Authors' response to referee comments on "Atmospheric odd nitrogen response to electron forcing from a 6D magnetospheric hybrid-kinetic simulation" by Häkkilä et al.

Please find below our answers (in blue) to the comments (in black).

Response to the comments of Referee #2

Review of "Atmospheric odd nitrogen response to electron forcing from a 6D magnetospheric hybrid-kinetic simulation" by Hakkila et al.
This study applies the WACCM model to simulate the effects of energetic electron precipitation in the Earth's thermosphere, mesosphere, and upper stratosphere, focusing on the impact on NOx and O3 levels. The study analyzes model runs with electron precipitation derived from magnetospheric hybrid-kinetic simulations using the combined Vlasiator and eVlasiator model framework. Additionally, comparisons are made with WACCM results incorporating simplified, nominal auroral precipitation maps parameterized by the geomagnetic Kp index (ranging from 0 to 5, with 0 indicating no auroral inputs). The findings indicate that auroral electron precipitation significantly enhances NOx concentrations during the polar winter, while its impact on upper stratospheric O3 is negligible. This study is very interesting, however, the following concerns need to be addressed.

Response to general comments: We thank the Reviewer for the insightful comments and questions regarding our manuscript. We appreciate the time taken to review our paper. We would like to point out a possible misunderstanding concerning the Kp parameterization. Setting the Kp index to 0 does not result in no auroral forcing in the parameterization, as can be seen in Fig. 4b. For this reason a separate reference run (REF) was necessary for comparisons in our study.

My biggest concern is that the electron precipitation estimated using Vlasiator-eVlasiator to drive the WACCM model seems to be fixed, not only spatially (precisely, in the geomagnetic coordinate system) but also temporally. This simplification significantly diminishes the potential benefits of using the sophisticated hybrid-kinetic simulation of particle precipitation, as compared to the simpler parameterization using the Kp index. Apart from a brief comparison of ion production rates in Figure 5, the study lacks detailed discussions that would adequately justify the preference for hybrid-kinetic simulations. To convincingly demonstrate the necessity and value of these complex and computationally intensive simulations, more comparisons and in-depth analyses should be conducted.

Electron precipitation is known to be highly variable energetically, spatially, and temporally. Our approach provides a unique methodology for the study of this auroral electron precipitation, as we employ a novel method for the production of the precipitating auroral electron fluxes through the use of Vlasiator. The Reviewer is correct in that this does not currently cover the temporal variability of the auroral forcing, but it does provide more information on the spatial and energetic distribution of the auroral electrons. This is a first step towards the use of more accurate electron driving in atmospheric simulations. Incorporating several eVlasiator runs with this now-proven methodology could allow for time-variable driving analysis, and in the future this could be used to produce more accurate parametric forcing of the polar MLTI.
We will add discussion on the ultimate usefulness of the the use eVlasiator in the revision. We will also expand the analysis of the ionisation rates in Section 3.1.2, and include analysis of momentary ionisation rates in addition to the daily averages currently shown in Figs. 4 and 5.

Clarifications regarding the Vlasiator-eVlasiator simulation are needed.

The proton-electron mass ratio is inconsistent between line 97 and line 115.

The mass ratio used in the 2D simulation in Alho et al. (2022) was larger than in the 3D simulation presented in this manuscript. The change was made to reduce computational costs. Differences between runs with different mass ratios were observed to be small, consisting of minor shifts in spatial structures.
We will clarify the manuscript to remove this confusion.

Lines 110-111: The upstream solar wind speed and electron temperature are significantly higher than typical values, while the solar wind density is considerably lower. Note that the obtained simulation results are used to drive the WACCM model over an extended period to represent typical precipitation conditions near Kp=1-2. Therefore, these settings are highly inappropriate.

We acknowledge that the driving conditions for the Vlasiator simulation do not match typical driving conditions. They represent conditions which are found during fast solar wind conditions, with a reasonable fast solar wind speed ensuring expedient initial condition formation, southward IMF to trigger efficient magnetopause reconnection driving global dynamics, and a low solar wind density in order to ensure the ion skin depth is similar to comparison 5D Vlasiator runs. A global 6D Vlasiator simulation requires significant computational resources to complete, and thus, it was not feasible to perform a new simulation (beyond the also-expensive eVlasiator run) for this purpose. As mentioned in Sect. 2.4.2, the driving conditions during the two DMSP overpasses used for scaling eVlasiator fluxes were associated with Kp values of 2 and 3.

Does eqn (1) specify the precipitating flux along the local magnetic field direction? Are magnetic mirroring effects considered?

The precipitating flux along the local magnetic field direction is specified by eqn. (1), and magnetic mirroring effects are considered. The bounce loss cone referenced on line 104 is the loss cone resulting from magnetic mirroring.

In Vlasiator, are electrons treated as a massless fluid?

Yes, in Vlasiator electrons are a massless charge-neutralizing fluid. Though considered massless and ensuring charge-neutrality, in MHD Ohm's law, the electron pressure gradient term is also included, assuming that inflow boundary electrons have equal temperature and density to solar wind ions, and that they evolve in an adiabatic fashion in the magnetospheric domain. This is a simplification, and the electron pressure term has only a minor contribution to global dynamics.

What are the boundary conditions near 4.8 RE? Do the models account for varying ionospheric conductances?

In the presented Vlasiator run, the inner boundary is a near-perfect conducting sphere with copy conditions for ion VDFs. A new ionospheric inner boundary, considering ionospheric conductances and field-aligned currents, is introduced in Ganse et al. (2024, https://doi.org/10.5194/gmd-2024-101). Using this model as a basis for eVlasiator runs in the future would be an interesting avenue of investigation.

The dates used for eVlasiator-DMSP calibration in line 135 are not consistent with the date used for magnetic field line mapping in line 356.

As explained in Appendix A, the date used for magnetic line mapping with the Tsyganenko 2001 model was selected to match equinox conditions, during which the geomagnetic dipole was almost perpendicular to the ecliptic plane. The reason behind this choice is that the used run of Vlasiator (and hence eVlasiator) for this study uses an untilted geomagnetic dipole. The geomagnetic activity level used as an input for T01 was chosen to be represented by a Dst value of –30 nT, consistent with mildly enhanced geomagnetic conditions as seen in the two DMSP overpasses. Note that our goal here is not to reproduce a real event, but rather to demonstrate a methodology, which is why we selected a parametrisation of the field line mapping as close as possible to the hypotheses (dipole alignment, driving conditions) used for the Vlasiator and eVlasiator runs.

Under the assumption of the non-tilted dipole magnetic field, the north-south asymmetry (in MLT-MLAT) is generally neglected, as seen in Figure 3. Explicitly clarify this in the text.

We will state explicitly in the text that lack of a dipole tilt will drastically reduce north-south asymmetry.

I don't understand how the calibration after the DMSP data along specific orbits can be useful, in physics. In particular, note that the calibration is temporally independent, while the model-data disagreement varies with time. Therefore, I suspect that even after applying the proposed calibration as in Figure B5, the ratio plots (similar to panels e-f in Figure B1 and Figure B2) will still show discrepancies of orders of magnitude.

It is inevitable that significant discrepancies still exist between the forcing data set (scaled eVlasiator precipitating electron fluxes) and the real measurements by DMSP. Indeed, as can be seen by comparing the DMSP observations shown in Figs. B1 and B2, the two events are characterised by order-of-magnitude differences, underlying how variable auroral precipitation can be despite similar driving conditions.
That being said, our aim in this study is not to obtain estimates of the atmospheric chemistry response to a given event, but rather to assess whether the long-term (over one year) forcing of the atmosphere by auroral electron precipitation using the Kp-based parametrisation of the fluxes can be improved by employing first-principle-based electron flux inputs. In that sense, scaling the eVlasiator fluxes based on two DMSP overpasses rather than only one helps in taking into account the high variability of electron precipitation. We do not expect to obtain a perfect match between the scaled eVlasiator fluxes and a given DMSP event, but we nonetheless try to reduce the discrepancy existing without the scaling (due to not all the processes leading to electron precipitation being present in eVlasiator).
While the results obtained in our study still have lots of room for improvement and have many limitations, we still want to emphasise that they are well beyond the current state-of-the-art, in the sense that eVlasiator is the first global model of near-Earth space based on solving the Vlasov equation for electrons and providing differential number fluxes of auroral electron precipitation. Further developments and improvements are naturally needed, but this study provides an initial evaluation of the benefits and shortcomings of our method to evaluate the atmosphere's chemical response to particle forcing associated with geomagnetic activity.

There are a few issues in atmospheric ionization calculations.

Line 176, the parameterization method of electron impact ionization is not applicable to incident energies below 100 eV. Nevertheless, it is adequate to consider only the incident energy range of 100 eV to 50 keV in this study, as <100 eV electrons do not penetrate below 140 km. See Fig 6.10 in Fang [2022], "Chapter 6.2—Fast calculation of particle impact ionization from precipitating energetic electrons and protons in the earth's Atmosphere" (https://doi.org/10.1016/B978-0-12-821366-7.00005-6)

Thank you for pointing this out. Indeed, spectral energy range of 50 eV to 50 keV is used in the ionisation rate calculation. The energy grid has 32 log-spaced points most of which can be seen in Fig. 2. Three of these energy grid points are below 100 eV. We have now removed those three points and calculated the atmospheric ionisation rates again. At the model altitude range considered here, i.e. below 140 km, the removal of <100 eV electrons from the spectrum does not change ionisation. As pointed out by the Reviewer, electrons with such low energy cannot penetrate below the model's upper altitude limit.
We have also re-examined the ionisation rates at the higher end of the auroral electron spectrum. Since the medium-energy electron (MEE) forcing in CMIP6, which was used in our WACCM simulations, already accounts for electron forcing at energies greater than 30 keV, we have also removed the eVlasiator derived auroral electron fluxes at energies 30–50 keV. This

avoids the possibility that the eVlasiator auroral forcing and the MEE forcing might partially overlap. The eVlasiator derived electron fluxes at these energies were so small, that this removal also had no significant impact on the results of our study. The final energy range of the eVlasiator-derived auroral electron input used in our WACCM-D simulation is 100 eV – 30 keV. As explained above, the adjustment of the auroral electron precipitation spectral energy range has negligible impact on the calculated ionisation rates and corresponding atmospheric response. We will add a brief discussion about this issue to Section 2.4.1 of the manuscript.

Line 177, the use of the NRLMSIS model for the ionization calculation introduces inconsistency with the WACCM-specified neutral profiles, especially for energetic electrons penetrating below 140 km. Are the resulting ionization rates above 140 km, as shown in Figure 2b, disregarded in the WACCM runs? If so, why not use the WACCM atmosphere directly to calculate the ionization?

The ionisation rate calculation requires an atmosphere which for the calculation was taken from the NRLMSISE-00 model. However, according to the CMIP6 procedure (Matthes et al., 2017), the ionization rates are then divided by the MSIS mass density which effectively removes the atmospheric “signature”. When the rates are used in WACCM, they are multiplied by the WACCM mass density profiles making the forcing consistent with the WACCM atmosphere.
We will note this in Section 2.4.1 of the manuscript.

Other minor comments:

Line 13, and throughout the paper, delete the space between numerical values and the percentage symbol (%).

We have used a space preceding the percentage symbol (%), as instructed in the International System of Units (9th edition, Section 5.4.7, https://www.bipm.org/en/publications/si-brochure).

Line 19, delete “unique”, or change to “particular”

We have changed this in the revised manuscript.

Line 30, change “solar energetic radiation” to “solar radiation”

We have corrected this in the revised manuscript.

Line 36, “There are three primary EPP sources of NOx”

We have changed this in the revised manuscript.

Lines 36-37, change “solar protons” to “solar energetic protons”

We have changed this to “solar proton events” in the revised manuscript.

In addition, what about “solar energetic electrons”?

Solar wind electrons do not have enough rigidity (momentum per charge) to penetrate the Earth’s magnetosphere and directly enter the atmosphere, unlike solar wind energetic protons which can enter the atmosphere at polar latitudes during big solar storms (referred to as solar proton events). Solar wind electrons are captured by the magnetic field of the Earth and stored e.g.

in the Van Allen radiation belts. The auroral electrons and the radiation belt electrons (or medium-energy electrons) therefore account for the precipitation of these electrons into the polar atmosphere. Though solar in origin, they are typically not referred to as solar energetic electrons, since they do not precipitate directly into the atmosphere but only after being energised by magnetospheric processes during magnetic storms.

Lines 42-43, rephrase the sentence. Auroral precipitation is a continuous phenomenon that occurs not only during substorms and has sources beyond just the magnetotail.

Thank you for pointing this out; we propose to rephrase this statement as follows in the revised manuscript: “Auroral electrons, with typical energies on the order of a few kiloelectronvolts, precipitate from the magnetosphere into the upper atmosphere in the polar regions, particularly along the auroral oval located most of the time between 60 and 75° geomagnetic latitude. While auroral precipitation occurs on a continuous basis, its flux is significantly enhanced during magnetospheric substorms, when the magnetotail is suddenly disrupted and launches a large number of electrons (and protons) of variable energies towards the ionosphere (Palmroth et al., 2017; Palmroth et al., 2023).”

Line 70, briefly explain “6D” (space and velocity space)

We have corrected this in the revised manuscript.

Line 74, what does “Cartesian 2D” refer to?

The mesh is discretised in Cartesian coordinates, and the spatial grid is 2-dimensional, the out-of-plane dimension having a thickness of a single cell only.

Line 81, what does “fields” refer to? It can easily be confused with “magnetic field” and “electric field”.

This indeed refers to both electric and magnetic fields. This has been clarified in the manuscript.

Line 86, the use of “at full strength” is not appropriate.

We have changed this to refer to actual strength. The reason this statement is included is to clarify that a reduced dipole strength, sometimes implemented in other global magnetospheric models, has not been used here.

Figure 1a, what does the color represent?

The colour represents proton pressure. We have updated Fig. 1a to include a colour scale and revised the caption.

Figures 1c-1e, what are the relative locations of the three points? Are they along one specific open magnetic field line? Why are the velocity space plots not organized in terms of parallel and perpendicular velocities? What findings are drawn from the comparison among these three plots?

The selected panels showcase the diversity of electron distribution functions found along those field lines which facilitate precipitation. They are provided for instructive purposes only. Maintaining the VDFs in Cartesian coordinates and indicating the magnetic field direction with an arrow showcases that they are from significantly different positions along the curved magnetic field line.

Line 128, swap the order of the two processes to align with the two items listed earlier in line 127.

Thank you for this suggestion; we will make the change in the revision.

Line 167, the sentence is confusing. What is the relationship between the NOEM-specified NO and the precipitating electron induced NOx at 140 km altitude? Is there any inconsistency here?

NOEM is used to set the upper boundary condition of NO concentration in WACCM simulations. This accounts for the production of NO at altitudes above WACCM's altitude range, and its exclusion would lead to a lack of NO at high altitudes. The use of NOEM in WACCM makes it necessary to set the Kp value for the VLAS simulation, as explained in Section 2.4.2 of the manuscript. We will try to clarify this further in the revised manuscript.

Lines 171-172, what is the relationship between "particle impact ionization" and "dissociative ionization"? What is "secondary electron dissociation"?

Particle impact ionization creates an electron-ion molecule pair (e.g. e and N_2^+), dissociative ionization also separates the ion molecule into an atomic ion and and a neutral atom (e.g. e, N^+, N). Further, if the created electron has enough energy, it can dissociate molecules itself. A review of these is given by Sinnhuber et al. (2012, https://doi.org/10.1007/s10712-012-9201-3).

Line 175, delete "temporal"

We have corrected this in the revised manuscript.

Line 185, briefly specify the recommended forcing conditions so that readers do not need to refer to the reference to understand the driving conditions.

The recommended CMIP6 solar and geomagnetic forcing, as used in this study, includes total and spectral irradiance as well as atmospheric ionisation rates resulting from solar protons events, medium-energy electrons, and galactic cosmic rays. This brief introduction is given in Section 2.4 (lines 162–166) of the manuscript. To avoid possible confusion and unnecessary repetition, we suggest restructuring Section 2.4, including its subsections, in the revised manuscript such that: (i) All descriptions of the WACCM simulations are combined into a single subsection 2.4.1, and (i) the production of the ionisation rates into subsection 2.4.2.

Line 195, I don't understand this sentence.

We suggest to reformulate this sentence in the revised manuscript as follows: "The eVlasiator-derived auroral electron forcing covers the full 24 hours of MLTs, and this forcing is repeated every day of the WACCM-D simulation."

Line 197, delete "and no Kp driven parameterized aurora", which is redundant

We have corrected this in the revised manuscript.

Line 197, it is my understanding that the REF run excludes auroral precipitation, but still includes SEP impact, according to line 263?

This is correct. All the WACCM-D simulations, including REF, include the recommended CMIP6 solar proton and medium-energy electron forcing. We have clarified this in the revised manuscript.

Line 206, how is the Kp index used to drive the VLAS run?

As stated in Section 2.4 (lines 166–168), NOEM uses the Kp index to determine NO at top of WACCM's altitude range. More precisely, WACCM makes use of NOEM to set the upper boundary condition of NO concentration. It is therefore necessary to set the Kp index for the VLAS simulation as well.

Line 220, I understand that these ionization rates are used to drive the WACCM model, not "from" the model.

Thank you for pointing this out. While the Kp-driven auroral electron forcing is calculated within WACCM based on the input Kp index, this is ultimately true. We have removed "from WACCM-D" from the title of Section 3.1.2 of the revised manuscript.

Figure 4, I don't see how altitude-integrated ionization rates can be useful. As dissociative recombination rates are altitude dependent, the efficiency of ionization in converting into ion/electron density increase also varies with altitude. This makes the integration of the ionization rate over altitude not meaningful.

The altitude-integrated ionisation rates are a measure of the total NOx production. NO production has been shown to approximately correspond to integrated ionisation rates with a factor of around 1.25, see, e.g., Nieder et al. (2015, https://doi.org/10.1002/2013JA019044) and Kirkwood et al. (2015, https://doi.org/10.5194/angeo-33-561-2015). It is true that the electron density resulting from the auroral ionisation is affected by the dissociative recombination. The NO density, however, is also affected by the recombination due to the balance of chemical production and loss, and transport. Nevertheless, we will update Fig. 4 to include the ionisation rates at select altitudes to better illustrate the vertical variability.

Line 233, what does it mean by "the lower boundary of the parameterization"?

This refers to the fact that WACCM's Kp parameterization of auroral electron forcing does not extend below about 95 km in altitude. We will clarify this in the revised manuscript.

Line 237, the polar cap excludes the auroral oval. You may want to change "polar cap averaged" to "polar averaged"

We will change this during the revision.

Line 269, where are the "troughs"? I cannot find them in Fig 7d.

The troughs are in reference to the upper stratosphere, depicted in Fig. 7f for the NH. Admittedly there is only one trough, not multiple. We will rephrase this to be more accurate in the revised manuscript.

Line 283, change "showing" to "due to"

We have changed this in the revised manuscript.

Line 293, change to "our results demonstrate the coupling between the magnetosphere and the atmosphere through electron precipitation", or something similar.

We will change this in the revised manuscript.

Line 303, change “at least” to “likely”

We believe that this would alter the meaning of the sentence, and cannot oblige in this instance.

Line 307, insert “be” prior to “considered”

We have corrected this in the revised manuscript.

Line 351, change “seed points” to “start points”? The word “seed” implies sources.

We will make this change in the revised manuscript.

Figure A1 caption, what are the thoughts behind the use of “7.5 RE”? In addition, change “Cartesian in MLAT-MLT” to “regularly spaced in MLAT-MLT”.

The value of 7.5 R_E used for field line tracing was empirically determined. Essentially, it ensures that this distance is sufficient to reach the transition region for all the closed field lines on the nightside in this run without extending unnecessarily far down the magnetotail or in the cusp for the open field lines. We will add this justification in the revised manuscript.

Figure B1 caption, “DMSP/SSJ (contour lines)”

We will make this addition in the revised manuscript.

Line 379, briefly explain why the high-energy component is missing

This is due to the sparsity threshold used in eVlasiator simulations, which discards velocity cells within which the phase-space density is below the threshold to keep the simulation computationally feasible. Since the phase-space density decreases near the edges of the velocity distribution, applying the sparsity threshold creates a sharp drop at those edges, which translates into a cutoff at high energies in the precipitating flux.
We will add this precision in the revised manuscript.

Line 399, delete “el cm^-2 s-1 sr^-1 eV^-1”? I think this is the ratio, not flux, that you are talking about.

Thank you for noticing this mistake; we will correct it in the revised manuscript.

Line 404 and throughout the paper, change “quantile” to “percentile”

Thank you for pointing out this language inaccuracy; we will replace “quantile” with “percentile” throughout the revised manuscript.