

## ***Interactive comment on “Denitrification, dehydration and ozone loss during the Arctic winter 2015/2016” by Farahnaz Khosrawi et al.***

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We thank reviewer 2 for the constructive, helpful criticism and the suggestion for revision. We followed the suggestions of reviewer 2 and revised the manuscript accordingly.

*Khosrawi et al. present a detailed analysis of polar processes occurring at high northern latitudes during the Arctic winter 2015/16. In particular, they compare simulations carried out with a nudged version of the EMAC CCM with a range of satellite and aircraft observations. The analysis presented in the paper is of high standard and explores an important and relevant topic within the scope of ACP and as such merits publication following revision. I have several comments the authors should address before publication:*

*General Comments:*

P5L25 The authors present their analysis averaged over a fixed latitude range (70-90N) rather than using a vortex following coordinate (e.g. by defining the edge of the vortex following Nash et al., 1996). Figure 12 in the manuscript shows the large zonal variation in temperature and chemical fields, and highlights that the vortex is neither centred on the pole nor circular. I wonder what effect using a fairly large area average has on the results compared to averaging only within the vortex. While I do not feel it necessary to redo the analysis in any way, I would like to see a discussion on how using a fixed latitudinal average may affect the results of the paper compared to only considering airmasses within the vortex.

In our analyses the usage of equivalent latitude is not mandatory since the separation between dynamics and chemistry is done by using the difference between the active (chemistry+dynamics) and the passive (dynamics only) tracer. However, in the frame of our analyses we have calculated ozone loss within an equivalent latitude band as well as within a geographic latitude band in order to quantify the differences in estimated ozone loss between the two approaches. Figure 1 and 2 in the supplement to this reply show ozone loss in mixing ratio and Dobson Units for both latitude and equivalent latitude. In terms of mixing ratios the result is almost the same (2.1 ppmv compared to 2.03 ppmv) while in Dobson Units the ozone loss on equivalent latitudes is approximately 10% lower (117 DU compared to 103 DU). Figure 3 shows that there are slight differences between the O<sub>3</sub> column time series between latitude and equivalent latitude, but that our result remain the same, namely that in contrast to the other recent Arctic winters very low O<sub>3</sub> values are found in 2010/2011. We added the following text in section 3.4: *Note that, rather than employing a vortex following coordinate as e.g. equivalent latitudes, we have chosen to perform our analyses on a fixed geographic latitude band. Such an approach is justified here because the use of a passive tracer allows dynamical and chemical processes to be separated, thus facilitating the quantification of chemical ozone loss. On equivalent latitudes the same amount of ozone loss in terms of mixing ratio is derived while in terms of column loss ozone loss is 10% less (103 DU).* In the

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conclusion the following text has been added: *Note that we did not use equivalent latitudes here since separation between chemical and dynamical processes is achieved via the passive O<sub>3</sub> tracer. On equivalent latitudes the same amount of ozone loss in terms of mixing ratio is derived while in terms of column loss ozone loss is 10% less (103 DU)*

*P3L22 While the authors have reference all the appropriate literature on the model configuration and description, and a detailed description of the EMAC model is not required, I would like to see further information on those parts of the model key to this paper. For example, section 2 should, in my mind, include a description of which PSC and aerosol types are included in the model, how sedimentation velocities are calculated, which heterogeneous reactions occur on aerosol surfaces, do uptake coefficients include temperature dependencies, etc. I feel this would significantly aid those not familiar with the EMAC CCM configuration.*

We agree that it would be worthwhile to provide more information on the parts of the model that are key to this paper. We added the following text briefly describing the PSC scheme and referring to Kirner et al. for more details: *The submodel MSBM simulates the number densities, mean radii and surface areas of sulphuric acid aerosols and liquid and solid polar stratospheric cloud particles. The formation of STS particles is calculated according to Carslaw et al. (1995) through the uptake of HNO<sub>3</sub> and H<sub>2</sub>O on the liquid binary sulphuric acid/water particles. Ice particles are assumed to form homogeneously at temperatures below T<sub>ice</sub>. For the simulation of NAT particles the “kinetic growth NAT parameterisation” is used. The “kinetic” parameterisation is based on the growth and sedimentation algorithm given by Carslaw et al. (2002) and van den Broek et al. (2004). The vapour pressure over ice is calculated according to Marti and Mauersberger (1993) and the vapour pressure over NAT according to Hanson and Mauersberger (1988). NAT formation takes place as soon as a supercooling of 3 K below T<sub>NAT</sub> is reached. The sedimentation velocity of ice particles is calculated according to Waibel et al. (1997) and for NAT particles according to Carslaw et al. (2002). Eleven heterogeneous reactions that occur on the surfaces of liquid and solid PSC particles are considered. A comprehensive description of the submodel MSBM can be found in Kirner et al. (2011).*

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*Specific Comments:*

*P1L3 There is no need to capitalize polar stratospheric clouds here, and it should appear instead as it does in the Introduction (P2L10). However, in the Introduction it should read PCSs within the brackets.*

This has been corrected.

*P1L18 This is at odds with P7L32, where the authors state maximum ozone loss is 120 DU. While 2 ppmv is the maximum mixing ratio difference, 100 DU is more representative of the average loss over mid March, and does not represent the maximum column loss. This also applies to the conclusions (P11L19).*

Thanks a lot for pointing this out. It should of course be the same amount of ozone loss in Dobson Units in all places of the paper. The exact amount is 117 DU. This has been corrected throughout the paper.

*I feel as well that it would be good to combine figures 7 and 8 so that total column differences appear below the  $\Delta O_3$  plot in a single panel and the reader can compare the column loss with the altitudes at which this is occurring.*

We would prefer to not combine figures 7 and 8 since these figures show ozone loss in different units, namely DU and ppmv and combining these may be confusing for the reader. However, to make a comparison of these figures easier we adjusted the time axes of figure 8, so that both figures have the same time scale.

*P3L4 I feel that having defined  $T_{\text{NAT}}$  and PSC, these should be used consistently throughout the manuscript in place of NAT existence temperature and polar stratospheric clouds.*

We agree and now the abbreviations  $T_{\text{NAT}}$  and PSCs are used consistently throughout the manuscript.

*P7L12I feel  $\Delta H_2O$  should be defined in the text as  $\Delta NO_y$  and  $\Delta O_3$  are. In fact, I feel each should be specifically defined in the text and figure captions (i.e. state  $\Delta O_3 = O_3 - O_3^*$ ).*

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We followed the suggestion and each of the deltas are specifically defined in the text and figure captions.

*P9L3 Is the Khosrawi et al. (2017) paper in prep, which it is in the reference list, or now published? If so this should be stated in the text. Further, if the paper is not yet available I do not feel that the reference should be included in this manuscript and reference to it removed (i.e. removed the sentence on P9L2-4. This also applies to the papers referenced on P10L27-28. Certainly they should say they are in prep if they are not yet published, and further if the findings of those studies are not key to this paper I do not feel they should be included.*

We agree and removed the sentences referring to Sinnhuber et al. (2017), Braun et al. (2017) and Johansson et al. (2017) since these studies are not key to this paper and it is not yet clear when these papers will be submitted and published. We would like to keep the Khosrawi et al. (2017) reference since this paper is ready for submission, but kept on hold due to the new MIPAS PSC product which is not published yet. We anticipate to submit this paper in autum. Therefore, we changed the status in the reference list from “in preparation” to “to be submitted”. Contrary to other journals as e.g. JGR, in the Copernicus journals the papers not published yet are listed with all other references in the reference list.

*P9L14 The simulations presented in the study are described as nudged in section 2. Therefore, surely any difference in temperature between the model and observations is a result of the nudged dataset and not the model. I feel saying ‘temperatures as simulated with EMAC tend to be slightly warmer than measured outside the polar vortex’ is misleading, as the temperature field is not being simulated freely. Presumably, in a free-running model the temperature biases would be significantly different.*

It is correct that the simulated temperatures in EMAC mainly reflect the temperature field of the meteorological analyses used for nudging the simulation. However, the EMAC temperatures and the temperatures from the ECMWF operational analyses, used in our analyses for nudging, are not 100% identical although they are very similar.

The EMAC temperatures are not replaced by ECMWF operational temperatures, but the internally calculated EMAC temperatures are pushed toward the ECMWF operational analyses. Therefore, small differences between EMAC and ECMWF remain. We changed the sentence as follows: *Temperatures in EMAC (nudged towards ECMWF operational analyses) tend to be slightly warmer than measured outside the polar vortex.*

*P9L28 Without providing further information this a difficult conclusion to follow. Can the authors be sure that chlorine activation is not just too weak? The assertion in the manuscript reads as though the chlorine activation is correct, but petitioning between other active chlorine species is the cause of the low ClO values, indicating too high Cl, Cl<sub>2</sub>O<sub>2</sub> etc. Can this be demonstrated by showing that ClONO<sub>2</sub> and HCl are well simulated? Looking at these species should highlight the ability of the model to capture chlorine activation. Here also ClO<sub>x</sub> should be defined.*

It is correct that a possible explanation could also be that chlorine activation is just too weak. We know from other comparisons that there are also differences between the simulated and measured HCl and ClONO<sub>2</sub>. Further, comparisons between different photolysis schemes performed by our colleagues at KIT (M. Sinnhuber and S. Versick) have revealed that the EMAC photolysis rates are too low at high solar zenith angles (>90°). ClO<sub>x</sub> is now defined in the text and the discussion on the differences between EMAC and MLS in ClO has been changed as follows: *However, the enhancement of ClO<sub>x</sub> (ClO<sub>x</sub>=Cl+HOCl+2·Cl<sub>2</sub>+2·Cl<sub>2</sub>O<sub>2</sub>) in the EMAC simulation is found at the same time as in the Aura/MLS ClO observation, thus indicating that the later increase in ClO is not necessarily caused by the activation of chlorine being too late in the model simulation but could also be caused by the partitioning between the active chlorine species. In EMAC the photolysis rates are calculated with the submodel JVAL (Section 2.1). JVAL is part of the standard configuration of EMAC that was also used in the EMAC simulations contributing to the Chemistry-Climate Model Initiative (CCMI, Jöckel et al., 2016) (note a similar configuration is used here apart from the resolution). An intercomparison of several photolysis scheme has*

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shown that JVAL provides lower photolysis rates at very high solar zenith angles ( $>90^\circ$ ) for e.g.  $\text{Cl}_2\text{O}_2$  than other schemes. Thus, the partitioning of chlorine containing species may be shifted for high solar zenith angles and thus could be the cause for the delay in the activation of ClO in the model simulation. However, to entirely rule out the cause for this difference further studies are necessary which however are beyond the scope of this study.

*P11L4 The model simulations are nudged, and so is it still true that the EMAC model has weak downwards transport in this configuration? I would have thought that nudging the model ruled out dynamical factors as likely causes of any biases in chemical fields when compared with observations.*

Vertical winds are not nudged in EMAC, but divergence and vorticity are. In EMAC, the vertical wind is calculated with the help of these two parameters. Nevertheless, despite the nudging, the vertical transport is underestimated. The results are improved when a higher resolution is used, but the problem that the vertical transport is underestimated remains.

*P11L9 A further complication here is surely that if the fine-scale features are not present in the ECMWF dataset used for nudging then the model could never accurately capture these features. Perhaps a discussion on this and to what extent will this limit the ability of your future T255 model to reproduce this structure is warranted.*

The following text has been added to the last paragraph of section 4.2 to discuss this: *However, it should be kept in mind that a good agreement between model simulations and observations can only be obtained if the model simulations are nudged towards meteorological analyses. It can be expected that comparison with free running model simulations would show larger differences. Further, the results are also limited by the accuracy of the meteorological analyses, e.g. resolving small-scale temperature fluctuations and mountain waves will still be problematic even when a T255 resolution is used.*

*P12L1-3 This is true only for nudged configurations where the dynamics is accurately*

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*captured, and would not be true of free-running models. I feel this is an important point which should be made to caveat the conclusion.*

To be more clear on this point we mention now at several places in the conclusions that a nudged EMAC simulation was used.

*Technical Corrections:*

*P11L29  $CIO_x$  should have a subscript  $x$ . Similarly subscripts should be used for  $NO_y$  in Figure 4.*

Thanks for pointing this out. This has been corrected.

*Figure 1 I feel contours should be used consistently alongside the shading in the figures to aid with clarity, as is done in the top panel in Figure 1. This could be applied to all the pressure vs time plots.*

We have tried this, but found that the addition of extra contours make the Delta and PSC plots too cluttered and thus harder to interpret.

*Figure 13 It looks like there are zeros used for multiple contours in the top panels ( $CIO$ ) in Figure 13, indicating the contour label does not have enough decimal places. This should be corrected.*

Thanks for pointing this out. The figure has been corrected.

*In a number of locations the grammar and sentence structure could be improved - I would encourage the authors to undertake another proof-read of the manuscript. The sentence on P9L30-32 should certainly be edited for clarity.*

We have performed another proof-read of the manuscript and hope that everything is correct now.

Figures are provided as supplement to this reply.

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Please also note the supplement to this comment:

<https://www.atmos-chem-phys-discuss.net/acp-2017-503/acp-2017-503-AC2-supplement.pdf>

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Interactive comment on Atmos. Chem. Phys. Discuss., <https://doi.org/10.5194/acp-2017-503>, 2017.

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