**Review for**

***Simulated mixing in the UTLS by small-scale turbulence using multi-scale chemistry-climate model MECO(n)***

**by Chau et al.**

---

**Summary:**

Chau et al. present in their study the mixing in the upper troposphere / lower stratosphere (UTLS) region, based on simulations with the multi-scale chemistry-climate model MECO(n). The study is interesting and very well written, contributing with novel results and insights in the turbulent processes leading to the mixing in the UTLS. The statements in the paper are well supported by the figures, which are of high quality. I have no doubt that the study will be of high interest to the community dealing with stratosphere troposphere exchange (STE) and the chemical and dynamical (stability) 'structure' of the UTLS region and the tropopause.
There are only few (major) comments that I invite the authors to consider. In particular, these are:

1) The passive-tracer test in Section 3.2 relies only on one turbulence indicator (Ellrod and Knapp's TI1), whereas there are many other indicators available (e.g., Richardson number as an indicator for Kelvin-Helmholtz instability, KHI). Hence, the 'validation' against this turbulence indicator must be considered with some caution. Furthermore, the turbulence indicators (TI1, TI2, Richardson number,...) are also not the truth, but may fail in recognizing turbulence and/or indicate turbulence where actually there is none. I suggest that the authors more carefully discuss the limitations (and potential) of the turbulence indicators in the passive-tracer test.

2) The three case studies, particularly the discussing of the delta tracer-tracer correlations are very interesting and inspiring! There are two aspects that might be improved, however. First, Subsection 3.3.1 comes with a short introduction on this type of diagram, which is nice. I think that the reader can even be more clearly be introduced on how to read these diagrams. A few additional sentences might be helpful. For instance, why is an L-shape indicative for asymmetric mixing, whereas a diagonal one is clearly pointing to symmetric mixing; where in these diagrams do we see mixing from stratosphere to the troposphere and vice versa. See also the specific comments below. Second, the three cases in Section 3.3 discuss in detail the mixing and tracer-tracer correlations, which is the key topic of the study. Still, it would also be interesting (at least to me) to learn somewhat more about the dynamical and thermodynamical 'setting' of the cases. For example, how does the wind field look like? How is the vertical stratification? Or, why do we see in Figure 5 mixing at a very distrinct location (blue/red dipole) but not at neighboring locations. I fully understand that these aspects are not the key topic of the paper, still some mesoscale context would be interesting.

3) A minor point on structure: I wonder whether Section 3.3.4 is actually needed, or whether the aspect of mixing normalization (to determine the importance of gradient vs. dynamically forced mixing) would better integrated in the three case studies. In short, the discussion of this effect is interesting, but maybe not necessarily in an onw subsection. In line with this, I wonder whether Figures 11 and 12 are needed in the main text, or could become part of some supplementary material? I have not a very strong opinion on that, but the authors might consider it. Furthermore, the statements in Section 4 (Conclusions) are rather general and vague. Some examples: L245 ("with different characteristics" → which?); L249 ("However, individual mixing events depend on the particular weather situation" → what

weather situation? Which ones have been studied in this paper?); L55 ("Both, the vertical tracer gradient and the dynamic and thermodynamic forcing, i.e. the stability and stratification, play important roles in the strength of vertical species exchange" → Maybe, that what we already would have expected! So, can you make a more nuanced statement about the relative importance?).

## Specific Comments:

- L17: aka PV tropopause; introduce 'potential vorticiy' before referring to it as PV

- L19: 'PV-tropopause is conserved' → I understand what the authors mean: that PV is conserved under adiabatic, frictionless flow conditions, and that thus the PV-tropopause behaves as a material surface under the these assumptions. The authors might rephrase, as 'tropopause is conserved' sounds a little strange.

- L27: affecting → affects

- Figure 1: Are really both panels needed?

- L88: COSMO(tbc) → What does 'tbc' mean?

- L95-98: Here, first the default setup of the 1D closure is described, whereas in the following text the actually used TKE-based scheme is described. Is it really necessary to describe the default scheme when it is not used? I see the authors' point to highlight in which way the default setup has been improved, but still wonder whether it is needed…

- L103-106: As before, do we need such a detailed description of the default setting? Or would be sufficient to just highlight in the text the improved setup?

- L116: Very minor detail: I think it should be ERA5 instead of ERA-5; and possibly start a new paragraph after 'EX-60 setup'?

- Section 3.1 (as discussed above): To which degree does this analysis depend on the specific section of the TI1 turbulence indicator? To which degree can the TI1 threshold to be assumed independent from the model resolution? Would you expect different results if TI2 and/or Richardson number is used instead of TI1? No detailed analysis is needed in my opinion, but a more critical discussion of the comparison betweem TI1 and the model TKE.

- Figure 5 (and corresponding text): I like the discussion on the tracer and inverted-tracer mixing, but wonder as a dynamic meteorologist why the mixingf only occur where it does and not at the other locations. Some meteorological background/context for the mixing events would be interesting, possibly supported by figures in the supplementary material?

- Figure 6 (panels c an d): Whereas panels a) and b) show straight diagonals, panels c) and d) exhibit some off-diagonal deviations. I wonder whether I correctly understand these. As an example, in panel c) in the lower-left quarter $O_3$ with vdiff corresponds to somewhat below-diagonal $O_3$ without vdiff. Does this mean that mixing (with vdiff) lowers the $O_3$ values?

- Introductory paragraph to Section 3.3.1: Possibly, introduce the reader even more carefully how to read the delta tracer-tracer plots (as explained above). Why does an L-shale indicate asymmetric mixing? Where in the plots do we see mixing from the stratosphere into the troposphere, where in the opposite direction? Somewhat refelcting on it, it becomes obvious? But why not helping the reader not familiar with tracer-tracer plots with 1-2 explaining sentences to get it at first reading?!

- L181: Minor detail; maybe start new paragraph

- L 185: ‘by dynamic instability’ → The term ‘dynamic instability’ is somewhat vague/unclear? I suggest that the authors introduce at some point in the manuscript very clearly what they mean with ‘dynamic instability’, and also set into contrast to other instabilities? Hence, if it is not a dynamic instability, what is it then? I assume that ‘dynamic’ refers essentially to the ones where wind (horizontal and vertical shear/deformation) is important, whereas a ‘static instability’ refers to one where a vertical profile becomes (thermo-dynamically) becomes unstable (e.g., if squared Brunt-Väisällä frequency becomes negative)? In essence, I suggest to carefully introduce these terms…

- L199: I get the basic idea, but what does |mixing| and |mixing| / |gradient| exactly stand for?

- L206-207: “This is a consequence of asymmetric strength and extension of the dynamical forcing, i.e., the stable layering of the stratosphere prevents deeper mixing into the stratosphere, whereas the lower static stability in the troposphere allows for deeper penetration of stratospheric tracers into the troposphere” → I am not sure whether I fully understand this argument. First, what exactly is ‘dynamical forcing’ referring to? The discussion in the ‘i.e.’ sentence is more about stability than on dynamics. Second, the asymmetry argument would also be true in case 1?! Hence, also there the stably stratified stratosphere inhibits a deeper mixing than the more weakly stratified troposphere? Maybe, the solution to this is in the comparison of Figure 9d) with Figure 10d), which shows squared N and clearly differs between the two? In short, some further explanations might help (1-2 sentences).

- L218-221: Please explain in greater detail how the scatter from the diagonal relates to irreversible mixing. I think I kind of get the basic idea, but some further details could be helpful.

- Section 3.3.4: As discussed above, consider including into the three case study sections. L234-236 remains somewhat vague, and would – with some more specific conclusions – fit nicely into Section 4 (Conclusions).

- L240: Have TSE and STE already been introduced? Has STE been used in the sense ‘stratosphere-to-troposphere exchange’, or did it refer to cross-tropopause transport in both directions`?

- Section 4 (Conclusions): As discussed before, try to bring more specific statements into conclusions.