

Answer to Referee 1 (2nd referee report received)

We would like to thank the reviewer for his comments. We agree with the referee that the text was a bit hard to follow in places and we hope that we could improve this by following both his and the other reviewers advices and suggestions for improvement. Since we received a comment from reviewer two before we received a comment from reviewer one, we are sometimes referring in this answer to the answer to reviewer 2.

Below, we comment on the first reviewers specific comments. For easier reference, we added a number to each comment. We use the following color coding:

Color coding:

reviewer comment

our answer

proposed change in manuscript

Review of "NO₂ vertical profiles and column densities from MAX-DOAS measurements in Mexico City" by Friedrich et al.

This manuscript discusses a newly developed profile retrieval code - the Mexican Max-doas Fit (MMF). Note: The first author's initials match the acronym, nicely done! The retrieval code consists of 2 parts, 1) an aerosol retrieval and 2) a trace gas retrieval using the previously retrieved aerosol profiles. This code is then used on 19 months of MAX-DOAS data measured at a location in Mexico City and the results are discussed. A comprehensive error analysis (which is great to see!) is also included in the manuscript.

It certainly is interesting to look at the complete 19 months NO₂ data set (e.g. see the discussed averages of the diurnal variation) but my guess is the more interesting studies (specially from an environmental view point) can be done by looking at individual days and using the right ancillary data to understand the NO₂ variability and what causes the observed peaks.

Overall, the manuscript is well structured and the figures and table are clear and straight forward to understand. However, in some places (e.g. in Section 5, Error analysis) the text can be somewhat difficult to follow, and the manuscript could gain from having another go at streamlining the text a bit more and simplifying the structure of some of the more complicated sentences.

1) Page 2, line 16: Replace 'giving' with 'with'

corrected

2) Page 2, line 17: Section 2 should be Sect. 2 for consistency, check whole manuscript

checked in whole manuscript, thank you!

3) Page 2, line 19: '(constituting the forward model)' - What exactly does this mean?

This means that the forward model in our case is a radiative transfer code and that we talk about radiative transfer codes here, because our forward model is a radiative transfer model, more specifically, VLIDORT.

4) Page 2, line 30: UNAM – can you please spell this out once

done at first appearance now, i.e. at the beginning of Sect. 2

5) Page 3, Figure 1, caption. Nice overview figure. For completeness, can you please also include a brief description of the yellow and red box in the caption.

Yes. As response to reviewer 2, we also made small adjustments to the figure, see answer to referee 2. The new caption is describing that version of the figure. We added to the caption:

“The yellow boxes represent the forward modelling steps. The red boxes are the inversion steps, using Thikonov regularization for aerosol retrieval and optical estimation (OE) for tracegas retrieval.”

As a response to (23) below, we also now added “& rates of change” in the orange and green boxes before the yellow “VLIDORT box”.

6) Page 3, line 3: Replace ‘large’ with ‘long’

corrected

7) Page 4, line 8: Typo: ‘receiving’

corrected

8) Page 5, line 4: Typo: ‘an average’

corrected

9) Page 5, lines 16-25: Why was O4 not retrieved using the same wavelength interval as NO2? The much older O4 XS from Hermans et al. 1999 was used for the O4 retrieval, why not Thalman and Volkamer (2013)?

Thalman, R. and R. Volkamer, Temperature dependent absorption cross-sections of O2-O2 collision pairs between 340 and 630 nm and at atmospherically relevant pressure., Phys. Chem. Chem. Phys., 15(37), 15371–81, doi:10.1039/c3cp50968k, 2013.

The windows for NO2 and O4 dscd fitting are chosen to enclose pronounced absorption lines for the species in question and are widely used windows. We agree with the referee that there are O4 windows that are closer to the chosen NO2 window (405 -- 465 nm) than our choice (336 -- 390 nm) and that it had been a better choice to use one of those (e.g. 450 -- 520 nm). However, the difference in middle wavelength had only been 22 nm less (i.e. +50 instead of -72). We would also like to refer to our answer to reviewer 3 question 2 regarding correction for aod. Regarding the choice of cross-sections, there was no specific reason for the choice of cross-section. We would like to refer the reviewer 1 to answer 1b to the mayor comments from reviewer 2, where we also include a test for changing the retrieval settings. Our main finding is that the effect of changing the cross-sections is small.

10) Page 5, line 26: Would it be possible to say something briefly here about how the errors were determined?

The dscd error is calculated directly within qdoas. We use this error as dscd error without any modification or addition. We refer the reviewer to pages 28 -- 29 ("Errors on Slant Column Densities) of the qdoas manual (http://uv-vis.aeronomie.be/software/QDOAS/QDOAS_manual.pdf) for details on the dscd error calculation within qdoas.

11) Page 7: The authors explain that the retrieval code was recently updated from using the Gauss-Newton scheme to the more stable Levenberg Marquardt iteration scheme. However, this is not really relevant for the work presented here and seems to unnecessarily complicate the discussion. Unless there is a compelling reason to keep this information, I suggest to drop the relevant equations and just briefly mention in a couple of sentences (or one paragraph) that the retrieval code has been updated and how. It would also be better to have all the variables explained straight after Equation (1) and not further down the page.

We fully agree with the referee. Referee 2 (first report received) had a similar comment. We moved all explanations regarding changes to the code into an appendix. This also leads to all symbols in Eq. 1 being defined right after its appearance. For details on the changes, please see the answer 2b to the major comments section from referee report from reviewer 2.

12) Page 7, line 6: Change to ‘non-linear’

corrected

13) Page 7, line 12: Change to ‘dimension which is the number of telescope’

done

14) Page 7, line 17: Change to: ‘equal to 1’

corrected

15) Page 7, line 23: Change to: ‘for the trace gas’

included “the”

16) Page 8, line 8: Change to: ‘with the LM iteration scheme.’

included “the”

17) Page 8, line 10: Change to: ‘algorithms. For example, there are’

Added “For example”

18) Page 8, line 20: Typo: ‘high speed’

corrected

19) Page 8, line 21: ‘instead of the 2x the number of layers calls’

corrected

20) Page 8, line 23: Jacobians always with capital J, also on Page 12 & 13

now capitalized everywhere.

21) Page 8, line 23/32 and footnote: Why not refer straight to LIDORT if only that part if used anyway?

VLIDORT and LIDORT are actually different code packages with different version numbers. Since it might be that they, of course by accident, include different “features” (i.e. bugs), we think that it is more accurate to state exactly which code and which version was used.

22) Page 8, line 32: Maybe replace with ‘For each simulated atmospheric layer,’

corrected

23) Page 9, lines 9-14: It is not quite clear to me how the rate of change is represented in Figure 1, can you please explain . . . or I might have misunderstood?

This was perhaps not clear. We did not refer specifically to the rate of change. We removed the sentence. However, we also realized that the rate of change as layer input was indeed missing in the diagram. We added “& rates of change” in the orange and green box before each of the yellow VLIDORT boxes.

24) Page 9, line 13: Should be either ‘enclosed’ or ‘included’ ?

enclosed

25) Page 9, line 21: Replace ‘is’ with ‘are’

corrected

26) Page 11, line 2: Comma needed after Qray

corrected

27) Page 11, line 14: ‘are assumed to be constant in all layers.’

corrected

28) Page 11, line 15: Replace ‘are’ with ‘is’

corrected

29) Page 11, line 16: Change to ‘density profiles in arbitrary units from . . .’

corrected

30) Page 11, line 17: Change to ‘heights h to provide

corrected

31) Page 11, line 19: I am not sure if all readers will know what is meant with an ‘intensive quantity’, maybe explain briefly in a footnote?

Ok, we add as a footnote: “bulk property which does not change when changing the size of the system”

We also noted that we did not explicitly mention the first step where we convert the relative intensive profile to an extensive one in the first place (for scaling) before we convert it back to an intensive one. Which is very confusing. We would like to change this by changing line 18 to “This profile, turned into a partial optical depth per layer by multiplying with the layer thickness, is scaled to match the total aerosol extinction from AERONET τ_{aer} . The profile is then converted back into an...”

32) Page 13, Equation 16: Rogue bracket or is something missing?

Opening bracket removed

33) Page 13, line 18: Gain is written in a strange font, on purpose (why?)? If not, please fix.

Changed to same font as AK everywhere

34) Page 13, line 21: 'produces'

corrected

35) Page 14, line 9: Add comma after fitting

corrected

36) Page 14, line 23: Change to 'AK matrices from the other errors.'

corrected

37) Page 15, line 1: 'the VMR(VMR)' – is that correct?

Yes, it describes the difference between subscript "VMR" and "pcol"

38) Page 15, lines 16/17: Why would the vertical aerosol extinction profile not be available?

Because the aerosol retrieval failed, or because it was judged to be a bad retrieval due to a large rms w.r.t. measured and simulated dscd

39) Page 16, Figure 4 caption, last sentence: 'an ideal'

corrected

40) Page 16, line 6: Add comma after 'operator' – makes this sentence a bit easier to read.

corrected

41) Page 17, Equation 25: Should that be 3% instead of 0.3%?

yes, corrected

42) Page 17, line 8: Should either be 'error . . . is' or 'errors . . . are'

corrected

43) Page 17, line 14: Comma after retrieval

corrected

44) Page 17, line 15: 'contributions: a) smoothing error and b) .. error.

corrected

45) Page 18, line 1: Comma after (2017)

corrected

46) Page 18, line 3: Could use 'dependent' instead of 'not independent'.

corrected

47) Page 18, line 5: Delete 'it'. Comma after 'However'

corrected

48) Page 18, line 9: Delete 'the' before 'VLIDORT'.

corrected

49) Page 18, lines 10/11: Add commas after '(2017)' and 'the residual'

First coma added, second would be incorrect, we believe

50) Page 19, Figure 6: The two solid orange lines are hard to distinguish, could use dash or dash/dot for one of them.

We agree with the reviewer and will change one of the orange lines to a dashed orange line.

51) Page 19, Figure 6 caption: Change to 'a) The square . . .' and delete full stop after 'total'

corrected

52) Page 19, line 3: Better: 'errors for No2 and O4 calculated'

corrected

53) Page 19, line 5: Change to 'errors' and delete 'fairly'

corrected

54) Page 19, line 7: Delete 'relatively'

corrected

55) Page 19, line 8: Something is not right with this sentence & it doesn't make sense as it is written. Maybe delete 'to' or rephrase altogether.

Changed to two sentences: "The error in the vertical column is smaller than the errors in the VMR profile for almost all layers (Fig.6). This can be explained by an anti-correlation in different partial column errors indicated by the full error covariance matrix."

56) Page 20, Table 1, caption: The last sentence is a bit hard to read; would help to add a comma after included and it needs a 'with' after better.

We reformulated to:

“However, if the algorithm error according to Wang et al. (2017) is included, the remaining error due to the uncertainty in the aerosol profile is slightly better: 9.3% instead of the 9.8% without O₄ retrieval.”

57) Page 20, line 2: Add comma after ‘In this section’

corrected

58) Page 20, line 4: Typo: ‘approx.’

corrected

59) Page 21, line 10: Typo: ‘Currently’

corrected

60) Page 23, line 1: I would rather say: ‘Generally, a better . . .’

corrected

61) Page 24, lines 8-11 and Figure 10: Would be really interesting to get higher resolved surface measurements as well, otherwise a small increase might be hidden in the surface data set as well. The peak only shows up clearly in the individual measurements with sufficiently high temporal resolution. Similar peak also shows up on Aug 15 and one could argue to some degree even on 9 Sep and 22 Dec with a bit of a time shift. Any idea what causes it?

We think this NO₂ enhancements might be transported from somewhere within the basin.

Definitely, surface data with higher temporal resolution would allow us to do a more in-depth analysis on a day-to-day basis, as mentioned to referee 2. We think, however, that such a detailed study would divert from the main objectives of the paper, which is to describe the methods and quality of these data.

62) Page 24, line 28: Change to: ‘This might have to do with the fact that during . . .’

otherwise something seems to be missing from this sentence.

Yes, indeed. corrected

63) Page 24, lines 20-23 & Page 26, Figure 11: Could you add a brief discussion here on the nicely (amazingly?) constant offset between surface and MAX-DOAS data, also including the uncertainties of both data sets in that discussion. Would you say that this is predominantly caused by NO₂ having strong emissions on the surface which are then just diluted over the vertical range which the MAX-DOAS measurements are covering?

Thank you for this comment. We added the following sentence at the end of the paragraph (Page 24, line 23). “Despite the fact that the offset in the curves for surface- and MAX-DOAS measurements appears to be nearly constant throughout the day, it would be interesting to investigate further how this offset varies in different seasons particularly when vertical mixing is not favoured”.

64) Page 26, line 1: Change to: ‘and certain trace gases. We . . . NO₂ at one . . .’

corrected

65) Page 27, line 1: delete ‘ ‘s’

corrected

66) Page 27, line 4: Add something like ‘Sinces this study, it has been . . .’

We take this suggestion

67) Page 27, line 10: Add ‘the’ before ‘NO₂’.

corrected

68) Page 31-34, References: There seems to be some doubling up of information, please check through all the references for correct formatting.

Thank you for the note on this, we looked over the reference formatting, see also reply to referee 2 on this subject.