

Interactive comment on "Composition changes

after the "Halloween" solar proton event: the High-Energy Particle Precipitation in the Atmosphere (HEPPA) model versus MIPAS data intercomparison study" by B. Funke et al.

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We thank C. Randall for helpful comments and suggestions. The "Referee's Comments" are noted first and then we give our "Reply:" to the comment.

In my opinion this paper should be published in ACP after the following comments, most of which are quite minor and may or may not require any changes to the paper, are considered. The authors will note that several of my comments relate to a single C5504

issue, that of how to interpret the differences between WACCM, WACCMp, and MIPAS. The electron effects are relatively small, but the paper emphasizes in several places the "better agreement" that would be obtained if electrons were not included. Given the large uncertainties in other quantities, I do not feel that this emphasis is justified (see below for details).

Reply: We fully agree that a possible overestimation of the electron contribution to ionization cannot explain the encountered differences in the NOy enhancements alone. Differences in other quantities definitely play a similar or even more important role. We have revised the whole manuscript in order to weaken the importance of possibly overestimated electron ionization in explaining the encountered differences.

Specific comments:

Title (and abstract and throughout): There are inconsistencies in the way the "Halloween" storm(s) is (are) described. If referring only to the SEP that occurred on 28 October, the singular form should be used (as in the title). But if referring to more than one storm, the plural form should be used. Gopalswamy et al. (GRL 2005) could be cited for a description of the events, but it would also be very helpful if, near the beginning of the paper (at least by the time Figures 4-5 are described), a timeline of the ionization events were presented. This should include, for instance, a listing of the main proton and electron precipitation events. Although this is available elsewhere, it is necessary for interpreting the results presented in this paper, and would make it much more convenient for the reader if the information were all in one place in this paper.

Reply: We apologize for the inconsistencies in the use of the term "Halloween" storm/event. In the revised version, we use this term only for the strongest SPE period 28-30 October 2003. We refer to the second (minor) event on 3-5 November as the "second event". Further, we have included a short description of these events in Section 3.2 (discussion of Fig. 4).

p. 9409, lines 20-22. The abstract states that the simulated NOy enhancements near

1 hPa are typically 30 overestimation of simulated electron-induced ionization. The paper describes the uncertainties in specifying the electron ionization source, but in my opinion does not provide compelling evidence that these uncertainties are the main explanation for the overestimate. As noted below, the argument that agreement between MIPAS and WACCMp (no EEP) supports EEP being in error is very weak – this would only be the case if EEP was expected to have a negligible effect. On the other hand, there is a long discussion, starting on page 9438, of other possible factors that contribute to the model/measurement (and model-to-model) differences. If anything deserves mention in the abstract, I believe it would be these other arguments.

Reply: We agree that also other possible error sources than deficiencies in the electron ionization modeling should be mentioned in the abstract. However, the systematic behavior of the model biases hints at a problem with the common set of ionization rates, although not necessarily restricted to the electron contribution. Therefore, the discussion of reasons for the NOy model biases around 1 hPa on page 9438 has been extended to other possible errors in the ionization rate calculation. Differences of the true and modeled atmospheric background state and/or transport schemes might also contribute, as already discussed on pages 9438-9442. However, these differences are more likely to produce a model dispersion rather than a bias of the model average. For the revised version, we have re-worded the corresponding part of the abstract in order to account for all possible error sources. It now reads: "Simulated NOy enhancements around 1 hPa, however, are typically 30is likely to be related to deficiencies in the used ionization rates, though other error sources related to the modelsÊij atmospheric background state and/or transport schemes cannot be excluded."

p. 9418, line 2: Consider citing Orsolini et al. (2005) as independent confirmation (but with better vertical resolution) of the MIPAS results.

Reply: We have included a reference to the work of Orsolini et al (2005) in the revised manuscript.

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p. 9423, line 5: The atmospheric parameters upon which ionization rates depend were taken from HAMMONIA and MSIS. How representative are these for the actual conditions during the Halloween storms, and are they a significant source of error?

Reply: Uncertainties of atmospheric parameters (density, altitude, composition, and temperature) used in the AIMOS calculations could indeed produce significant errors in the modeled ionization rates. These parameters, taken from HAMMONIA and MSIS calculations, might differ from the actual atmospheric conditions during the Halloween SPE. For instance, up to 20 K differences between HAMMONIA and MIPAS temperatures show up in Figure 7. In the revised version, a discussion of this error source has been included in the paragraph on page 9438, dealing with possible reasons for the overestimation of modeled NOy enhancements.

p. 9430. Is SOCOL free-running, or nudged to ECMWF?

Reply: SOCOL and SOCOLi are free-running models. This has now been clarified by including "free-running" instead of "-" in Table 3.

p. 9434, top: I would argue that EMAC does a fine job below 1 hPa.

Reply: It is true that EMAC, though being nudged in the troposphere only (as HAMMO-NIA), does a good job below 1 hPa. For this reason, we only mention HAMMONIA (not both weakly nudged models) in the revised version when referring to an overestimation of stratospheric temperatures below 1 hPa.

p. 9434, lines 6-7. The text states that the stratopause temperatures are too high in several models. Since Figure 7 does not show the individual model results (as opposed to differences), this cannot be inferred from the figure. Is it clear that the stratopause temperature is too high, or is it possible that the stratopause height in the models is just shifted vertically from that observed?

Reply: Free-running models (B2dM and SOCOLi) and those which are nudged to meteorological in the troposphere only (i.e., HAMMONIA) tend to overestimate the observations inside the polar vortex by more than 15 K around approximately 1 hPa or slightly below, while polar mesospheric temperatures are considerably underestimated by these models (more than 25K in the case of SOCOLi). This behavior is related to a lower polar stratopause height (but similar stratopause temperatures) compared to the observations. Slightly too high stratopause temperatures are found in EMAC, CAO, B3dCTM, FinROSE, and WACCM simulations. These models also tend to have a higher stratopause compared to the observations, particularly in the case of WACCM. The KASIMA model yields generally good agreement with the observations in the polar regions, however, overestimates stratopause temperatures in the 50–60N region. In the revised version, the text has been updated accordingly.

p. 9434, lines 10-11. The text states that no significant trend can be observed in the models or observations. For the most part, this is true. Yet around 1 hPa or slightly above WACCM starts out near or slightly higher than MIPAS, and ends after 27 Nov with an 10-15 K low bias. This is interesting in that WACCM is nudged up to 40 km, which suggests that its temperatures near 1 hPa should be reasonable. It would be interesting to read a comment on this.

Reply: It is correct that WACCM is forced by MERRA/GEOS-5 meteorological reanalysis data up to 40 km. Above that level the forcing is reduced linearly, so that the model is free-running at altitudes higher than 50 km. In principle, temperature deviations at pressure levels above approximately 2 hPa (see also the second dashed line from bottom in Fig. 8, indicating the 40 km mean geometric altitude) could be related to the relaxed forcing above 40 km. Below, WACCM results show only small variations compared to the observations. Regarding the different temperature response of WACCM above 2 hPa compared to other nudged models, we recall that the latter are nudged to ECMWF reanalysis data, while the WACCM run is based on MERRA data.

p. 9434. Please define the CH4 meridional anomalies (i.e., to what are the anomalies referenced?).

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Reply: The relative meridional anomaly is defined as percentage deviation from the 40-90N average at each vertical level. This definition has been included into the revised version.

p. 9435, lines 18-19. To say that the general behavior of CH4 is qualitatively reproduced by the models seems to be an overstatement, given that several of the models predict very different (opposite) behavior in the mesosphere.

Reply: We agree that the agreement between the observed and modeled temporal CH4 variations is rather poor, particularly in the mesosphere. We have therefore weakened this statement in the revised version by stating: "This general behavior is partly reproduced by the models but important differences with respect to the vertical structure and magnitude exist".

p. 9435, last paragraph. This explanation seems to leave out the possibility that NOx might be produced via particle ionization in air that has already descended. Thus air with high CO and high NOx does not *necessarily* indicate descent of a NOx enhancement. Is it possible that by neglecting these air masses, you are underestimating the actual particle effects?

Reply: We agree that our method does not allow for distinguishing the NOx content in descended air masses that has been produced in the upper atmosphere prior to the descent from that produced in situ by high-energy particle precipitation. We only know that air masses with high CO abundance are likely to be affected by EEP indirect effects. These indirect effects, however, are not well represented in atmospheric models in general. For models not including the lower thermospheric source region this short-coming is evident. But also models with higher lids tend to underestimate the indirect EEP contribution for reasons that are currently not fully understood. Therefore, we prefer to exclude these air masses from the intercomparison in order to avoid potential biases. Regarding the possible underestimation of actual particle effects, but it does

so in both model and observations. We would like to recall that the aim of our study is to assess the ability of atmospheric models to reproduce SPE induced composition changes, not to assess the magnitude of these changes itself.

p. 9438, lines 16-18. Referring to the NOy overestimate near 1 hPa, the text states, "A possible overestimation of electron ionization is also supported by the better agreement of the WACCM simulation without electrons (WACCMp) with the observations." This would only be the case if you really do not expect a significant effect from electron ionization. Although the quantification of the electron effect is uncertain, as described well in the text, is it really expected to be negligible? If this can be supported, it would be an important conclusion. But given the large spread in the model results at 1 hPa, which (as written) suggests that something else is causing large errors, there seems to be little, if any, justification for inferring such a conclusion. I therefore suggest deleting this statement.

Reply: In the revised version, the corresponding paragraph reads: "A possible overestimation of electron ionization alone, however, cannot explain the mismatch between modeled and observed NOy increases of up to 50(WACCMp) yields 20electrons. Even when assuming that electrons do not contribute to the SPE-induced ionization at stratospheric altitudes, only about half of the differences between modeled and observed enhancements could be explained. Additional ionization by alpha particles, included in CAO, FinROSE, SOCOL, and SOCOLi contributes only by approximately 5within 40–90N, hence increasing the SPE-related NOy enhancements only marginally. Other possible error sources in the ionization rate calculation are related to uncertainties of the GOES proton flux observations and to the spatial interpolation scheme for particle fluxes. Also, uncertainties of atmospheric parameters (density, altitude, composition, and temperature) used in the AIMOS calculations could produce errors in the ionization rates. These parameters, taken from HAMMONIA and MSIS calculations, might differ from the actual atmospheric conditions during the Halloween SPE. Apart from possible deficiencies in the ionization rate calculation, also differences of the true and

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modeled atmospheric background state and/or dynamical conditions could contribute to the encountered model overestimation of NOy enhancements. However, such differences are likely to produce a spread in the modeled NOy increases rather than a systematic bias compared to the observations."

p. 9442, lines 10-15. Related to the last paragraph on p. 9435: doesnÊijt this (excluding model and observed NOy profiles where MIPAS CO was higher than 1 ppmv) ignore air parcels that had descended and subsequently experienced particle ionization? Also, given the very poor agreement shown in Figure 14, I would question whether the geographic locations of the COenhanced air parcels observed by MIPAS are the same as in the simulations. If they are not, is the exclusion of profiles based on MIPAS CO values really effective? I think that this could (should) be easily checked (not necessarily presented) by making a figure similar to Figure 14, but for CO.

Reply: Regarding the first point, see reply above. Concerning the possible mismatch of modeled and observed CO-enhanced geolocations, we agree that this could be an issue. However, pronounced NOx-descent related to EEP indirect effects occurs only in the observations. None of the models simulate a significant indirect EEP NOx increase in the vertical range of interest throughout November. In this sense, the filtering is principally relevant for excluding the observed CO- and NOx-enhanced air masses.

p. 9442, line 18. The text states that Figure 15 shows the NOy enhancements "related to the SPE, only". Perhaps I have a misunderstanding (which would also be reflected in my last comment) – to what does "the SPE" refer? Is it only proton ionization? Is it proton + electron ionization, but only during the SPEs in late October and early November? This could perhaps be clarified by referring directly to Figure 4.

Reply: We refer to direct (i.e., in situ) NOx production in the stratosphere and mesosphere related to high-energy protons and electrons during the Halloween events. We are not interested in NOx production at higher altitudes before the event that might have descended into the vertical range of interest during the period of 26 October – 30 November. In the revised version, this has been made clearer by stating in the caption of Fig. 15: "Note that observations exhibiting CO abundances higher than 1 ppmv have been omitted in the averaging in order to exclude the contributions from descended NOx produced by EEP at higher altitudes before the Halloween stroms." In the body text, we will state, "Figure 15 shows the temporal evolution of the observed and modeled NOy enhancements (related to the SPE-induced in-situ production, only)".

p. 9442-9443. The last paragraph on 9442, which continues onto page 9443, discusses the overestimate of NOy by WACCM, attributing the overestimate largely to the "excess production during the second event" from electron ionization. WACCMp matches MIPAS quite well for most of the time period, below about 0.2-0.3 hPa, which leads the authors to conclude that the electron ionization must be in error. But rather than matching, shouldnÊijt there be a persistent underestimate in WACCMp, since it neglects the electron source? I agree that electron ionization errors are likely contributing to the overestimate. However, in keeping with my previous comments, it is not clear to me that the electron errors are necessarily any worse than other contributing errors.

Reply: We agree that the better matching of WACCMp with MIPAS (compared to the nominal WACCM run) does not necessarily imply that electrons do not contribute at all. Nevertheless, the very good agreement of WACCMp and MIPAS is worth to mention. Further, the comparison of WACCMp and WACCM allows for the identification of the electron-related contribution to the excess NOy layer descending in the course of November. In the this sense, we have re-written the paragraph in the following way: "It is interesting to notice that the WACCM simulation without electron-induced ionization yields better agreement with the observations than the nominal simulation throughout the period under investigation (see Figure 16). Additional NOy buildup related to electron-induced ionization is even more pronounced during the second event (4–5 November) below 0.4 hPa compared to the main proton forcing (see right panel of this Figure). The NOy increase caused by electrons during the second event contributes with 5–10ppbv to the excess NOy layer, descending during the following weeks."

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p. 9451, last sentence. The text notes that the model simulations overestimate the seasonal buildup of ozone in the mesosphere. What conclusion should be drawn from this? Related information is given on the bottom of page 9453, but the implications of the results are still unclear.

Reply: The principal conclusion to be drawn from the overestimated seasonal ozone buildup in the mesosphere is that it masks residual (HOx-related) ozone depletion induced by the SPE. This has been added to the revised version. A detailed investigation of the encountered differences in the seasonal ozone buildup among the models and the observations is beyond the scope of this paper, though an interesting topic for future studies.

p. 9452, lines 15-16. The text once again points out the better agreement with MIPAS of WACCMp than WACCM. Although the implication is unstated, the reader is left to infer that the conclusion to be drawn from the results is that the contribution to ozone loss by electron precipitation is negligible. As noted above, it is not clear that the results support this conclusion.

Reply: We have deleted the sentence "It is interesting to notice that the agreement of the WACCM simulations with the observation is better when excluding the electron contribution" in the revised version.

p. 9453, lines 13-15. Similar to my previous comment: The text states that the differences between WACCM and MIPAS "could be significantly reduced when excluding the electron contribution to atmospheric ionization." That is a true statement, but is excluding the electron contribution justified?

Reply: In the revised version, we have deleted the sentence "WACCM simulations with and without electron-induced ionization, however, suggest that these remaining differences could be significantly reduced when excluding the electron contribution to atmospheric ionization"

p. 9454, lines 8-11. This repeats the statement that "agreement between models and observations could be [even] improved when excluding the electron contribution to atmospheric ionization." While the agreement might be improved, is it improved for the wrong reason?

Reply: In the revised version, we have deleted the sentence "On the other hand, WACCM simulations with and without electron-induced ionization suggest that the agreement between models and observations could be even improved when excluding the electron contribution to atmospheric ionization"

p. 9462, middle paragraph. Same issue as above. In order for this paragraph to warrant so much space in the conclusions, it is necessary to show that WACCMp agrees better with MIPAS for the right reasons; that is, that electron ionization really should not be a significant contribution. Otherwise, turning off the electron precipitation is just a proxy that compensates for some other source of error.

Reply: Related statements have been deleted in the corresponding paragraph of the revised version that reads now: " Simulated NOy enhancements around 1 hPa are on average 30 higher than indicated by the observations, while an underestimation of modeled NOy of the same order was found in the mesosphere. The systematic behavior in the stratosphere suggests that these differences are related to the simulated ionization rate profile shape, though other error sources related to the modelsÊij atmospheric background state and/or transport schemes cannot be excluded. WACCM simulations without inclusion of electroninduced ionization allowed for distinguishing the electron and proton-related contributions to the NOy enhancements. An upper stratospheric excess NOy production by electron-induced ionization of 5-10 ppbv (20these simulations, particularly after the minor second event around 4–5 November."

Figures:

The text in Figures 1-3, 15, and 25-26 is so small that it is very, very difficult to read when printed. Also, the white dashed lines often disappear, so they should be made

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thicker.

Reply: We agree that Figures 1-3, 25, and 26 are very small and difficult to read in the ACPD version. These figures will be significantly enlarged in the final version (ACP formatting).

Figure 3 labels: Chlorine should have a lower case I, not upper case.

Reply: The labels of Figure 3 have been changed accordingly.

Figure 6. Is the middle panel WACCM with application of averaging kernels? This would seem to contradict the sentence on the top of page 9433 that states, "...as modeled by WACCM with and without application of averaging kernels. In the latter case, the vertical distribution is broader and slightly shifted towards lower altitudes." Perhaps this should say "In the former case."?

Reply: The Reviewer is right. The text has been changed accordingly.

Figure 12 caption: Omit "model" before "multi-model mean". Also, it appears as though the single model, SOCOLi, is skewing the model results. Would a median be more representative of the models?

Reply: "model" before multi-model mean has been omitted. We also checked the use of a median value and it turned out that differences with respect to the arithmetic mean are not very pronounced.

Figure 14 description (page 9441). This figure shows exceptionally large discrepancies between the models and MIPAS. Yet it gets relatively little discussion in the paper. Most of the discussion centers on the SOCOLi results, which appear to be anomalous even among the very disparate results from the other models. This figure seems to be pointing to a systematic flaw in the models, and in my opinion deserves more discussion. Perhaps the description of SOCOLi was supposed to be illustrative of what is wrong with all of the models; if so, this should be made more explicit. Reply: We have extended the discussion of this figure, including the other extreme of modeled NOy distributions; being B2dM with extremely pole-centered NOy increases. Figure 14 highlights one of the less expected result of our study, namely, that transport processes are very important for the overall NOy budget even on the time scale of only a couple of days. The added text to the revised version reads: "On the other hand, B2dCTM shows the most polecentered NOy distribution among the models. As a consequence, NOy enhancements in the 70–90N region reach highest values of up to 60 ppbv (twice as much as observed), although the 40–90N average (see Fig. 12) is below the multi-model mean at this pressure level. This behavior is related to the very strong but small vortex in this particular model, probably as a result of its relatively poor horizontal resolution. The high dispersion in the latitudinal extent of the modeled NOy distributions, showing up already two days after the onset of the main proton forcing, is rather unexpected and highlights the importance of transport processes on a very short timescale."

Figure 21 caption: The caption states that differences between modeled and observed averages are shown, but I think that only the changes in N2O5 since 26 October are shown. Reply: The Reviewer is right. The caption has been changed in the revised version accordingly. Figure 22 caption: Same issue as with Figure 21.

Reply: As above.

p. 9425, line 7: Is it really 3402 K, not 3400 K?

Reply: Yes, 3402 K (in terms of potential temperature) is the correct upper lid of B3dCTM.

All other encountered typos and/or suggested technical corrections have been corrected/included.

Interactive comment on Atmos. Chem. Phys. Discuss., 11, 9407, 2011.

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