

Response to Reviewers

August 29, 2025

We thank the editor and referees for the comments. Reviewer comments are in **bold**, while our responses are in normal text.

Response to Reviewer 3

The authors have made an effort to implement the major comments, and I think the readability of the paper has improved as a result. However, I still have a question regarding the final comment about the Analysis of Mixing and Exchange. I understand that the delta tracer-tracer correlation is not suffering from the limitations of the traditional tracer-tracer correlation related to accumulation effects. Setting aside the issue of the method's applicability - since two experiments have to be performed to find the delta tracer-tracer correlation - the authors might address the issue raised in question 5 of the original review: Can the fluxes be computed directly from the simulation data and used to support the findings not from the tracer-tracer but from delta tracer-tracer correlations.

As mentioned in the previous response, the delta tracer-tracer correlation shows the accumulation of a single process on the tracers, while the fluxes calculated by the COSMO turbulence scheme show the instantaneous mixing, at that time step. First of all, it will be impossible to output and store all of the fluxes at every time step. Second, it will most likely show something similar to the TKE or the mixing coefficient, basically showing the region where mixing happened. The delta tracer-tracer correlation or the cross-section of the difference plot (figure 8) shows the consequence/accumulation of the mixing, taking the meteorological conditions into account. Unless we are in an ideal situation where only vertical mixing will modify the tracer distribution (without any horizontal advection from previous potential vertical mixing upstream), we can directly use the fluxes to compute the tracer mixing. Otherwise, the fluxes cannot directly determine the tracer mixing.

Response to Editor

1) Motivation and scientific question - As it comes now, the manuscript does not convey a sufficiently new or important message. The importance of UTLS composition, of the role of turbulent mixing in shaping it and of the issue of how well high-resolution simulations can capture it, is beyond any question. However, after reading your manuscript I am struggling to disentangle the motivation and goal of your manuscript. Was the aim to produce a detailed case study of turbulent events above Scandinavia? To test the skill of high-resolution simulations for turbulent mixing in UTLS? To test the performance of the parameterisation and get more insight in how the turbulence scheme by Doms et al works? Or to introduce a

novel delta tracer methodology for analysing the mixing in the models?

The key focus of our study is the representation of tracer mixing in the UTLS by turbulence in relatively coarse grain models. We conducted a systematic analysis of the impact of turbulence on tracer mixing in model simulations, which, to our knowledge, has never been published in such a detailed way. Most of the literature focus on turbulence in a dynamical point of view, but not the impact of the turbulence on tracer mixing. We are not trying to analyse the turbulence representation itself but rather the representation of turbulence and related tracer mixing. We analyse if the tracer mixing can be either deduced from the tracer gradient or other related forcing. We reformulate in the introduction from

Considering the increasing trend of CAT, and the link between turbulent mixing and STE, and hence the radiation budget, it is crucial to investigate the relation between CAT and mixing of chemicals in the UTLS. The main objective of this study is to analyse the representation and the efficiency of turbulent tracer mixing in the UTLS utilising the multi-scale climate chemistry model MECO(n).

to

Considering the increasing trend of CAT, and the link between turbulent mixing and STE, and hence the radiation budget, it is crucial to investigate the relation between CAT and mixing of chemicals in the UTLS. However, previous studies mainly focus on the dynamical aspect of turbulence (Kaluza et al., 2021; Muñoz-Esparza et al., 2020), but not on tracers. The main objective of this study is not to analyse the representation and strength of the turbulence itself, but to systematically analyse the impact of turbulence on tracer mixing in the UTLS. For that purpose, a novel diagnostic, namely the delta tracer-tracer correlation is used within the multi-scale climate chemistry model MECO(n). Consequently, the main objective of the study is on the resulting effects on the tracer distributions caused by turbulent mixing. Note to differentiate between the mixing itself, i.e., the "dynamical" mixing represented by e.g., the TKE, and the local effects on the tracer distributions provided by the mixing and the tracer gradient and further effects of the mixing, i.e., the downwind changes in the tracer distributions, originating from the mixing and subsequent processes, e.g., advection. Especially, the latter can further enhance vertical differences in tracer concentrations in case of modified vertical gradients of the respective tracers.

2) Do I understand correctly that you are interested only in the part of mixing that is unresolved by the model and is mediated by the Doms et al. (2018) parameterization scheme? If so, the scheme needs to be detailly introduced in the paper, including all the underlying physics and technical details and review of previous validation efforts of the scheme.

We are interested in how the parameterized turbulence by the Doms et al. (2018) impacts the tracer distribution. However, since we do not have any new model development on the scheme, it will be inappropriate to include the detailed description of the scheme in the manuscript. We have already briefly introduced what related mechanism the scheme is based on. The turbulence scheme is originally designed for and well-tested in the boundary layer. It is known that in turbulence schemes in other model like ECHAM5, which have originally been designed for the boundary layer, the turbulence is dampened in the free atmosphere, it does not change the tracer distributions significantly. Therefore, we would like to address how the COSMO turbulence scheme works on tracer mixing in the UTLS. Nevertheless, we extend the description of the used turbulence scheme from:

COSMO also provides another newer turbulent scheme based on prognostic turbulent kinetic energy. The K_ψ in this prognostic TKE-based scheme is determined by the Blackadar length scale, stability functions and the turbulent velocity scale which is based on the prognostic TKE

equation. The latter scheme is used in this study. Details for the turbulent schemes can be found in the documentation of the COSMO model by Doms et al. (2018).

into

COSMO also provides another newer turbulent scheme based on prognostic turbulent kinetic energy. The K_ψ in this prognostic TKE-based scheme is in the form of:

$$K^H = q\lambda S^H$$

$$K^M = q\lambda S^M$$

where K^H and K^M are the turbulent diffusion coefficients for heat and momentum respectively. They are computed by the corresponding stability functions for scalars (S^H) and for momentum (S^M) which are determined by the flux-Richardson number, the turbulent length scale λ (which is assumed to be the Blackadar mixing length) and the turbulent velocity scale $q = \sqrt{2\bar{e}_t}$ where $\bar{e}_t$ is the turbulent kinetic energy (TKE). The latter scheme is used in this study. Details for the turbulent schemes can be found in section 3 (3.3.2 for the used scheme) of the COSMO model documentation by Doms et al. (2018).

3) Thorough meteorological analysis of the case studies needs to be done, including identification of regions of dynamic (e.g. Ri) or static instabilities (e.g. using potential temperature contours).

We now added the Ri plots next to the horizontal wind plot as requested by the previous reviewer. The dynamics like vertical wind shear or static stabilities should be able to be derived from the color code of the scatter plot as well. We have rearranged the manuscript; instead of having a specific section for the synoptic situation, we merged it into every case study to improve the readability of the manuscript. The original section from L170–L190 also merge into the case study of case 1.

4)The methodology of computation of tracer-tracer and delta tracer correlations needs to be clarified, because right now it is not clear how they were constructed from the model fields (e.g. sampled over fixed volume regions over time of the simulation?)

We have now added a new section Delta tracer-tracer correlation to explain the concept of it. We added in the manuscript In order to investigate the tracer mixing in the UTLS, we introduced a novel diagnostic, namely a delta tracer-tracer correlation, which is a similar concept to the tracer-tracer correlation, but makes use of the model capabilities. While the tracer-tracer correlation can be compared to the real world, the delta tracer-tracer correlation is a correlation between the differences of the tracers from model experiments. Instead of showing the mixing as an accumulation affected by other processes, it shows the impact of a single process (and potential subsequent advection differences). It requires 2 pairs of tracers (one pair of stratospheric and one pair of tropospheric). The difference of each pair, is a particular process being deactivated on one of the tracers in the model to investigate the impact of it. In our study, it is the turbulent vertical diffusion (vdiff). The detailed released tracers are described in section 3.2. The delta tracer-tracer correlation can also be used to determine the direction of vertical mixing. Several distributions are expected for different scenarios: (1) Concentrated distribution at the center [0,0] if no vertical mixing takes place at all; (2) Diagonal distribution for bi-directional mixing, where both tracers change at a similar rate, causing the data point spread along the diagonal. The bi-directional mixing could be either balanced or imbalanced, meaning an even (case 1, spread equally from the center [0,0]) or uneven (case 2, spread unequally from the center [0,0]) spread along the diagonal. Balanced bi-directional mixing indicates a similar amount

of stratospheric tracers being exchanged with the tropospheric tracers, while imbalanced bi-directional mixing indicates a different amount of stratospheric tracers being exchanged with the tropospheric tracers. It could be attributed to different situations, details are discussed in the following cases. The upper left section of the diagram indicates the downward mixing of stratospheric tracers into the troposphere since at the same grid, there are increasing stratospheric tracers and decreasing tropospheric tracers. And the lower right quadrant indicates the opposite, with decreasing stratospheric tracers and increasing tropospheric tracers i.e. upward mixing of the tropospheric tracers. Scatter further away from the center indicates irreversible mixing, as the composition of the air masses is substantially modified, and the tracer is mixed irreversibly into the grid, i.e., instantaneously horizontally mixed. Additionally, this scatter is caused by initial differences from the mixing which are then amplified by (mostly horizontal) advection into regions where the vertical gradient of the tracers are different. Those different gradients can originate both from the tracer mixing event itself further upstream or from specific meteorological conditions, e.g., tropopause folds with strong gradients. Scatter away from the diagonal (case 3) indicates that the mixing occurs in a region with a different tracer gradient, a non-local effect introduced by other processes like horizontal advection acted on the mixed tracer. The scatter away from the diagonal gives an indicator that the mixing is non-local but the strength of mixing itself is still solely contributed by the turbulent mixing.

For the delta tracer-tracer plot in the manuscript, we plot every grid point between 100 to 350 hPa on the cross section that is indicated in Fig. 6, 12,15 (the plot of geopotential height).

In the updated manuscript we have now separated the synoptic section into each case with the location of the analysed case and added in the manuscript **It is conducted using every grid point between 100 hPa to 350 hPa at the indicated location on Figure 6.** to emphasize it. However, this diagnostic should theoretically be working for a different selection of the data, as long as the deactivated process is modifying the tracer in that dataset.

5) Section 3.1 does not have any good meaning and should be omitted from the revision. Definitely, the analysis presented cannot be used for the argumentation (however vague):” To conclude, the model is able to represent turbulence at a reasonable position (and time).” Or was the intention to test the skill of the Ellrod index in detecting the turbulence in the model?

We would like to keep the comparison between TI and TKE to show the consistency between grid scale wind field and the turbulence scheme. To test whether TI is able to detect turbulence in the model is part of the purpose. We have now also added a comparison with measurements to show the link between the model TKE and observation. We have now added in the manuscript **We also compare the model results with the last flight in the GW-LCYCLE II campaign (Witschas et al., 2023) on the 1st of February in northern Scandinavia. We derive a measure of turbulence from the high frequency measured N₂O (Lachnitt et al., 2023) and link it with the model TKE. We computed a 31-point running standard deviation normalized with the variability of the window for N₂O. The running standard deviation shows the N₂O fluctuation from the background in a short period of time while the normalization eliminates the effect of a tracer gradient due to the changing flight altitude or large-scale exchange of air masses. Figure 5 shows the model TKE at the flight time with the normalized running standard deviation of the measured N₂O. It shows that the derived turbulence signal often coincides well with the simulated TKE (figure 5a); the stronger signals (higher percentiles, figure 5b) coincide with the higher model TKE as well. This indicates that there is a reasonable degree of consistency between the derived turbulence signal from the measured N₂O with the simulated turbulence.**

We reformulated the argumentation from **To conclude, the model is able to represent turbulence at a reasonable position (and time)**

to

To conclude, the model grid scale wind field is consistent with the model turbulence scheme and can detect the occurrence of turbulence in the model.

L29 local changes in the energy budget

Corrected.

L30 affecting-*i* affect?

Corrected.

L67 the MESSy-fied - MESSy abbreviation has not been defined yet

Corrected

L129 conducted in the supplement

Corrected

L131 ..hence the mixing - a verb is missing?

Corrected to [hence the mixing is more frequent](#)

.. the Ellrod index does not fully representing?

Corrected to [fully represent](#)

Figure 5 and a majority of the following figures - the units are missing! Also what is the meaning of the (kg-1kg-1) unit? If the unit is indeed correct, why not to write kg-2?

The units is now added and corrected.

Caption of Fig. 5:.. difference (vdiff on - off) (c) Inverted O3-like tracers, (d)O3-like tracers at 2016-02-05 18:00. - Please rephrase for clarity.

Changed to [and \(c\) difference \(vdiff on - off\) of the Inverted O3-like tracers \(mol/mol\), \(d\) difference of the O3-like tracers \(mol/mol\) at 2016-02-05 18:00.](#)

L180-181:.. as the cross section of Figure 5. - in Figure 5? Btw. where is the cross-section located?

It is indicated in the map of geopotential height at the section of synoptic situation. It is now merged into each case studies for clarity.

L187 Figures 6c and 6d show Sections 3.3.2-3.3.4. define the tracer differences and the whole delta tracer-tracer correlation by equation and discuss the results more rigorously.

Figure 6c and 6d are the tracer-tracer correlation instead of delta tracer tracer correlation.

The intention of these graphs are to guide the readers before directly diving into the new delta tracer-tracer correlation. And therefore it is only discussed briefly.

L205.. The delta tracer-tracer correlation can also be used to determine the direction of vertical mixing. - but later in the text you mention only 1) no vertical mixing and 2) bi-directional mixing scenarios! Please pay attention to proper definition and discussion of mixing regimes, including balanced/unbalanced and reversible/irreversible regimes invoked later in the text. The part of the manuscript showing the results of delta tracer-tracer decomposed according to dynamical quantities and then normalized by the gradient is the strongest part of the paper that can elucidate how the turbulent parameterization works. But, more detail is needed how the plots were constructed.

They are now explained in the new section delta tracer-tracer correlation. We added in the manuscript In order to investigate the tracer mixing in the UTLS, we introduced a novel diagnostic, namely a delta tracer-tracer correlation, which is a similar concept to the tracer-tracer correlation, but makes use of the model capabilities. While the tracer-tracer correlation can be compared to the real world, the delta tracer-tracer correlation is a correlation between the differences of the tracers from model experiments. Instead of showing the mixing as an accumulation affected by other processes, it shows the impact of a single process (and potential subsequent advection differences). It requires 2 pairs of tracers (one pair of stratospheric and one pair of tropospheric). The difference of each pair, is a particular process being deactivated on one of the tracers in the model to investigate the impact of it. In our study, it is the turbulent vertical diffusion (vdiff). The detailed released tracers are described in section 3.2. The delta tracer-tracer correlation can also be used to determine the direction of vertical mixing. Several distributions are expected for different scenarios: (1) Concentrated distribution at the center [0,0] if no vertical mixing takes place at all; (2) Diagonal distribution for bi-directional mixing, where both tracers change at a similar rate, causing the data point spread along the diagonal. The bi-directional mixing could be either balanced or imbalanced, meaning an even (case 1, spread equally from the center [0,0]) or uneven (case 2, spread unequally from the center [0,0]) spread along the diagonal. Balanced bi-directional mixing indicates a similar amount of stratospheric tracers being exchanged with the tropospheric tracers, while imbalanced bi-directional mixing indicates a different amount of stratospheric tracers being exchanged with the tropospheric tracers. It could be attributed to different situations, details are discussed in the following cases. The upper left section of the diagram indicates the downward mixing of stratospheric tracers into the troposphere since at the same grid, there are increasing stratospheric tracers and decreasing tropospheric tracers. And the lower right quadrant indicates the opposite, with decreasing stratospheric tracers and increasing tropospheric tracers i.e. upward mixing of the tropospheric tracers. Scatter further away from the center indicates irreversible mixing, as the composition of the air masses is substantially modified, and the tracer is mixed irreversibly into the grid, i.e., instantaneously horizontally mixed. Additionally, this scatter is caused by initial differences from the mixing which are then amplified by (mostly horizontal) advection into regions where the vertical gradient of the tracers are different. Those different gradients can originate both from the tracer mixing event itself further upstream or from specific meteorological conditions, e.g., tropopause folds with strong gradients. Scatter away from the diagonal (case 3) indicates that the mixing occurs in a region with a different tracer gradient, a non-local effect introduced by other processes like horizontal advection acted on the mixed tracer. The scatter away from the diagonal gives an indicator that the mixing is non-local but the strength of mixing itself is still solely contributed by the turbulent mixing.

L243 ..figure 9d....figure 7d of case 1 have a similar N2 on both ends - You mean

11d and 9d?

Corrected

L255 2-;two

Corrected

L256 s most likely due to the advection, considering the completely different wind field in Figure 8 and tropopause in Figure S17 - This feature has to be disentangled (maybe a 3D resolved overturn encompasses the unresolved turbulence region) and the methodology suggested by Ref3 can help here.

We further compared the TKE and the mixing (difference of the tracer with/without vertical diffusion), the mixing is located at the downwind region of the high TKE values region, unlike the other two cases, where the mixing has a better correlation with the model TKE. This also proves what we replied to reviewer 3 that the mixing fluxes themselves do not necessarily represent the mixing since they only show the instant mixing effect but ignore the post-mixing accumulation by the meteorology. We now reformulate in the manuscript from

The scatter away from the diagonal unlike the other two cases is most likely due to the advection, considering the completely different wind field in Figure 8 and tropopause in Figure S17, the strong horizontal advection in the region of strong horizontal gradients changes the background ratios in addition to the vertical mixing and thus introduces additional mixing during each time step compared to the other cases.

to

The scatter away from the diagonal unlike the other two cases, where the modeled TKE is better correlated with the mixing (not shown), is due to the advection, the mixing shown in Figure S17 and S22 located at the downwind region of the high TKE region (Figure S21). In the earlier time, the mixing region (Figure S22, left panel) is more co-located with the high TKE region (Figure S21, left panel). After several hours, the mixing region (Figure S22, right panel) propagates to the downwind region while the high TKE region (Figure S21, right panel) remains at the same location. The strong horizontal advection in the region of strong horizontal gradients changes the background ratios in addition to the vertical mixing and thus introduces additional mixing during each time step compared to the other cases. The wider the scatter is, the more, e.g., tropospheric tracer depletion is found at similar stratospheric tracer values.

L262 ... such that the mixing is almost equally balanced. What does this statement about the mixing type mean?

The mixing type is now mentioned in the new section delta tracer-tracer correlation in the manuscript **Balanced bi-directional mixing indicates a similar amount of stratospheric tracers being exchanged with the tropospheric tracers, while imbalanced bi-directional mixing indicates a different amount of stratospheric tracers being exchanged with the tropospheric tracers.**

L272-273 To conclude, vertical turbulent mixing by CAT in the model simulations leads to an enhanced and significant tracer mixing in the UTLS region. - Is there any novelty in this statement? This seems to come from the definition of the turbulence parameterization.

Even though the general statement is not new, we now have a systematic proof that the model has a suitable representation of turbulence in the UTLS and it has a corresponding effect on

tracer redistribution.

L275-276 Strong dynamical forcing like vertical wind shear could lead to mixing even in the stable atmosphere with a typical stratospheric N^2 value. - This is a textbook knowledge, intensively studied under the term dynamic instability?

We now changed in the manuscript to [This confirms the findings of Kaluza et. al. \(2021\) and Kunkel et al. \(2019\) that strong dynamical forcing like vertical wind shear could lead to mixing even in the stable atmosphere with a typical stratospheric \$N^2\$ value.](#)

L280 provides a reliable tool - this was not assessed in the manuscript

We think that the model simulation now shows that we have reasonable turbulence and associated mixing, considering we have now added comparisons with the observation, we think it is a suitable tool. The manuscript now changed to [provides a suitable tool.](#)

L283 ..MECO(n) is presented.-¿ MECO(n), is presented.

Corrected

L286 .. balanced and imbalanced bi-direction mixing - balanced/imbalanced mixing has not been defined/introduced before. I had the impression that the motivation was to analyze the direction of mixing. Nevertheless, there is a great potential to define the different mixing regimes robustly and provide a systematic analysis on these aspects in the revision

We have added in the manuscript [Balanced bi-directional mixing indicates a similar amount of stratospheric tracers being exchanged with the tropospheric tracers, while imbalanced bi-directional mixing indicates a different amount of stratospheric tracers being exchanged with the tropospheric tracers.](#) in the section introducing the delta tracer-tracer correlation.

L287-289 The simulated turbulent kinetic energy (TKE) is spatially and temporally well matched with the (post-simulation) diagnosed Ellrod Index, showing the model is able to generate turbulence in the UTLS in agreement with the gridscale wind field data from the model output. - ¿ I assume that the Doms et al. parameterization has been validated before against observations.

We do not find any proper documentation where the UTLS turbulence in COSMO was compared against observation, since it was mostly designed and tested for the boundary layer. And sparse studies are focusing on the performance of the turbulence scheme in UTLS. We can only find one study from Muñoz-Esparza et. al. (2020) that tested it for WRF.

L293-294 ...which located near the tropopause (case 1) experiencing the strongest mixing considering the high vertical wind shear and tracer gradient. -¿ please rephrase.

Changed to [which located near the tropopause experiencing the strongest mixing due to the high vertical wind shear and tracer gradient \(case 1\)](#)

L295.. when measurement data is available. - you mean that there are not any data even from targeted campaigns existing that would be suitable for validating

the model?

Some measurement is available, but an ideal measurement data would be something like a pseudo-lagrangian measurement which can better distinguish between the mixing and the post-mixing effect. We now changed to [when a more comprehensive measurement dataset is available](#).

L300 .. both, the forcing or the pre-existing tracer gradients are the dominant drivers for the exchange. -¿please rephrase

Change from [Depending on the individual situation, both, the forcing or the pre-existing tracer gradients are the dominant drivers for the exchange.](#)

to

[Depending on the individual situation, either the dynamical forcing or pre-existing tracer gradients \(or both\) can be the dominant drivers for the exchange events.](#)

L302-305 These events can be irreversible, i.e., the exchange of tracers happens along the diagonal of a delta tracer-tracer correlation, leading to a disturbance of typical stratospheric or tropospheric chemical compositions in the respective parts of the atmosphere with implications for climate, e.g., via the radiative impact of exchanged species. - From the definition of a delta tracer-tracer correlation, these events are unresolved in the model and mediated by the parameterization, hence inherently irreversible. However, is this unresolved process the only irreversible mixing process in the model given that your resolution may be sufficient for resolving parts of the overturning?

In MECO(n), other sub-grid scale processes like gravity waves could potentially affect the dynamics of the turbulence, but the gravity waves themselves do not affect the tracer mixing ratios directly. As we are switching off the turbulence mixing for the specific tracers, the turbulence is the only irreversible mixing process for tracers in the model, beyond the subsequent advection which amplifies the changes originating from the parameterised vertical diffusion.