs before comparing against the retrieved CO_2 observations, or (b) subtract the component that is likely due to the prior from the retrieved CO_2 observations ($\mathbf{X}_{\mathbf{CO2}}$ **-** $\mathbf{X}_{\mathbf{prior}} = \mathbf{X}_{\mathbf{satellite}}$) and apply Eq. 4 to the model outputs (e.g., Frankenberg et al. 2006, Bergamaschi et al. 2007, Basu et al. 2013, Saeki et al. 2013). We use the latter approach in the real data simulations:

$$\mathbf{z} = \mathbf{X}_{\mathbf{CO2}} - \mathbf{X}_{\mathbf{prior}} - \mathbf{h}^T\mathbf{A}\mathbf{b} \qquad (5)$$

where $\mathbf{z}$ are the processed observations used in the inverse model and $\mathbf{b}$ is the CO_2 background or clean air boundary condition.

An exception is that we did not include $\mathbf{x}_\mathbf{a}$ in the synthetic data simulations – because it cancels out. Let us suppose that we include an *a priori* CO_2 profile in the synthetic data. We would generate the synthetic satellite data ($\mathbf{X}_{\mathbf{CO2}}$) using the equation outlined above: $\mathbf{X}_{\mathbf{CO2}} = \mathbf{X}_{\mathbf{prior}} + \mathbf{X}_{\mathbf{satellite}} + \mathbf{h}^T\mathbf{A}\mathbf{b}$. Before running the inverse model, we would apply Eq. 5 and subtract $\mathbf{X}_{\mathbf{prior}}$ from the synthetic satellite. As a result, the term $\mathbf{X}_{\mathbf{prior}}$ cancels out.

Specific comments:

Line 52-53: “Rather, these models are often used to calculate the product of H or HT and a vector (e.g., a vector of estimated CO2 fluxes)”. Here, a vector of estimated CO2 fluxes is not an appropriate example. Usually, the vector is the gradients of your objective function with respect to simulated targeted species, here in your study, simulated CO2 profiles.

We have removed this example from the manuscript. We originally added an example because it was requested by a different reviewer. Chemical transport models are often used to calculate the product of **H** and a vector of estimated CO_2 fluxes. By contrast, the adjoint of a chemical transport model is often used to calculate the product of $\mathbf{H}^T$ and a vector, and that vector can vary depending upon the application and specific inverse modeling approach used. For example, that vector will differ depending on whether one uses a gradient-based method for minimizing the inverse modeling cost function (as mentioned by the reviewer above) or whether using a different approach like the minimum residual method (e.g., Saibaba and Kitanidis 2012). To avoid any confusion, we have removed the text in parentheses.

Line 55-56: “The model output must be interpolated to the locations of the observations, often referred to as the observation operator.” Partially correct. The key part of the observation operator, here in your study, is the application of satellite a priori, averaging kernels and pressure weighting function.

We have removed the term “observation operator” from the text to avoid confusion.

Line 59-66: I wonder how different are the gradients at the first iteration between using reduced data and using full data, in terms of spatial distribution and magnitude?

We did not calculate gradients as part of the inverse modeling simulations in this manuscript. We found the minimum of the inverse modeling cost function directly (aka, analytically) instead of using an iterative minimum-finding algorithm. We have added text to Sect. S3 that provides additional detail on the equations used to minimize the inverse modeling cost function.

References:

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