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Atmospheric Measurement Techniques Discussions

Interactive comment on "Improved water vapour spectroscopy in the 4174–4300 cm^{-1} region and its impact on SCIAMACHY HDO/H$_2$O measurements" *by* R. A. Scheepmaker et al.

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The authors thank the referee for his/her review of the paper.

> 1) The new line list is provided as supplementary data. The authors state that that the format is the HITRAN one, however this is not totally true as the information on the assignment of the lines is missing. As this new line list is based on a combination of two initial lists it is not trivial to just replace the hitran08 data by those new data.

The referee is right: the format we have used is the old (100-character record) HITRAN format. In the revised version of the manuscript we will change this to the new HITRAN

format (160-character record), including information on the assignment of the lines, etc.

> 2) Missing lines: Since (a) Jenouvrier et al reported more lines than Hitran in the same spectral range, (b) with the higher sensitivity towards H2O of the atmospheric observations, have the authors checked that some residuals might come from missing lines in the line lists. This is mostly true for low intensity lines.

We have not performed such a check for missing lines, as the goal of our study was to further improve the already existing line parameters from Jenouvrier et al. Also, a check for missing lines will be hindered by changes in the residuals caused by already existing lines. Unfortunately, such hindrance will especially be strong for low intensity lines.

> 3) high residuals in Fig. 1 (commented on p8545, lines 10sq): I do not understand why the fact to cut the complete range into 4 pieces introduce noise at the limits. Could the authors explain. What is the need of this cutting? why not select widely overlapping ranges if the cutting is absolutely needed? The authors state that this is not a big problem as the limits were chosen where no strong water lines lie, however it seems to me that the strong lines will never be a problem but low intensity ones might. Moreover the 4212-4248 cm-1 region which is used in the following contains such a limit, was it wise?

The cutting was needed to decrease computation time and the resulting edge effects are a by-product of the convolution algorithm. In fact, the forward model always runs over a wider window than the actual fit-window, so there already is an overlap. And although the weak lines can be uncertain, they are only affecting their direct vicinity, while strong lines, on the other hand, have extended wings that will overlap with many lines throughout the retrieval window. This makes the weak lines a lesser problem compared to the broadening parameters of the strong lines.

> 4) factor of 5 between self and pressure broadening. I am surprised of such a factor, certainly for water which is a very complex molecule regarding its spectroscopy. Would

it be possible to consider the self broadening parameters from the HITRAN/Jenouvrier databases and only fit the pressure broadening. Would then the ratio of 5 still be observed?

We have performed an experiment very similar to the one suggested by the referee: using a laboratory spectrum of pure water (no air) we fitted the self broadening parameters, keeping pressure broadening fixed. This was followed by using a mixed spectrum (water and air) to fit pressure broadening, keeping self broadening fixed. After these fits the average ratio between self/pressure broadening was 5.02 \pm 0.76. Furthermore, we performed laboratory fits and retrievals in which we adopted different ratios between 4.0 and 6.0, and found that the exact ratio used has hardly any impact on the retrieved deltaD (impact less than 4 per mil).

> 5) in the line list, all isotopologues are present. Did you consider them separatedly in the fit of H2O (as done for HDO)? In the same order of idea: would it be possible to consider 2 (or more for the other isotopologues) correction factors to correct for the "concentration" of H2O/HDO/... in the Jenouvrier sample spectrum (described on p8543, lines 10-20).

Yes, throughout our work we have considered all isotopologues separatedly (so with H2O we normally mean H216O). If with "correct for the concentration" the referee means an individual adjustment of the vertical column density per isotopologue: no, this is not possible in our setup. It would be possible, however, to correct for unnatural abundances of other isotopes through a correction factor on the line intensities, like we did for HDO (described on p8544, lines 26-28). We have checked, though, but found no evidence for unnatural abundances of the other isotopes, except for HDO.

> 6) Figure 4: Top panel is not readable Panels B,C, D: is it not misleading to compare results using the new list and that of Jenouvrier below 4200 cm-1, since Jenouvrier did not produce any data in this region (p8544, lines10-18). The positive residual at about 4185 cm-1: could it be a missing H2O line, not present in the HItran database, or a line

from another species?

The remark on the top panel of Fig. 4 was also made by referee #1. We are aware of this difficulty, but on this scale this was the best readability we could achieve. The main purpose of panel A is to show that there are many overlapping lines and that there is strong absorption by water. We think that this is clear from the current figure. We provide a zoom in Fig. 5, also to show some absorption lines and the overlap from Fig. 4 in more detail.

The referee is right that it is a bit misleading to treat the Jenouvrier and HITRAN line lists separatedly below 4200 cm-1, while in effect these line lists are the same in that region (since we extended the Jenouvrier list with HITRAN parameters below 4200 cm-1). Differences in the line lists above 4200 cm-1, however, could in principle still affect the residuals below 4200 cm-1. Nevertheless we will remind the reader of the similarities between the two line lists below 4200 cm-1 in the caption of the revised version of the manuscript.

About the positive residual at 4185.23 cm-1: it is difficult to say what is the exact cause of this. Around this wavenumber we find an H216O and an HDO line very close together. In the laboratory water spectrum we can remove the residual by an increase in the air broadening coefficient of the HDO line (from 0.0982 to 0.1128 cm-1 atm-1) and a simultaneous increase in the pressure shift parameter of the H2O line (from 0.003780 to 0.00984 cm-1 atm-1, together with a smaller increase in the pressure shift of the HDO line from 0.00000 to 0.003281 cm-1 atm-1). The Paramaribo spectrum, however, still shows a residual in this region. This suggests that there is no need for a missing H2O line, and that the residual is caused by another species. At the same time a missing H2O line can not be fully excluded, as the vertical column density of water vapor at Paramaribo was about 26 times higher than in the laboratory and the missing line could be strongly overlapping with the existing lines.

Interactive comment on Atmos. Meas. Tech. Discuss., 5, 8539, 2012.