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RC1: 'Comment on acp-2022-616', Anonymous Referee #1, 20 Nov 2022 reply

This is a paper on an important subject: vertical redistribution of tracers by parameterized convective mixing in CTMs. Two models are compared and run with and without convective mixing. Many of the model differences can be explained by the differences in convection. In that sense, the paper has a clear message.

Having said this, I think that the analysis itself is rather superficial and raises a couple of questions. Off-line models rely on parameterizations of the parent meteorological models. The authors mention that "time-averaging" in the transfer to the GCM may lead to biases. However, no results are presented that specifically address effects of temporal averaging.

We agree that this is a critical thing which needs to be investigated. While this was also previously mentioned in Yu et al 2018 paper, we have been unable to convince either reanalysis center to do this which requires special output from NASA and/or ECMWF. Without access to driving meteorology at resolutions higher than 3 hours, e.g. 5 min, 15 min, 30 min, etc, it is impossible to investigate time averaging errors of subgrid scale motions. Therefore, it is unfortunately beyond the scope of this paper. It is our thought that papers like this one should serve as motivation for national agencies to better support the evaluation of these uncertainties in light of the importance to studies of trace gases and climate.

Apparently, this paper is an interim report of ongoing investigations. Likewise, the fundamental differences between the parent models (GEOS having a one-updraft-detrainment scheme and IFS a more involved updraft-downdraft separation) is untouched.

This is true but the updraft strengths are an order of magnitude stronger than the downdraft strengths for the ERA schemes, implying that when the updraft strengths of ERA are 2X that of MERRA, the downdrafts from ERA are a second order difference. We've added the summed ERA-I downdraft fields in figure S9 for completeness. We've also clarified this in the text (addition of underlined text):

While the RAS and Tiedtke convective parameterizations are different, we can still perform qualitative comparisons of the upward convective mass fluxes from the parent models under investigation here. While the

downdraft component from TM5 is important, it is an order of magnitude weaker than the updraft component as can be seen in Figure S9.

Figure S9 portrays the differences in convective mass-fluxes. Large differences are apparent, but explanations of impact are lacking. As an example, it would be very instructive to investigate the vertical redistribution of a non-well-mixed column of tracer after e.g. several time-steps.

We feel the impact is somewhat intuitive. For example, ERA-Interim based convective mass fluxes, which feed into TM5, are clearly much stronger than MERRA2's throughout the entire vertical column with local maximums over the equator and midlatitudes (S9). The effect of this mixing difference is quite clear in the results in Fig 1f and 1l, where (1f) is fluxing a *positive* CO2 and (1l) is fluxing a *negative* CO2. We agree that single column tests would be interesting but it is not quite clear how to proceed with that as any effect beyond what we mentioned above (first order type effect) needs to be advected in order to produce the emergent tracer differences you see in Figure 2 for example.

This brings me to another important point. Vertical mixing of tracers is extremely non-linear, with a well-mixed column as the end-point. In that respect, I was surprised to read that the GEOS-Chem mass fluxes assume a well-mixed column (whenever convection appears), both for convection (line 121) and for PBL diffusion (line 132). There must be an explanation for these choices, which obviously have a huge effect on mixing, but maybe I do not completely understand the reason for this choices.

Line 121 doesn't say this. It says:

"Furthermore, whenever convection is found within a gridcell, the GEOS-Chem convection code triggers a complete mixing in the atmospheric column beneath the lowest level with convection."

Recall that GEOS-Chem mixed up to a *diagnostic* (from parent GEOS model) PBL height (PBLH variable), it doesn't have to match parent PBL mixing exactly. What we state here is that when convection is present in the column, it is essential that this convective mixing has access to the surface fluxes of that grid cell. One can imagine, if for example the PBLH is determined to be at the 5th vertical level of the model and the convection starts in the 7th vertical level, that one would end up with two disjoint mixing cycles where the convection can't "see" the surface. In real life, this would

be quite unrealistic but in "model world", this could happen. In that sense, We find the fact that it well mixes the *lower* atmosphere up to the first convective layer to be a wise decision.

In summary, my feeling is that a more in-depth analysis of the vertical mixing and the underlying choices in the parent models is needed to fully understand the huge differences presented in this paper. The current analysis, while interesting, raises many unresolved questions, which need to be addressed to bring this paper beyond an update in ongoing investigations.

We don't disagree with this assessment. However your summary is what we hope people should conclude from this paper. CTMs are largely simple, but not necessarily inaccurate, reimplementations of their parent models. In the case of this analysis, we feel more work, i.e. funding, research, etc, is needed to investigate the vertical mixing of trace gases in the parent ECMWF and NASA models, where the *big* differences seem to be. The fact that TM5 and GEOS-Chem produce very different trace gas profiles is not necessarily because *they* are very different, but likely because the driving parent meteorology is quite different. The authors here are GEOS-Chem and TM5 users and don't have the access, or resources, to run tests on the parent meteorology models. Again, fair assessment.

Some minor points:

Around line 95:

"This mixing matrix takes on the form of a tri-diagonal banded matrix with nonzero entries up to the cloud top, with nonzero non-diagonals allowing nonlocal mixing between all levels with convective activity within a single convective timestep."

I do not understand how nonlocal mixing between all levels can occur when the matrix is tri-diagonal banded. This only allows exchange between adjacent layers (like diffusion). The concept of convection is that important for this paper that the reader needs to obtain full understanding of the modelled process. This does not help: maybe a figure and/or example is more illustrative.

We agree that this was not written clearly in the text. The entire section has been rewritten to explain the form of the convective mixing matrix and to describe the convective parameterizations of the ERA-interim simulation,

The procedure to build the convection matrix **starts with a tridiagonal banded matrix, but then the column mass conservation and flux boundary constraints at the bottom and top of the column lead to this banded form being "filled" in, allowing the nonlocal mixing we referred to. We've rewritten this as:**

"The no-mass-flux boundary condition at the surface and convective top, along with a mass conservation constraint, determine the off-diagonal values of this mixing matrix. This permits nonlocal mixing among all levels with convective activity within a single mixing operation. For a complete description of this procedure in the TM3 model we refer readers to \cite{Heimann2003}."

Moreover, I think the convective parameterization in the "TM5-parent" ECMWF IFS model needs to be outlined in the paper (as for GEOS). This parameterization changed over time, and the ERA-I version needs to be properly described, see e.g.:

https://www.ecmwf.int/sites/default/files/elibrary/2021/20198-ifs-documentation-cy47r3-part-vi-physical-processes.pdf, chapter 6.

We agree that the documentation/descriptions for the changes in IFS can be difficult to find, we feel that Dee et al 2011, as referenced in the text provides the best description we could find of the state of the IFS model for ERA-I as it pertains to TM5. The reference pointed to is good but recent and only documents recent version of the IFS from v41 onwards (in contrast to v31*).

Figure 2 is interesting, but hard to read. First of all, units are missing. Second, the outer panels axis labels are unclear. Third, without an obvious reason the color in the outer panel changes from black to red.

Units added and colors set to "black" for all side integral plots. Don't understand about why outer panel axis labels are unclear, I've added 90S and 90N to the plots, these are simply zonal averages of the interior plots so unsure of what is "unclear".

In figure 3 once more the unit is missing.

Added title and included units, <u>XCO2 (ppm).</u>

Figure S1 is not useful without proper explanation of the symbols and nomenclature in the caption.

Added full description consistent with what was presented in caption of Schuh et al 2019, where figure originated from.

I also upload the annotated pdf that contains some small additional remarks.

Comments on annotated manuscript:

Reviewer asked why only remove mass difference for 2016-2018.

The small global mass differences were removed from 2016-2018 which were the only years under analysis here, they could have been removed from previous years during the spinup, doesn't have any effect on this analysis. We have changed text to reflect this:
"We found a small non-conservation of tracer mass in GEOS-Chem, with a monotonic loss of about 0.25\% in fossil fuel \ce{CO2} over the period 2000-2018. Non-conservation of natural fluxes was about half as small. The global mass differences for these tracers were removed from the concentration data before analysis."

Reviewer asks to change GC to GEOS-Chem.

Reviewer is correct. We have changed GC to GEOS-Chem everywhere.

Reviewer highlighted Fig2 without comment.

Fig 2 modified with respect to earlier comments.

Reviewer asked for IFS version to be mentioned earlier in manuscript.

We added IFS model version to description of TM5 in Methods based on this and earlier comments.

Comment on IFS/Tiedtke: Reviewer says Tiedtke is only the basis for calc of convective fluxes at various levels. We've changed text to read:

"The IFS uses the Tiedtke convection scheme (Tiedtke et al 1989) to provide upward and downward plume entrainment and detrainment mass fluxes at each model level and as a means to represent shallow, intermediate, and deep convection."

Reviewer questions the TM3 reference for Heimann et 2003, we've rewritten more clearly:

"Both GEOS-Chem (Stanevich et al 2018) and TM5 (based on the TM3 model convection implementation from Heimann et al 2003) interpret convective mass fluxes from their parent models to drive relatively simple mixing schemes."

Reviewer says this sentence isn't supported by paper:

"Flux inversions using in situ measurements, which are more prevalent at the surface, should be much more sensitive to modeled vertical diffusion in the PBL than flux inversions using column average data."

We've changed the text to reflect the reviewer's comments to:

"We have shown that for the simulation of concentrations near the surface, diffusive mixing in the PBL has a bigger effect than deep convection. It can therefore be expected that inversions based upon in situ measurements would be more sensitive to modeled vertical diffusion in the PBL than modeled deep convection."

Reply

Citation: https://doi.org/10.5194/acp-2022-616-RC1

- **RC2**: 'Comment on acp-2022-616', Anonymous Referee #2, 19 Dec 2022 reply

The authors have conducted an evaluation of the impact of uncertainties in atmospheric transport on the distribution of CO2 in the GEOS-Chem and TM5 chemical transport models (CTMs). They examined the contribution of convective and diffusive transport toward discrepancies in the models and found that differences in convection between the models are strongly linked to the differences in the modeled CO2. They noted that although convective transport is the main contributor to the CO2 differences between the models, PBL diffusivity is also a contributing factor. The manuscript is short and well written, and builds on the previous study of Schuh et al. (2019). Characterizing transport errors in CTMs is critical for improving the fidelity of tracer transport in the models and we think the manuscript will be a valuable contribution to the literature in that context. I therefore recommend the manuscript for publication after revisions to address my comments below.

Main Comments

The experiments are focused on convective and diffusive transport, but it is unclear what constitutes "diffusive transport" here. Vertical diffusion can be specified in different ways in models. As far as I am aware, GEOS-Chem has imposed vertical diffusion only in the PBL. And based on the manuscript, it seems that TM5 has vertical diffusion imposed throughout the troposphere. If that is the case, turning off diffusion will have very different impacts in the models, emphasizing mainly the PBL influences in GEOS-Chem. Furthermore, the caption in Figure S2 seems to imply that the effects of vertical diffusion is about PBL mixing. I find the discussion about vertical diffusion confusing. How vertical diffusion is specified in the two models needs to be better described and the discussion needs to be clarified as to whether the focus is mainly on PBL mixing.

Technically, we agree, TM5's vertical diffusion in the free trop means that the diffusion effect isn't entirely in the PBL. We've removed "(~PBL mixing)" from S2 caption. Furthermore, while we agree it is difficult to entirely characterize TM5's free tropospheric vertical diffusion (e.g. effect in upper trop), we find the vast majority of the effect, relative to our research question, occurs in the PBL. This is supported in Figure S2. We've modified text (~ line 102) to now read:

"While vertical diffusion is imposed throughout the free troposphere, that mixing is almost negligible above the diagnosed planetary boundary layer top. "

Minor Comments

1. Page 4, line 97: Are the vertical diffusive fluxes in TM5 added throughout the vertical column? How are the diffusive fluxes computed?

The support for the vertical diffusion in the TM5 is given by Louis et al 1979, referenced in Krol et al 2005's TM5 description.

2. Page 4, line 106: What was the improvement in mass conservation that was implemented in version 12.0.02 of GEOS-Chem? My understanding was that the update was primarily to address the simulation of dry air masses.

   You must be quite familiar with this as these changes are subtle and not many folks understand them. You're also correct. The technical

doc clearly says the CO2 global mass was constrained and similar across both the "wet mass advection" and "dry mass advection" cases. The switch to dry mass advection is often times (and we believe here from experience) desired in order to produce smoother local tracer gradients in time and space, which can be affected by quickly varying water budgets.

We've changed the previous sentence:

We use the version 12.0.2 of GEOS-Chem which has improved mass conservation (Lee and Weidner, 2016) and tracer advection over previous versions, but also includes modifications to more correctly simulate the impacts of variable water vapor content and dry air mass.

To:

We use the version 12.0.2 of GEOS-Chem which has improved tracer advection, and smoother local tracer gradients in time and space, over previous versions due to transporting tracers with dry air mass as opposed to wet air mass (Lee and Weidner, 2016).

3. Page 4, line 114: Should there be an "of" between "Scheme" and "Moorthi and Suarez"?

   Corrected.

4. Page 6, last line: The PBL differences in TM5 in Figure S2g are much larger than those in GEOS-Chem. How does PBL mixing differ between the two models? How is PBL mixing parameterized in TM5?

   PBL mixing for TM5 is described in Krol et al 2005, where the PBL mixing follows Holtsag and Moeng 1991. The non-uniform vertical profile of mixing in the PBL from TM5 is the source of the larger PBL mixing differences near the surface compared to the GEOS-Chem well mixed PBL.

   We've changed the TM5 methods text to capture this:

   "While vertical diffusion is imposed throughout the free troposphere, that mixing is much stronger within diagnosed planetary boundary layer, following Holtslag and Moeng (1991) as described in Krol et al. (2005). Mixing from the surface is explicitly

modeled as layer-to-layer diffusion, and as a result there are often strong vertical gradients in TM5 near the surface, for instance due to large northern midlatitude fossil fuel CO2 emissions."

5. Page 10: Figure 4 is too small. It is difficult to see the spatial patterns on the plots and the text on the colorbars is impossible to read.

   I removed the labels on the xaxis and yaxis which should be obvious in "lat"/"lon" and added 50% bigger labels for the Titles and the Colorbar axis.

6. Page 13, lines 295-296: The study of Prather et al. (2008) should be referenced in this discussion about the convergence of a CTM's transport.

   We appreciate the reviewer pointing out this important reference. Authors assume the CTMs should converge to some solution and find varying degrees of evidence for this across two CTMs running with same parent met. Changed the following text to:

   "*Ideally*, one would desire a CTM's transport *to* asymptotically converge to the parent model's transport as model spatial and temporal resolution increases to the native resolution of the parent model, but this has not been demonstrated. *It is worth noting that past work (Prather et al 2008) utilizing two CTMs acting on the same parent meteorology has demonstrated the difficulty in characterizing this convergence."*

References: Prather et al. (2008), Quantifying errors in trace species transport modeling, PNAS, https://doi.org/10.1073/pnas.0806541106.

Reply

Citation: https://doi.org/10.5194/acp-2022-616-RC2