Point-by-Point Responses to Anonymous Referee #3

We thank Anonymous Referee #3 for their time and effort in reviewing our work and appreciate their recommendations for ways to improve the manuscript. Following many of their suggestions, we believe the revised manuscript is an improvement upon the original submission. The referee comments below are taken from https://doi.org/10.5194/egusphere-2023-2227-RC3.

This document provides a point-by-point response to Referee #3. The responses follow the sequence: (1) comments from the referee, (2) authors' response, (3) authors' changes in manuscript.

1.1 Referee Comment

"Tribby and Wennberg argue in "An analysis coordinate transform to facilite [sic] use of in-situ aircraft observations for flux estimation" that simulated ethane and propane fields from the GEOS-Chem transport model run at three different horizontal resolutions look similar when the chemical tracer is plotted on a latitude versus potential temperature coordinate, although they look different when plotted on a latitude versus pressure coordinate. They then conduct a simple optimization in which the simulated mole fractions are compared to observed mole fractions from the ATom campaign, at the same latitude and potential temperature, and scaled to match. Tribby and Wennberg report that the scale factor is within 10% for simulations whose resolution ranges from 4x5 deg to 0.5x0.625 deg. They use this agreement to conclude that the use potential temperature as the analysis coordinate for comparing simulated to observed tracers could save time and money associated with chemical transport modeling."

1.2 Author Response

We have made substantial changes to the analysis and no longer present a Bayesian approach. We substantially revised the manuscript to focus on an analysis approach by creating pseudo data for ethane and propane as sampled by the DC8 aircraft during the Atmospheric Tomography (ATom) aircraft mission. We sample simulations from the highest resolution (0.5 x 0.625 degree) GEOS-Chem High Performance v14.3.1 and then evaluate the correlation of these pseudo data with lower resolution simulations and simulations sampled +/- 5 days from the pseudo data. We apply a simple statistical analysis that illustrates the value of potential temperature as a vertical coordinate in comparing sparse observations with a GCM.

1.3 Manuscript Changes

Figures 4-8.

2.1 Referee Comment

“The analysis in the paper was insufficient to substantiate this conclusion, and major revisions and additional writing are required before the paper is suitable for publication.There was no counterfactual presented, in terms of how close the optimization scale factors would be if a comparison were conducted in latitude/altitude space rather than latitude/potential temperature space. This comparison is critical to evaluate the authors’ conclusion about the benefits of the proposed coordinate transform.”

2.2 Author Response

See RC1 author response 6.2 for that addresses reasoning for change in approach. We now present a simple linear regression analysis, RMS, and RMSE that quantify the differences between the coordinate transform.

2.3 Manuscript Changes

Figure 4-8.

3.1 Referee Comment

“There was no argument offered for the appropriate spatial resolution at which fluxes could be optimized. While the methods were not clear, I got the impression that the authors were optimizing fluxes uniformly or perhaps zonally, both of which would be coarser than what is desired for many chemical species. The authors do not show whether (or how) this approach could be used to improve flux optimizations at continental, regional, or local scales, where fluxes would be optimized on a 2-d grid rather than a zonal a.”

3.2 Author Response

As the Referee pointed out, this study focuses on constraining sources at large scale (coarse). In Tribby et al. 2022, using θ coordinate, we evaluated zonal errors in emission sources that were most clearly visible using summer data when the lifetimes of ethane and propane are shorter (Figure 3,4 in Tribby et al. 2022).

3.3. Manuscript Changes

No changes.

4.1 Referee Comment

“The spatial scales of the chemical transport model were also coarse compared to that which would be desired for some applications (e.g., 10s of km), and it is not clear whether this approach would add value at those scales.”

4.2 Author Response

Even under those types of situations, traditional lat/lon/time/altitude approach can be problematic if sources are misattributed in space. (We are not trying to show this here.) Nevertheless, our new analysis approach shows that potential temperature can mitigate time and resolution errors when comparing coarse GCM simulations to sparse observations.

4.3 Manuscript Changes

Figures 4-8.

5.1 Referee Comment

“The authors simulate the chemical fields using fluxes that had previously been optimized in Tribby et al., 2022. Can this approach work when there are spatial biases in the distribution of prior fluxes fluxes (for example, zonal, meridional, or seasonal biases) imposed in the chemical transport model? If so, what are the limitations that are important for users of this approach to take into account?”

5.2 Author Response

The simulations have been previously optimized in Tribby et al. 2022 when there was a spatial bias in the distribution of underlying emissions. Using potential temperature as a dynamical coordinate supported revision of the underlying emissions grid. We added additional language detailing limitations for using this approach.

5.3 Manuscript Changes

Lines 53-60.

6.1 Referee Comment

“The authors describe the results plotted in Fig. 3 as being more consistent across resolutions than those plotted in Fig. 2, although the results for February 23 look quite different among the three resolutions even in Fig. 3. On this day, there are elevated concentrations in isolated patches within the middle of the free troposphere apparent in the 0.5x0.625 deg simulation, but not in the other simulations. The ATom observations are not shown for this day, so it is not clear whether the elevated concentrations were observed or whether they are an artifact of the the transport model. In either case, the paper should discuss what characteristics of the meteorology on this day lead to the result that the potential temperature approach does not lead to convergence among the various resolutions.”

6.2 Author Response

While some days are predicted to have slightly higher mole fractions, these data did not appear to significantly affect or skew the new RMS, RMSE, or slope comparison analyses.

6.3 Manuscript Changes

Figure 4-8.

7.1 Referee Comment

“In general, the paper read as incomplete. It is noteworthy that the paper did not have a Discussion or Conclusions section. This should be remedied before a revision is considered. It ends abruptly and leaves the reader with many questions, and it is surprising that the paper went out for review. The methods section lacked sufficient detail to understand the simulations and emissions inventories underlying the simulations. I am not familiar with Tribby et al., (2022), and relevant aspects of the methodology, results, and conclusions should be summarized briefly so that readers of this paper are not required to do an in-depth read of that paper. The results section did not contain the relevant analysis and documentation to substantiate the conclusioins [sic] (as described above), and the lack of discussion meant that it is not clear what the caveats of employing this method were.”

7.2 Author Response

See new Methods, Discussion and Conclusions section.

7.3 Manuscript Changes

Lines 52-251.