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Atmospheric Chemistry and Physics Discussions
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# *Interactive comment on* "Characterizing model errors in chemical transport modelling of methane: Using GOSAT $XCH_4$ data with weak constraint four-dimensional variational data assimilation" *by* Ilya Stanevich et al.

**Anonymous Referee #2**

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The authors propose a novel method to quantify errors in transport modelling. It uses GOSAT measurements within a new assimilation framework. In particular, the authors propose to use part of the knowledge provided by the adjoint of the transport model to constrain model errors. I am personally a great enthusiast of using the adjoint in a more comprehensive way than what is currently done by the community. Therefore, I recommend supporting the authors in their efforts to do so, and their work should make an interesting contribution to the community.

However, the present state of their manuscript requires significant changes, clarifica-



tions and rearranging before suitable for publications.

## 1 General comments

### 1.1 Structure

With the current structure and organization, it is hard to filter the take away messages. Some details are missing, other are not necessary. I have some doubts on the choice made by the authors in the way they split the content of their work between the present manuscript and the sister paper in GMD (gmd-2019-248). At lot of details about the method itself is given here, while it would be more suitable for a model description paper in GMD. Also, many details about the method, in particular the tuning choices, are set aside, while they are critical for validating the reliability of the approach. Similarly, all the OSSEs would make more sense in a GMD paper.

Only the part directly concerning real data would be suitable for an ACP content in my opinion, as well as the discussion on model resolution?

I suggest the author dramatically reconsider the way they organize their presentation of their work to help the reader navigate through the results.

### 1.2 Weak constraint vs Strong constraint

The authors insist on sticking to the 4D-VAR formulation of the surface flux inversion problem. Such an approach, following the work from the numerical weather forecast community, is artificial and ends up in clumsy and artificial formulations. Even though the equations are correct, they are uselessly complicated. The surface flux inversion problem is a 3D-VAR problem, the time step of the NWF community having no meaning in our case (the author implicitly acknowledge this fact by putting the emissions in the model parameters $\mathbf{p}$).

I may be wrong, but the author's formalism could be easily replaced by the classical inversion equation, simply adding model bias in the control vector. Thus, the matrix $\mathbf{Q}$ would only be a sub matrix of $\mathbf{B}$, and the Lagrangian terms would not be needed; they would be implicitly solved for in the problem as a 4D CH4 atmospheric source/sink in the transport model.

### 1.3 Period of interest

The authors chose a very short period of interest (4 months) in 2010. This seems to be guided by the availability of validation data.

Such a duration is very short considering the global atmospheric transport patterns. The author show that the biases in the initial conditions can be corrected quite quickly, which would excuse the short period. However, what about long-term biases?

In the present conditions, the WC inversion seems to only allow for short term corrections, at the cost of a loss in the mass balance. It would then limit the inversion conclusions to very regional patterns, reducing the interest of running global models...

### 1.4 Uncertainty matrices

It feels that your results are so dependent to the subjective choice of $\mathbf{Q}$ that they are hardly exploitable. It is already rather challenging to find a balance between $\mathbf{R}$ and $\mathbf{B}$ in a classical inversion. The final taste of the work as it is describe is that the method does not really fit its purpose. Quantifying biases would be as efficient with simple forward simulations as it is presented...

I am convinced that the use of the adjoint to quantify model errors is a good approach,



but with the author's framework and no additional data, it seems quite impossible to deduce any conclusive results...

## 2 Specific comments

- p.2 l.24: regional and global scale
- p.2 l.33: "assume that the model is perfect": this statement is misleading; the so-called strong-constraint inversion never assumes that the model is perfect. Errors are represented in the $\mathbf{R}$ observational error matrix. Of course, in most inversion framework, the $\mathbf{R}$ matrix is too simple and misses most of the error patterns, but that is only a technical choice in the application.
- p.4 l.7: EDGAR 2004 is quite outdated; could the author justify such a choice?
- p.4-6 Sect. 2.2.1: This section mixes observation information with preliminary studies and side conclusions. Shorten and put results in the results section if really needed or in Supplement, or in a GMD style paper
- p.6 Sect. 2.2.2: a lot of information is given about the instrument precision and techniques; are such details really needed in a OSSE paper?
- p.7 l.20: $\mathbf{p}$ vary over time? it is not clear from equation (1)
- p.7 l 26: it is not clear at all what are the dimensions and spaces of the object presented here
- p.8 eq.3: are $\mathbf{Q}$ and $\mathbf{R}$ always the same for each $i$? by design, you make it impossible to have temporal correlations in the observation space. It is often the case in practice in classical inversions, but should be highlighted as a limitation of this formulation

- p.8 l.10: 4D-VAR artificial and makes it hard to understand. Justified in NWF where the state is directly optimized with respect to observations, but our interest is p (surface emissions). We rather do 3D-VAR!!!
- p.8 eq.4: should $\mathbf{H}$ be $\mathbf{H_i}$? should be different at each so-called time step?
- p.8 eq.4: The Lagrangian factor part would be automatically solved with a 3D-var SC including a 3D source-sink atmospheric term...
- p.9 l.11: What is exactly the size of $u_i$? and what are i standing for? days? minutes? It is not fully clear from the text neither as it changes over the course of sections...
- p.10 l.1: It is a big problem to assume diagonal $\mathbf{B}$ (as well as diagonal $\mathbf{Q}$) as you give too many degrees of freedom to your inversion compared to the number of observations
- p.10 l.17: the choice of $u$ is very shortly justified (and unconvincingly); consider extending such justification or all the results appear untrustworthy
- p.10 l.20-30: very clearly and accurately written paragraph stating the limitations of the method. But later sections contradicts the acknowledgement of the limitations
- p.11 l.3-6: important sensitivity results! should be more extensively detailed, either in the result part, or supplement, or GMD companion paper...
- p.11 eq.4: is there a link with the cost function? the use of $J$ is misleading; the equation is artificial and does not make sense. If the purpose is to introduce the total sensitivity in eq.12, the author should rather change both eq 11 and 12 and write them with the adjoint of the model, evaluated at an increment observation vector equal to 1 at every GOSAT obs.



- p.12 l.15: with less extreme situations, the balance between $\mathbf{Q}$ and $\mathbf{B}$ is expected to be even more subtle...
- p.12 l.27: not clear what tuning you are talking about; please consider adding a table detailing all the OSSE and inversion set-ups to help the reader
- p.12 l.35: negativity bound: ad-hoc unjustified choice; might be reasonable, but needs some details
- p.13 sect.3.1: more than 2 full pages, 8 figures, a lot for one section... consider splitting
- p.13 l.27: fig.3 may be misleading; it shows the integrated 'footprint' of GOSAT observations, but the inversion uses increments depending on the deviation from the prior and observations (or truth)
- p.14 l. 7: I disagree. It only shows that the matrix $\mathbf{Q}$ you chose is incorrect for that set-up... it feels that your results are so dependent to the subjective choice of $\mathbf{Q}$ that they are hardly exploitable
- p.14 l. 31: again, it only shows that $\mathbf{Q}$ is ill specified
- p.14 fig.6: Right column: Due to ill specified Q, WC applies correction upwind in the Atlantic ocean to improve the situation over the Amazon bassin. This could be highly misleading for diagnosing model errors!
- p.15 fig 6-7-8: why not including SC in these figures for comparison?
- p.15 fig.11 and last OSSE: I didn't really get this last OSSE. why initial conditions at different dates? In the end, it is probably on of the most important OSSEs as it show the capability of the WC to correct for long-term errors; but the way it is presented makes it hard to understand

- p.18 l.34: is it really necessary to extent ACE-FTS profiles to compare with GEOS-CHEM? can't you produce real equivalents?
- p.19 l.30: such results is quite obvious with a one month assimilation window; please comment accordingly...
- p.20 l.5-10: Gives the impression of fitting pre-conceived conclusion at all costs... the results are not convincing in that direction

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