

Referee Comment 3 (RC3) by Vivienne Payne

This paper describes an approach for quantifying impacts of spectroscopic parameters on radiative transfer model simulations and on atmospheric retrievals that accounts for correlation between different parameters. This is an important consideration which is often ignored in other studies. The paper also an example of the application of the approach to downwelling microwave radiative transfer calculations and retrievals. The work is thorough and makes a useful contribution to the body of work on quantifying retrieval uncertainties associated with spectroscopy. The paper is generally well organized and well written. I recommend publication after addressing the comments below.

We thank the reviewer for the positive feedback.

As the authors state in the conclusions, the approach is applied to one particular widely used microwave absorption model. This should also be stated clearly in the abstract and made clear at the beginning of Section 2. Section 2 would initially seem to imply that the “review of absorption model equations” is also general, but the descriptions of the parameterizations of resonant and non-resonant absorption are particular to the MPM-based family of models. Not all atmospheric absorption models use these same parameterizations. As the authors are aware (since on page 2, within the introduction, the authors cite Long and Hodges [2012], which describes impacts of different choices of line shape parameterization on calculations of absorption for the 0.76 micron O2 A-band utilized by the Orbiting Carbon Observatory and other remote sensing instruments), there are models out there for other wavelength regions that use non-Voigt line shapes for resonant absorption. Also, the description of non-resonant absorption does not apply, for example, to the widely used MT_CKD continuum model. It would seem to make sense to move the material in sub-section 2.4 up to the start of Section 2 in order to make it clear that this review of absorption model equations is not general.

Agreed. We added text to the abstract and the beginning of Section 2 to underline that the approach is applied to one particular microwave absorption model. We prefer not to move the whole Section 2.4 at the beginning of Section 2, as Section 2.4 mentions parameters that are defined in Section 2.1-2.3.

Abstract: “The approach is applied to a widely-used microwave absorption model (Rosenkranz, 2017) and radiative transfer calculations in the 20-60 GHz range”

Section 2: “The following Sections describe the resonant and non-resonant absorption components and the parametrization as defined in the family of absorption models considered here, i.e. R98 and R17 as well as others introduced in Section 2.4. Therefore, the review presented here applies specifically to this family of models. However, the presented approach can be considered as generally valid for any absorption model.”

Page 2, lines 50-54. The need to account for correlation between uncertainty estimates for different spectroscopic errors is general to all wavelength regions, and this is good to emphasize. The authors list a few examples of studies that discuss the impact of spectroscopic uncertainties on remotely-sensed profiles. There is one microwave example, one sub-mm example and one

visible (0.76 micron) example. The authors might consider adding examples in other wavelengths. Possible examples for the thermal infrared region include Alvarado et al., [2013] and Alvarado et al [2015]. Possible examples for the near infrared region include Connor et al., [2016]. For disclosure: I happen to be a co-author on each of these particular suggested references... I am sure there are also others if you wanted to look for alternatives.

- Alvarado, M. et al., Performance of the line-by-line radiative transfer model (LBLRTM) for temperature and species retrievals: Recent updates evaluated with IASI case studies, Atmos. Chem. Phys., 13, 6687-1711 (2013)

- Connor, B. et al., Quantification of uncertainties in OCO-2 measurements of XCO₂: Simulations and linear error analysis, Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2016-128, 16th June 2016

Agreed. We now emphasize that the need for spectroscopic uncertainty characterization is general to all wavelength regions. The references above as well as Alvarado et al., 2015 have been added. Thanks for pointing this out.

Page 3, line 81: Please make it clear that “the absorption models” means a particular set of microwave absorption models.

Agreed. The sentence has been modified as “the considered microwave absorption model”.

Page 4, line 125: Hill (1980) is a pretty old reference. Does “analogous” mean alternative Voigt parameterizations? Do the authors know if anyone has re-visited fits of line shape parameterizations to microwave experiments since then?

To remove the ambiguity, the sentences have been modified as follows: "...for water vapor ($Y_i \cong 0$) (Ma et al., 2014). Then for water vapor, the line-shape function reduces to the van Vleck–Weisskopf profile: Eq(4).

The van Vleck–Weisskopf profile was demonstrated to fit experimental data well on the 22-GHz line (Hill, 1980) and the 183-GHz line (see Fig. 5 and related references from Tretyakov, 2016); also, Koshelev et al. (2018) found that speed-dependence effects amount to less than 1% deviation with respect to the van Vleck–Weisskopf profile near 22 GHz."

Page 7, lines 220-223. Does water to air mixing ratio (r'_{w2a}) here mean that in theory the mixing between oxygen lines would be altered by the presence of water vapor?

Please consider some more words here for additional clarification. Are there any calculations out there to suggest that the line mixing for oxygen should look different in wet vs dry air?

Correct. The mixing between O₂ lines should be different in dry and wet air from very general considerations. A polar water molecule as a colliding partner for an O₂ molecule acts significantly different from N₂ or O₂. However, no such calculations are available to our knowledge. The following sentence is added for additional clarification: "Line mixing depends on the off-diagonal elements of the collisional interaction matrix, while the diagonal elements of that matrix give the line width parameters. Therefore both mixing and broadening depend on the type of perturbing molecule; but because of the absence of either calculations or relevant measurements for r'_{w2a} ,

the model assumes $r'_w2a=r_w2a$. We believe that the possible systematic impact of this assumption is smaller than other model uncertainties discussed in this paper".

Page 12, line 1: Have these line intensities and lower state energies changed between the HITRAN 2004 and HITRAN 2016 compilations?

Yes. However, R17 uses the HITRAN 2004 values. In fact, updating intensities by more accurate values will result in significant deterioration of the model if the mixing parameters are not redefined. The latter is the subject of another analysis which shall be published soon. This does not affect the work presented here, as differences between HITRAN 2016 and 2004 values are within the stated uncertainty. We added the following sentence to the revised manuscript: "Although newer calculations are available (HITRAN 2016, Gordon et al., 2017), the differences are within the assumed uncertainty."

Page 12, line 377: Later in the paper, there is a reference for the JPL catalogue. Please also add the reference here.

Done. Thanks.

Page 14, line 438-439: please add citation/reference for the 22 GHz line intensity for clarity here.

Agreed. We add the reference to HITRAN 2012 (Rothman et al., 2013) for the 22 GHz line intensity and Payne et al. (2008) for line width.

Page 16, line 500: Please provide more information here on the indirect method used in R18.

Since we believe the method used here is more rigorous than the one previously used in R18, we prefer to leave the details to that reference. However, to provide some general information, we changed the following sentence "estimated using a more indirect method in R18" to "estimated in R18, by means of an analogy with data from Payne et al. (2011)."

Page 25: How does the uncertainty associated with spectroscopic parameters compare to the uncertainty associated with instrument noise for these examples? Please comment.

Interesting question. We checked the instrument noise contribution, i.e. the diagonal terms of \mathbf{Cov}_m in Eq. (39). It results of comparable magnitude (with respect to the absorption model parameter contribution), though with different vertical shape and little dependence on climatology. We have added this information at the end of Section 5.2.

Page 28, lines 873-874: "the laboratory and field measurements". Although these are presumably referenced in Tretyakov et al. 2016, this is a very interesting point for many potential readers of

this paper and therefore it would also be helpful to include the references for these laboratory and field measurements here directly also.

Correct, the references for the laboratory and field measurements are given in Tretyakov et al. 2016. Although we could report the same references here, we prefer to refer to Tretyakov et al. 2016 only, as it collects results from at least 6 different sources to produce the figure (their Figure 19) leading to the conclusion we reported.

Typos/word choice

Page 9, line 259: “from the microwave to **the** far infrared range”

Page 10, line 303: Please consider replacing “retrieved” with “determined”, since “retrieved” has its own other meaning in this context.

Page 10, line 312: Please consider replacing “involved” with “associated”.

Page 10, line 313: Please consider replacing “retrieved” with “taken”.

Page 11, line 342: “of which 37 ****are**** within the 60 GHz band, one ****is**** at 118 GHz and the remaining 11 ****are**** in the sub-mm range”

We thank the reviewer for spotting the above typos and making suggestions for word choice. We have accepted them all.