

General comments

This article is about improving the parameterization of denitrification in the WACCM model with the help of MIPAS measurement data.

The paper is scientifically sound, well written and well structured. I recommend to publish the study with (relatively) minor revisions.

Having said this, I think I have two major comments. I have put all my comments into the "specific comments" section.

The first one is the comment to lines 90–93 (see below). I think you are doing a little bit of a strategy of "least effort" here. I think some more discussion and analysis would really be helpful and increase insight and maybe even improve your parameterization.

The second major comment is to lines 165–167 (see below) and Figure 4. This one really worries me. The ozone values are off by an order of magnitude here. I hope that there this some simple explanation for this, e.g. a simple mistake in the labels of the x axis. Or maybe I am just too tired after doing this review in one piece in only 6 hours, and can't think clearly anymore ;-).

While this paper is quite technical, the improvement of model parameterizations is clearly an important topic, and as such the manuscript is well suited to ACP. Having said this, it would also be an obvious candidate for publication in GMD, but I have no strong opinion on the journal this article should be published in.

Best wishes, Ingo Wohltmann

Specific comments

- Title: This manuscript is specifically about the WACCM model. This should also be reflected in the title. Please add "WACCM" to the title in some way. For the same reason, you could also add that you use MIPAS data in the title.
- Lines 38–40: "Accounting for denitrification is an important process in chemistry-climate models, which is why many parametrizations with different levels of detail have been developed to account for the microphysics and sedimentation of NAT particles in these models (e.g., Wegner et al., 2013; Zhu et al., 2015; Kirner et al., 2011; Weimer et al., 2021)."

I am a little bit surprised that you are talking only about chemistry-climate models (CCMs) here, and not about chemistry and transport models (CTMs). This is all the more surprising since you use the specified dynamics version of WACCM here (SD-WACCM), which is effectively a CTM.

There are some obvious omissions in the citations that you give here. The first that comes to my mind is the implementation of denitrification into the CLaMS model by Groß et al., doi:10.5194/acp-5-1437-2005 (there are also follow-up papers), which is based on the Lagrangian DLAPSE

scheme (Carslaw et al., doi:10.1029/2001JD000467) that has also been used in other models.

I probably have a small conflict of interest here, but if you like, you could also cite the implementation of DLAPSE into my model ATLAS, Wohltmann et al., doi:10.5194/gmd-3-585-2010.

But surprisingly, you also don't cite your own implementation. As far as I can figure out, the denitrification scheme in WACCM is based on the scheme described in Considine et al. (2000). Wouldn't it make sense to cite that here? Wegner et al. does not exactly deal with the details of the denitrification scheme.

- Same topic: I would really like to see a short and concise account of the methods used to model denitrification in CCMs and CTMs here. This really is not required to be detailed or complicated, just a short overview. I think that would be helpful for the reader.

- Line 48: "...other datasets may also be appropriate but here but here we use MIPAS for this initial test".

You probably anticipated a comment here and tried to avoid it by stating this. Nevertheless, I will give the comment here anyway ;-). There are some obvious additional candidates for comparison with measurements. The most obvious one is MLS, in particular since there is a much longer time series extending into the present.

- Line 49 (and lines 11–12): If you would use other measurement sources than MIPAS, you could also show results for HCl here. HCl seems to be quite an obvious omission here.

- Line 64: "...using a simple upwind scheme."

I would add Considine et al. as a reference at the end of the sentence, since this is where it is actually described in detail.

- Same topic: I think it wouldn't hurt to shortly describe how the denitrification scheme works, even if you repeat information from some older papers, since this is central for your study. I think this would help the reader, who is not required to gather this information from other papers then.

This could give the reader an idea how microphysical processes as nucleation, sedimentation (fall velocities), growth and evaporation are handled here in a simplified fashion.

- Lines 67–68: "...observed NAT particle abundances may therefore not be the best guide for this parameter choice."

I agree, and will therefore not comment on this or other details of PSC measurements.

- Line 69: "Here we have had the benefit of the unusual NH year 2020"
Exactly. But since you use MIPAS data here, which ends in 2012, you are not able to compare to just this winter, which could be relatively easily compensated for by using a different measurement data set like MLS.

- Line 71: I think it would increase the insight of the reader in what is happening in your model greatly if you would mention that decreasing the NAT number density will increase the particle sizes and the fall velocities, and hence, the efficiency of denitrification. Maybe you mention that somewhere else in the paper and I missed it.

This is under the caveat that I understand correctly how your denitrification scheme is working.

- Line 90–93, 99, General approach with pdfs in the polar vortex in the altitude range 30–150 hPa: I understand the benefit and elegance of your approach to have a single and comprehensive metric (integrated difference of the WACCM and MIPAS pdfs) that you apply for improving your parameterization, but I think this very condensed metric may hide some important things.

In particular, 30–150 hPa is a HUGE altitude range, where all kinds of parameters change significantly (pressure, partitioning of species, NAT threshold temperatures and so on). Isn't it a bit dangerous to throw everything into one pdf here?

I think it is required that you at least go into SOME more detail here. That would not only allow more insight into what is actually happening, but may also help to improve the parameterization.

E.g., I would really like to see a comparison of MIPAS and WACCM using an HNO₃ vortex mean profile that shows regions of denitrification and renitrification. This could also be done as a function of time and altitude for individual years.

Or, since the two pdfs may agree although identical values are located at spatially very different locations (in altitude or horizontally), it would also be helpful to do some simple "sanity checking" and to provide some simple plots like contour plots of HNO₃ at a given altitude level for several dates (in different years).

- Line 100: "In order to make the datasets comparable, we remove the profiles from both WACCM and MIPAS data where negative values occur in the measurements."

Does this significantly affect the results? If not (what I suspect), it may be worth noting. I write this comment because removing profiles with negative values from a noisy measurement data set can easily introduce a positive bias when e.g. applying a mean or looking at the pdf.

- Line 115: Probably only when the ozone sonde measurement is inside the vortex? Might be worth noting.
- Line 118: Why these two years? Warm and cold NH winter?
- Line 126: But I think it also shows that compared to the effects of denitrification, the effects of heterogeneous chemistry on HNO₃ are usually quite small. Might be worth noting. Would also be nice to have a citation for this, but since this is kind of textbook knowledge not often stated explicitly, it might be hard to find.
- Line 161: "There is also a clear signature of heterogeneous chemistry in the ClONO₂ distributions."
... which I don't find surprising when you switch off the ClONO₂+HCl activation reaction.
- Line 161: "ClONO₂ is formed faster in early spring than HCl"
I don't really know what to make out of this sentence. Do you want to discuss the fact here, that depending on temperatures and hemispheres, chlorine deactivation is sometimes predominantly into HCl (SH, maybe cold NH winters) and sometimes predominantly into ClONO₂? That effect will depend on the Cl/ClO ratio and hence on low or high ozone, and it will depend on denitrification.
- Line 163–164: "ClONO₂ volume mixing ratios that are too low compared to MIPAS, it is notable that the maximum values are increased by about 1 ppbv and then are comparable to MIPAS in all simulations with heterogeneous chemistry."
That's interesting. Switching off heterogenous chemistry should impede activation of ClONO₂ into active chlorine and impede ozone depletion. But why does this seem to "cut off" the highest ClONO₂ values? Do you have an explanation? Seems not straightforward to me.
- Line 165–167: Now, I am confused. When switching off heterogenous chemistry, I would have expected MUCH higher ozone values (a few ppm). Am I misunderstanding something here completely or is there something going wrong here (e.g. the values at the x axis not being correct)?
And the ozone values in the northern hemisphere seem to be suspiciously low in all cases. Values of below 0.3 ppm are normally never observed in this altitude range, even with ozone depletion.
I have the impression that something is clearly going wrong here.
- Lines 168 and following: Why don't you compare to ozone from MIPAS here? Would somehow be consistent to the rest of the manuscript. I would also find it interesting not only to see the differences, but also the mean ozone profiles.

- Lines 207–208: Isn't it a little bit over the top to argue with the Kolmogorov-Smirnov test here when it can be easily seen from the figures that the distributions are still different? I think that could be shortened.
- Supplement: I think it wouldn't hurt to mention what species you are showing in the plots. In the moment, you can only deduce that from the figure numbers in the main manuscript given in the caption.

Technical corrections

- Line 124: Typo "cpmpared"