Authors' reply to ‚Report #2 by Referee #2'

The authors would like to thank the Referee #2 for the constructive and encouraging report.

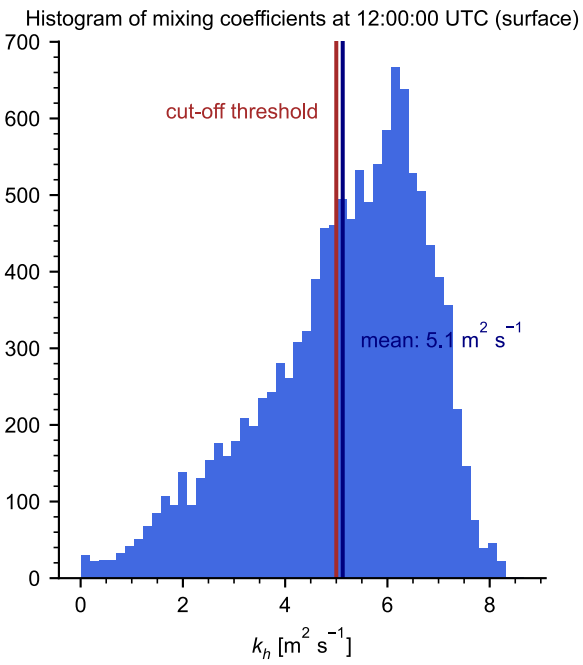
Below, the authors respond to the report point by point. The Referee's comments are printed in blue, and the authors' responses in black.

Major comments:

The clipping of the k_h would have also an effect during the day, near the top of the boundary layer, and it is plausible that k_h during daytime shows important variability and might be often below the thresold of 5 m2/s. I wonder if this could explain the significantly lower NO2 daytime concentrations of the run S-YSU+5, compared to S-YSU (Fig. 5)? This should be elucidated. My impression from the results shown is that overall, that "clipping" might be better than "no-clipping", but that the 5 m2/s threshold is a bit arbitrary and might be too high.

The Referee rightfully points out, that the mixing coefficient may fluctuate across the model domain and time, and may oftentimes fall below the clipping threshold.

At the surface, this is certainly the case, as demonstrated by the histogram below. The histogram was drawn for S-YSU at noontime at all locations of the UBA stations, i.e. the model cells from which the diurnal cycles in Fig. 5 and Fig. 6 were computed.



Clearly, the Referee's suspicion is correct: Enhancing the clipping threshold to 5 m^2 s^{-1} does affect daytime mixing (although much less than at nighttime) and this is certainly the cause of the differences observed between S-YSU+5 and S-YSU during daytime.

The authors agree that the clipping threshold could be deemed arbitrary. Here it was chosen to result in a reasonable trade-off between nighttime overestimation and noontime underestimation.

The Referee rightfully points out, that the clipping should affect the top of the boundary layer, where the average mixing coefficients are close to zero at all times of the day. This may result in slightly different model behavior in the 1500 - 2000 m altitude range. However, NO_2 concentrations are comparably low at such altitudes and a slight manipulation of the mixing strength in these layers is expected to be negligible in our validation study.

Sect. 3.1 was changed to mention the spatiotemporal variability of the mixing coefficient and the possible effects on daytime NO_2 concentrations at the surface.

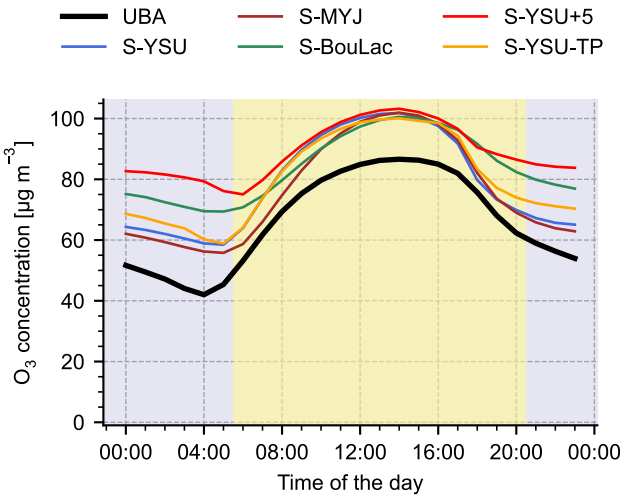
The histogram was added to the Appendix of the article.

My impression from the results shown is that overall, that "clipping" might be better than "no-clipping"

The authors would like to clarify that there is no case of „no-clipping" presented in their manuscript. The original WRF-Chem code already has clipping implemented. The simulation run S-YSU+5 only merely a higher clipping threshold.

Minor comments:

What does the clipping at 5 m2/s to the modelled ozone?



The left-side Figure shows the diurnal O_3 cycle at the surface for all relevant model runs.

Clipping the mixing coefficient to 5 m^2 s^{-1} **increases** the nighttime O_3 concentration (contrary to NO_2, which was found to be reduced instead).

This could relate to reduced titration via reactions such as $NO_2 + O_3 \rightarrow NO_3 + O_2$, which act as an O_3 sink at nighttime.

Notice that the same behavior is observed equally for all other model runs, for which the clipping threshold remained at its original value.

l. 374-375 "Based on the large uncertainties of mixing and chemistry during nighttime, it is more adequate to evaluate the model perormance during daytime": I had the impression that the discrepancies at nighttime were the main motivation for the S-YSU+5, so this statement is puzzling.

This statement refers to the fact, that the NO_x concentrations depend on NO, and the NO chemistry at nighttime seems to be somewhat misrepresented by the model (in particular, the build-up of the morning peak).

The sentence was removed from the manuscript, seeing that a full comparison (at nighttime / daytime / noontime) is presented directly afterwards anyways.

l. 462 Saying that total NO2 does not change at all is of course an exaggeration. Changing the vertical profile in the PBL has an impact on horizontal transport, deposition, and the convolution with the TROPOMI vertical profile of sensitivity. Please rephrase.

The sentence was rephrased to: „This is expected, seeing that in first order, the tropospheric column is a measure of total NO_2, which may vary only slightly across these simulation runs.“

l. 443 : No, the study of Poracu et al. did not derive corrections to the diurnal cycle of emissions.

Neither the attached file with marked-up differences, nor the revised version refer to Poraicu et al. in l. 443. The authors assume that the Referee is referring to l. 525 ff. (in the marked-up differences) instead. The authors have referred to what Poraicu et al. (2022) describe in their abstract:

„Using a mass balance approach, we determined a **new weekly profile of NO_x emissions** (…)“

It is therefore possible, that similar corrections will be derived for the diurnal temporal profiles in the future, which is the statement made in l. 525 ff.

l. 610: The justification for an overestimation is not convincing. Indeed, MAX-DOAS stations are located in cities, but the problem might be more an issue of representativeness than of biased emissions.

The authors have decided to remove the statement in question, seeing that a consistent overestimation of the MAX-DOAS data seems no longer evident. Except for the station „Uccle“, it can be argued that S-YSU+5 represents the MAX-DOAS data altogether without no significant positive bias.

All other minor comments and technical comments were taken into the revised manuscript as suggested by the Referee, without explicit mentioning.