

Mainz, 3 January 2022

Dear Michel van Roozendael,

please find a revised version of the manuscript amt-2021-213 according to the minor revisions suggested by the reviewer.

Concerning the main issues:

(1) re-include datasets with temperature inversion (during day time)

This seems to be a misunderstanding: daytime temperature inversions are not skipped from the analysis: They are included in the global maps as well as in the presented histograms and the listed standard deviations.

Only for the investigation of possible dependencies on humidity (Fig. 10) and surface altitude (Fig. 11) we had to skip temperature inversions, as they would otherwise dominate figures 10 and 11 and would generally hamper the systematic analysis of weaker effects.

For clarification, we have modified the last sentence of Sect. 5.2 to

“As the impact of temperature inversions on δ_T is quite strong, we skip profiles with temperature inversions of more than 2 K for the investigation of the effects of humidity (Sect. 5.3) and surface altitude (Sect. 5.4) in order to avoid interference of different effects.”

(2) use a different day in Sect. 5 for ECMWF data set than the one used for fitting.

We now moved the results for 18 December from the Supplement to Figures 3 and 7. In addition, we now also point out that the deviation of 0 for 18 June is a consequence of the fit being made for this day directly in the caption of Fig. 7.

The uncertainties given in the text already refer to the value from 18 March, which is based on a different data set than the one used for fitting.

(3) better follow the AMT guidelines regarding the usage of "quantity/ unit" notation instead of "quantity [unit]"

We appreciate the reviewers wish for consistent formatting according to journal guidelines. The format of units in figure labels is not directly specified in the current AMT guidelines. Obviously, Copernicus has to take some action here as the format used in most publications (“quantity [unit]”) is not in accordance with SI brochure and green book.

We have contacted the Copernicus editorial support on this matter, and they are now aware of this inconsistency. However, as it will probably take some time to be specified by Copernicus (as this would affect all journals, not only AMT), we would like to keep the figures as they are for now.

In the case that Copernicus specifies the format in short time, we will modify the figures accordingly.

Below we respond in detail to the further issues raised by the reviewer.

Kind regards,

Steffen Beirle

The revised version of the manuscript entitled "Calculating the vertical column density of O4 from surface values of pressure, temperature and relative humidity" does address most of the reviewers comments or, where the authors disagree, they give arguments for not changing, just as they state in their answer.

In terms of structure, the manuscript improved and is now easier to follow. Adding references to specific equations and subsections in the appendix also makes it easier to follow.

In terms of validation datasets, two of the three datasets increased greatly in number of measurements compared to the original submission. I also acknowledge the extra section on temperature inversions, however, I think it is misleading to exclude temperature inversions from the analysis and urge the authors to re-include them in the analysis to reflect fairly the ability and shortcomings of the proposed method since temperature inversions cannot be detected from just measuring the surface values of temperature, pressure and relative humidity and hence their results could be unfairly biased to better values when intentionally taking out temperature inversions from the comparisons in Sect 5.

This seems to be a misunderstanding: daytime temperature inversions are not skipped from the analysis: They are included in the global maps as well as in the presented histograms and the listed standard deviations.

Only for the investigation of possible dependencies on humidity (Fig. 10) and surface altitude (Fig. 11) we had to skip temperature inversions, as they would otherwise dominate figures 10 and 11 and would generally hamper the systematic analysis of weaker effects.

For clarification, we have modified the last sentence of Sect. 5.2 to

“As the impact of temperature inversions on δr is quite strong, we skip profiles with temperature inversions of more than 2 K for the investigation of the effects of humidity (Sect. 5.3) and surface altitude (Sect. 5.4) in order to avoid interference of different effects.”

Likewise, I urge the authors to use a different day for the ECMWF dataset in Sect.5 than the day which was used for the fit.

We now moved the results for 18 December from the Supplement to Figures 3 and 7. In addition, we now also point out that the deviation of 0 for 18 June is a consequence of the fit being made for this day directly in the caption of Fig. 7.

The uncertainties given in the text already refer to the value from 18 March, which is based on a different data set than the one used for fitting.

I mostly checked the new submission with track changes i.e. document amt-2021-213-author_response-version1.pdf. However, I see now that there are actually differences between that version and what was submitted as a new version, likely exclusively attributable to latex issues with the diff package [and hence nothing the authors could influence]. See for example page 11 (page 32) in the former document, last sentence of Sect. 3.2 "For further details see Appendix B0.1 and B0.1" and compare this with the last sentence of the document which was submitted as new version as amt-2021-213-manuscript-version2.pdf (page 9): "For further details see Appendix B1.2 and B1.3". Please ignore comments that refer to non-existing sections or multiple figure numbers if you find them correct in the not-track changed version. Line numbers below refer to the track changed version.

Yes, the incorrect labels in the tracked-changes version are caused by latexdiff.

(1) Since the authors only consider in their validation daytime VCDs (see also Sect. 3, especially lines 209- 212), the title should reflect this limitation. Please add this to the title accordingly.

We have modified the title to “Calculating the vertical column density of O4 **during daytime from surface values of pressure, temperature and relative humidity”**

(2) Regarding following the AMT guidelines:

(a) I disagree with the authors that the use of "quantity/ unit" in axes labels and table headings is only a recommendation. I have also never "noted" that it is only a recommendation either. Please read carefully the AMT author guidelines (<https://www.atmospheric-measurement-techniques.net/submission.html#math>):

"

In addition, the SI and IUPAC recommendations should be followed:

SI brochure

IUPAC Green Book, 3rd edition

IUPAC Gold Book

"

Collins dictionary says about the use of the word "should"
([#2](https://www.collinsdictionary.com/dictionary/english/should)) :

"

You use should to give someone an order to do something, or to report an official order.

All visitors should register with the British Embassy.

The European Commission ruled that the company should pay back tens of millions of pounds.

"

Hence, it is more an obligation than a recommendation to follow the guidelines (or recommendations) of the SI brochure and the green/ gold book. The point is that AMT uses "should be followed" not "it is recommended to follow" or "authors are encouraged to follow".

(b) The argument that the authors give " Thus we prefer to provide units in brackets in figure axis, which is also commonly done in most of recently published AMT papers", is not a valid argument for the validity of their choice; it is merely a statement about the state of quality control at AMT regarding their own guidelines.

(c) Even if following the guidelines of the green book and the SI brochure were just a recommendation:

Who will follow these guidelines, if not even the chief editor of the journal which publishes these guidelines/ recommendations follows them? People in power should set good examples and follow (at least their own) recommendations, otherwise recommendations do not make any sense and could be removed all together.

(d) There are good reasons why AMT refers to the SI brochure and the green book. For a motivation for these guidelines, check out the preface of the green book, where it reads on page IX:

"The purpose of this manual is to improve the exchange of scientific information among the readers in different disciplines and across different nations"

Including the unit in round brackets in an axis label (or table heading) is common in some areas (e.g. physical review letters prefers the notation with round brackets is even recommended: <https://journals.aps.org/prl/authors/axis-labels-and-scales-on-graphs-h18>; but keep in mind that the article in question was not submitted to APS but to AMT; AMT has different style guidelines, as cited above), square brackets are in fact used to give units of a quantity as follows: [quantity] = unit, e.g.: [T] = K. Using square brackets in axis labels around units is simply not correct and should never be used. Using round brackets is accepted, but has certain disadvantages: It can be easily mistaken as a multiplication factor whereas it really should be the denominator of a quotient. Hence, labeling a distance axis as "distance (m)" could be interpreted as "distance \times meters". This is incorrect. What is labeled on the ticks on the x-axis in the graph is "distance $\overline{\hspace{1cm}}$ meters" (a plain number); the notation "distance/ m" does not leave any room for interpretation and will be understood correctly independent on your field or background. A very instructive explication in German (see the original

from the BIPM linked on the AMT homepage) can be found in the German version of the SI brochure: "https://www.ptb.de/cms/fileadmin/internet/publikationen/ptb_mitteilungen/mitt2007/Heft2/PTB-Mitteilungen_2007_Heft_2.pdf", as in the original, in Sect. 5.3.1 (especially page 174 [corresponding to page 33 in the pdf]).

We appreciate the reviewers wish for consistent formatting according to journal guidelines. The format of units in figure labels is not directly specified in the current AMT guidelines. Obviously, Copernicus has to take some action here as the format used in most publications (“quantity [unit]”) is not in accordance with SI brochure and green book.

We have contacted the Copernicus editorial support on this matter, and they are now aware of this inconsistency. However, as it will probably take some time to be specified by Copernicus (as this would affect all journals, not only AMT), we would like to keep the figures as they are for now.

In the case that Copernicus specifies the format in short time, we will modify the figures accordingly.

(3) Regarding the authors answer about the criticism of the limited datasets:

I acknowledge that the authors increased the number of both ECMWF and WRF and I agree that this is a sufficient coverage now. However, two comments here:

(a) regarding the GRUAN dataset, I would still like to mention that more than 70% of their ~6300 datasets come from 3 stations, and hence, I do not agree that that is a good coverage.

We agree that GRUAN does not provide good spatial coverage. However, spatial coverage is provided by the ECMWF data, while GRUAN provides very good temporal coverage for some stations.

Note that we do not claim “good coverage” for GRUAN in the manuscript.

(b) from the authors answer on page 5 from document amt-2021-213-author_response-version1.pdf, I understand that the authors submitted the first version of the manuscript in the middle of the process of creating the validation data set, anticipating the full results based on a subset of just ~15%. This is certainly bad practice and should be avoided in the future. It was highly inconsistent (2 months vs a few days) and confusing in the first version.

We will avoid this in the future.

Minor comments:

line 44: "this study" is ambiguous: does it refer to "the current study" (maybe better refer to the specific Sect. 4.1) or to "Wagner et al." (better use: "that")?

We have modified “this study” to “the current study”.

line 51: To which equation does "The final equation" refer to?

We skipped the reference to “The final equation” in the introduction.

Table 1: I think "deviation to" should be "deviation from"
(<https://www.collinsdictionary.com/dictionary/english/deviation> or
<https://dictionary.cambridge.org/dictionary/english/deviation>) (likewise l.195)

Corrected.

line 88: Are the authors sure that they want to refer to Eq. 19 here? This seems to have nothing to do with the derivation here?

Yes, thanks, the latex labels were mixed up here. We corrected this reference to Eq. 6.

line 264: Please check the references here, it currently reads Appendix B0.1 and B0.1 There is not even any B0, Appendix B starts (as it should) with 1. (page 31, page 52 in the document.)

The wrong references are caused by latexdiff. In the plain pdf, the references are correct.

line 284/285: "correlation ... are found". "is"?

Corrected.

Figure 1: The frequency is defined as points in some "square" area made of Δx time Δy ? Please give more detail here, otherwise the quantitative description in the color bar is not meaningful (of course, the qualitative message still comes across and I think it's a very good idea). Same for Fig. 5, 10, 11.

We have added the following specification to the caption of Fig. 1:

“Frequency per pixel is color coded, with a binning of 100 pixels for both x and y axis, as in all 2D frequency distributions shown below.”

For most of these figures: The inclusion of the colour bar in either one or all subplots is inconsistent. Consider to include it as a separate axis instead. (Although it is not wrong as it is now since multiple colour bars are included where the colour scale differs between subplots. Still it seems not very pleasing for the eye as it is now.

We would like to keep the color bars inside the figure. An additional axis on the right or bottom would shrink the actual plots, which are quite small already.

Additionally, e.g. in Fig. 10, the colour bar lacks the top axis while it is present in e.g. Fig. 11).

The top axis is present in all color bars – this might be a zoom issue of the pdf viewer?

line 311: "too low" with respect to what? Why "too low"? They are not "too" low?

We added “as compared to a polytropic atmosphere with the same O4 VCD”.

Figure 8: Caption refers to "top" and "bottom" in a figure where only left and right are present. Please include horizontal separation lines between the stations. Are the authors serious in including stations with single digit numbers (Beltsville, Darwin, Nauru, LaReunion) here?

We have corrected “top” and “bottom” to “left” and “right”.

We added faint separation lines between the stations.

We see no reason to exclude stations with low number of sonde launches from this figure: of course the statistics are rather poor for these sites, which is marked by faint color as noted in the caption. However, we found it worth showing that also for these stations no unexpected behavior or larger deviations could be observed.

line 303: "agreement to"?

We would follow the recommendation of the Copernicus copy editor here.

Fig. 7: Please choose any of the other 3 days here (or best all) and not the day which was used for fitting the parameters. Using the day used for fitting does not make sense. So replace Fig.7 by Fig. C2. Especially, because your argument of "But there is also a considerable reduction of SD from 1.6% for δT to 1.0% for δRH " (line 366) is not that strong any longer if you actually consider days that were not used for the fit, the SD only decreases from 2.0% to 1.8% (Mar), from 1.6% to 1.3% (Sep) and from 1.3% to 1.2% for Dec.

We now moved the results for 18 December from the Supplement to Figures 3 and 7. In addition, we now also point out that the deviation of 0 for 18 June is a consequence of the fit being made for this day directly in the caption of Fig. 7. We also add the SD for 18 December to the discussion in the manuscript.

The uncertainties given in the text already refer to the value from 18 March, which is based on a different data set than the one used for fitting.

line 495: I acknowledge the footnote here, I was at first a bit puzzled here.

Yes, this was confusing on first sight.

line 513: Maybe better "equation"?

We would follow the recommendation of the Copernicus copy editor here.

line 614: "Note that the for a"? Remove "the"?

Corrected.

Figure B1: Please increase the space between the map and the x- and y- axis labels. Also: There are four "Fig. B1" (at least in the version with track changes), comment is about the first one.

Done.