

Interactive comment on “MAX-DOAS observations of the total atmospheric water vapour column and comparison with independent observations” by T. Wagner et al.

T. Wagner et al.

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Reply to Reviewer #1

General Comments: The paper presents a new approach to derive water vapour vertical columns from MAXDOAS measurements in the yellow and red spectral range. The experimental setup and the retrieval method are clearly described. The resulting water vapour vertical columns are compared with different independent data sources (ground based and model data as well as satellite measurements). My main point of criticism is that the errors of the derived VCDs are not sufficiently discussed. Overall,

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the manuscript is well written and may be published in AMT after some corrections addressed below.

Author reply: We thank this reviewer for the positive assessment of our manuscript. We agree that a sufficient error discussion was missing in the original version of our manuscript. We added such a discussion in the revised version (new section 2.8). Before we give our detailed replies to the individual reviewer comments (see below), we give a short overview on several major changes of the revised version of our manuscript.

A) We implemented a new cloud discrimination scheme based on clearly defined conditions and quantitative thresholds. This scheme is similar to that presented in Wagner et al., 2011. Since no zenith view measurements are made in the current study, we used those made at an elevation angle of 70° . However, since the observed radiances and also the retrieved O₄ DSCDs for this elevation angle not only depend on SZA but also on the relative azimuth angle, the calculation of the normalised radiance and O₄ AMF is more complicated than in Wagner et al. (2011). Thus we decided not to apply a radiance threshold, because of the strong dependence of the radiance on the relative azimuth angle. For similar reasons we relaxed the threshold from 0.7 to 1 for the normalised O₄ AMF. These changes affect the separation between ‘thin’ and ‘thick’ clouds. Because of the strong dependence of the radiance on the relative azimuth angle, we also slightly modified the discrimination scheme between clear sky and ‘thin’ clouds. Instead of investigating the temporal variation of the normalised radiance, we investigated the temporal variation of the radiance after applying a high pass filter to the diurnal variations for individual days. We expect that this change has only a small impact on the discrimination between clear sky and ‘thin’ clouds. Overall, the application of the new cloud classification scheme led to substantial changes of the classification results. The fraction of clear days increased from 20% to 38%, the fraction of ‘thin cloud’ cases decreased from 74% to 44%, and the fraction of thick cloud cases increased from 6% to 18%. The large change in the frequencies of clear sky

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and thin cloud cases is caused by the rather coarse criteria for the detection of cloudy situations: In many cases, when the discrimination scheme indicates clear sky conditions, the presence of clouds is clearly obvious from inspecting the diurnal variations of cloud sensitive quantities, especially the colour index. In spite of these differences, the results of the correlation analyses for MAX-DOAS measurements made under clear sky or thin clouds are only slightly affected by these changes. We introduce the new cloud classification scheme in section 2.7 (old section 2.6) and explain the resulting differences. We also added a new figure (Fig. 9) illustrating the different steps and conditions of the cloud classification scheme. We updated the correlation analyses (Figs. 14 – 17) for the new sub-sets for clear, thin cloud and thick cloud conditions.

B) We added a detailed discussion of the error budget in the new section 2.8. The total error is based on uncertainties of the spectral retrieval and the treatment of the atmospheric radiation transfer. In most cases the latter dominates the total error. We add a formula (new equation 8) for the determination of the total error of the H₂O VCD and display these errors in Fig. 11 (old Fig. 10).

C) We added clear criteria for the selection of wavelength ranges and elevation angles. These are based on fit errors in both spectral ranges for the whole time series of measurements. Here, for O₄ smaller values are found for the green spectral range, and for H₂O smaller values are found for the red spectral range. For the selected combination of elevation angles (20° and 70°), the standard deviation of the derived O₄ VCDs is smallest for the whole time series. We also added the respective information in sections 2.2 and 2.3. We added a new table showing the standard deviation of the O₄ VCDs derived from the different combinations of elevation angles (new table 2).

D) Detailed discussions of H₂O profiles and the variability of the layer height We added a figure showing the average diurnal variation of the H₂O layer height (new Fig. 19). A systematic increase is found for the combination of MAX-DOAS and in-situ observations as well as for ECMWF data. We also investigate the variability of the H₂O profiles over the measurement site based on ECMWF data (new Fig. 20) and the suitability

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of an exponential function to describe the height dependence. It is found that above the boundary layer, the exponential function fits well to the observed profiles. However, close to the surface, the H₂O concentration is typically smaller than the extrapolated values of the fitted exponential function. This explains the systematic difference (about 400m) between the fitted scale height and the layer height calculated according to equation 9 (in the revised version). We discuss these findings in section 3.8 (in the revised version).

E) We also added a new figure showing the average diurnal variation of the H₂O VCD found in different data sets (new Fig. 13). A systematic increase of the H₂O between 7% and 11.4% is found for a period of about 12 hours.

Specific Comments:

1. p. 6245/6246: Why is a Fraunhofer reference spectrum required (except for maybe the Ring correction)? As stated in the first paragraph on page 6245, always the same Fraunhofer reference spectrum is used in this study. Therefore, it should cancel out in eq. (2), i.e. one could use the SCD instead of the DSCD. Please explain.

Author reply: Maybe there is a misunderstanding here? A Fraunhofer reference spectrum is needed in each individual fitting process to remove the strong Fraunhofer lines. Since we use the same Fraunhofer reference spectrum for the analysis of all spectra, its contribution indeed cancels out in equation 2:

$$\text{SCD}(a) - \text{SCD}(b) = [\text{DSCD}(a) + \text{SCD}(\text{ref})] - [\text{DSCD}(b) + \text{SCD}(\text{ref})] = \text{DSCD}(a) - \text{DSCD}(b)$$

2. p. 6245, last paragraph: As stated in this paragraph, H₂O data are taken from the wavelength interval 608–680 nm and O₄ from 543–620 nm (with the argument that the scatter of the data is lower in these spectral ranges). As H₂O and O₄ SCDs are determined from the same spectral analysis, wouldn't it be more consistent to use O₄ derived from the same spectral range as H₂O for the correction described in section

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2.5? As shown in Fig. 3 the DSCDs of O4 (and also H2O) derived in the two spectral windows differ somewhat (not only by scatter, also by absolute values). Could this have an impact on the results?

Author reply: In principle, using H2O and O4 results from the same wavelength interval would be more consistent. However, not only the difference in wavelength range but also in vertical distribution affects the combination of the absorptions of H2O and O4. So in any case, we would have to apply a correction factor to account for the different scale heights. The correction factor used in our study is 1.25; if the O4 results were taken from the same wavelength range as the H2O results, the correction factor would be slightly different, but the accuracy of the correction factor would not be significantly better. Since the accuracy of the O4 analysis is significantly higher in the green spectral range, we prefer to use the O4 results from this spectral range.

3. p. 6247, 3rd paragraph: As described in Wagner et al. (2003), the saturation correction is determined from numerical simulations. What assumptions on the atmosphere have been made in these simulations, and how dependent are the results described in the present manuscript on these (a-priori) assumptions? Furthermore, the factor 1.25 used in eq. (5) is determined from radiative transfer simulations. What assumptions have been made there, and what are the dependencies on these settings (e.g. atmospheric profiles, SZA)? Please justify that the statement that the retrieval does not depend on a-priori information (made several times in the paper) is still valid under these conditions.

Author reply: We investigated the influence of variations of the H2O profile on the retrieval using ECMWF data. We found that most profiles (>95%) have scale heights between 1.5 km and 3 km. The resulting errors of the retrieved H2O VCD are <15%. We added this information in the new section 2.8. We agree that our statement on the independence from of a-priori information was misleading, and we changed the manuscript at several places. We agree that several assumptions made, e.g. on the H2O profile shape, constitute indeed a-priori information. The important point of our

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retrieval, however, is that it does not depend on explicit a-priori information for individual observations. We added this information at several places in the revised version (abstract, introduction, conclusions).

4. p. 6247, last paragraph: Looking at Fig. 4, the application of the O4 correction using a 30% threshold seems to result in an exclusion of most of the data at lower relative azimuth angles, which corresponds to the morning data (as stated on p. 6248, l. 15/16). Could the exclusion of these data be an additional reason for the larger differences to the GOME-2 satellite data (overpass in the morning)?

Author reply: This is a good idea, and in principle we agree that excluding many data during late morning could explain part of the discrepancies between MAX-DOAS and satellite data. However, since the average diurnal variation of the H2O VCD is rather small (see new Fig. 13), the exclusion can probably only explain a small fraction of the observed discrepancies (a few percent). We added the following information to section 3.6: 'It might be interesting to note that on clear days, often MAX-DOAS measurements in the late morning (close to the satellite overpass) are skipped by the application of the O4 selection criterium, because for these observations the small RAZI can lead to strong errors of the geometric approximation (see section 2.5). However, since the diurnal variation of the H2O VCD is on average small (see Fig. 13), this should have only a very small effect (a few percent) on the comparison between MAX-DOAS and satellite observations.'

5. p. 6252, l. 21–24: 'While the diurnal variations of the DSCDs of H2O and O4 still show some scatter, the radiance, the colour index, and the O2 DSCDs show a rather smooth variation (except towards the end of the day).' Looking at Fig. 9 (left), the variation of O4 seems even a bit smoother than the variation of O2.

Author reply: Many thanks for this hint! We exchanged O4 and O2 in the revised version of our manuscript.

6. p. 6253, l. 9–11: Has the categorisation of all 40000 measurements been done by

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visual inspection and, if yes, why? According to the description in Wagner et al., 2011, it should be possible to define an automatic procedure for this which would probably give more reproducible results and could be also applied to further MAX-DOAS data sets.

Author reply: As explained in point A) above, no zenith sky observations are available for our measurements. This complicates the application of the original cloud discrimination scheme introduced in Wagner et al. (2011). Thus in the revised version we applied a slightly modified version of this scheme. We also included a new figure (Fig. 9) illustrating the individual steps and conditions of this modified scheme.

7. p. 6260, l. 25/26: 'Our retrieval algorithm is fast and robust and can yield the H₂O VCD and associated uncertainties...' What are these uncertainties and how are they determined? There is no discussion of errors except for the statement on p. 6256 l. 17/18 that 'the deviation of the measured O₄ VCD from the true value is a good measure for the accuracy of the H₂O VCDs retrieved from MAX-DOAS'. This is however a more qualitative statement, and it essentially means that the quality of the H₂O VCDs is similar to the performed O₄ correction – shouldn't the quality be better after this correction? Please give an estimate of the error of the derived H₂O VCDs, preferably split up into the different potential error sources including the error on the derived SCD from spectral fit and additional systematic errors due to assumptions in the saturation and/or O₄ correction (e.g. from assuming a constant true O₄ VCD or from assumptions in radiative transfer simulations).

Author reply: As described in detail in point B) above, we added a detailed discussion of the total error budget in the revised version (new section 2.8). In addition to uncertainties of the spectral retrieval, the dominating contribution is usually caused by the radiative transfer effects. The latter can be well quantified by the deviation of the retrieved O₄ VCD from the true value. We defined this error indicator now in a specific equation (Eq. 7 in section 2.5). We also give a formula for the total error (equation 8 in the new section 2.8 on the total error).

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The correction based on the retrieved O₄ VCD (Eq. 6) leads to more accurate H₂O VCD. However, from radiative transfer simulations it follows that the deviation of the (corrected) H₂O VCD from the true H₂O VCD increases for cases of 'complicated' radiative transfer, e.g. for small RAZI, high aerosol loads or (broken) clouds. In such cases, also the deviation of the retrieved O₄ VCD from the true O₄ VCD increases. Thus the magnitude of this deviation can be used to quantify the error of the H₂O VCD (caused by radiative transfer effects). We added this explanation to the new section 2.8.

Author reply: It is true that our saturation correction does not account for the wavelength dependent effects of atmospheric radiative transfer. We investigated this effect in more detail using high resolved radiative transfer simulations. For extreme cases (high H₂O VCDs, no clouds and aerosols), the resulting errors are up to 7%. These errors are small compared to other uncertainties (see new section 2.8) and are thus ignored in our retrieval. We added the respective information to sections 2.3 and 2.8.

8. Table 2 & Figs. 12–15: The quantities $\langle A=B \rangle$ and $\langle A \rangle = \langle B \rangle$ given in Table 2 and Figs. 12–15 are not mentioned/discussed in the text.

Author reply: We now introduced these quantities at the beginning of section 3.6. We also discussed the derived values for each of the comparisons.

Technical Corrections: 1. p. 6252, line 4: I suggest to make this a separate section (2.7) instead of a subsection of 2.6 as there is no other subsection.

Author reply: We followed the suggestion of the reviewer.

2. p. 6258, line 5: I suggest to make this a separate section instead of a subsection of 3.6 as there is no other subsection.

Author reply: We followed the suggestion of the reviewer.

3. Fig. 2: The titles of the two sub-figures do not match the wavelength axes.

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Author reply: We corrected this figure.

4. Fig. 3: Even when scaled to a full (portrait) page size the text in the sub-figures is barely readable. Please increase the font size.

Author reply: We increased the font size of the text of this figure and hope it is now better readable. (we also expect that in the final version this figure will be print on one full (portrait) size).

5. Figs. 5 & 8: Does Fig. 5 show a ratio of VCDs (as stated in the label of the y axis) or a ratio of the VCD ratios shown in the lower sub-figures of Fig. 4 (as stated in the caption)?

Author reply: Indeed, these figures show ratios of VCD ratios. We changed the labels accordingly.

Reference

Wagner, T., Beirle, S., Brauers, T., Deutschmann, T., Frieß, U., Hak, C., Halla, J. D., Heue, K. P., Junkermann, W., Li, X., Platt, U., and Pundt-Gruber, I.: Inversion of tropospheric profiles of aerosol extinction and HCHO and NO₂ mixing ratios from MAX-DOAS observations in Milano during the summer of 2003 and comparison with independent data sets, *Atmos. Meas. Tech.*, 4, 2685-2715, doi:10.5194/amt-4-2685-2011, 2011.

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