Response to Referee #2: Greenhouse gas profiling by infrared-laser and microwave occulation: Retrieval algorithm and demonstration results from end-to-end simulations

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We thank the reviewer for the detailed and very careful review and the helpful and constructive comments which we will all take into account in the revision of the paper. Please see our detailed responses below (comments of reviewer italicized, author response below each comment).

In order to make sure that the revisions we intend to do as quoted below refer indeed to the paper version where we will implement them, we refer in our response to the pages and line numbers of the official AMTD paper version. We understand, however, that the reviewer had a different version.

General comments:

- **Comment on spectroscopic errors:** *One issue that I think is missing is the sensitivity of the results to spectroscopic errors. Could uncertainty in the knowledge of the spectral lines change conclusions? Please discuss briefly, e.g., in a discussion section.*
  As errors due to uncertainty of spectroscopic parameters is a separate issue of introducing time-constant errors (or offsets from "true"), but not time-varying biases, we did not address it here. We did discuss these errors and related spectroscopic measurement requirements in Section S2 of Kirchengast and Schweitzer (2011), as well as in the specific paper of Harrison et al. (2011) (not yet cited in the AMTD paper version yet since very recent but meanwhile in press). Spectroscopy "simply" needs to be improved prior to launch to within the requirements as discussed in these references and as such does not change conclusions of this paper. We agree, however, that we should at least briefly refer to this issue which we will add in the revised paper on p. 2281, line 9, two sentences as follows "Errors in spectroscopic parameters are not considered in this study because, on the one hand, they lead to essentially time-constant retrieval errors only with negligible effects on observing GHG variability and, on the other hand, their reduction is a separate matter

of spectroscopic laboratory work. Kirchengast and Schweitzer (2011), section S2 therein, and Harrison et al. (2011) discuss the requirements and needs for reducing spectroscopic errors to within ∼0.1 % in detail."

- **Comment on the word "grid":** *Use of the word "grid": I tend to think of a "grid" as a 2D mesh of, e.g., horizontal and vertical lines crossing each other, but in this manuscript it is used for the collection of 1D levels. Is there any precedence for that use in other papers? Please consider using the word "levels" instead of "grid" throughout the paper if you agree that this would be more correct. I will use "levels" in my comments below.*
  We carefully reconsidered the use of this term and can at several places where suitable change to "levels" which we will carefully do. But if we refer to the full vertical profile vectors as an entity then terms like vertical grid, height grid, time grid appear quite simpler and we have seen it (and used it) in several previously published papers.

Specific comments:

- **Comment to Page 1, line 10:** *"... did not yet exist" reads awkward in the abstract. I suggest to rephrase or skip sentence. Next sentence could for example read "Here we introduce an algorithm... ", which in my opinion would be sufficient and to the point.*
  Ok, we then prefer and will change to "...is not yet available."
- **Comment to Page 2, line 24:** *I suggest skipping sentence on "Subsequent work. . . ". It doesn't belong in the abstract.*
  We carefully considered this but since the second last sentence of the abstract again emphasizes that this particular study treated clear-air conditions we prefer to keep this last sentence as it consicely provides valuable perspective to important next work that shall deal with cloudy air.
- **Comment to Page 2, line 30–31:** *Perhaps "This proposed... " instead of "This new.... " and "would enable... " instead of "... enables... ", since the LMIO technique has not yet been realized.*
  Ok, done.
- **Comment to Page 2, line 54:** *It is not clear why the Schweitzer et al. (2011b) citation appears separately from the ones just above. How has the prepared airplane-to-airplane demonstration been part of establishing the expected performance of LMO? Maybe sentences should be re-arranged.*
  Ok, we will stricken the extra sentence on the prototype instrument, we agree it appears somewhat misplaced here, and will start the next sentence with "Very recently a detailed..." (this one sentence is kept separate since this most recent study is immediately relevant for this study).
- **Comment to Page 6, line 168:** *For completeness, I think the 5 frequencies*

used for the LMO ought to be mentioned in the parenthesis here.
Ok, we will extend to "(5 channels, 17.25 GHz, 20.2 GHz, 22.6 GHz, 179 GHz, 182 GHz)".

- **Comment to Page 6, line 189:** *"The related altitude levels are determined to within 10 m accuracy.". But the altitude is the independent variable in the retrievals. Thus, as I see it, the altitude is in principle exact and all errors should be attributed to the atmospheric variables (one could imagine the output levels to be fixed in the algorithm and the retrieved parameters interpolated to these levels). Please consider removing the sentence if you agree.*
  Ok, we will make clear that also the altitude accuracy estimate is a result of Schweitzer et al. (2011b) by attaching it with a semi-colon to the previous sentence, i.e., on p. 2281, line 16, we will change to "...for the specific humidity; the related altitude levels are determined..." And yes, altitude is then used as independent variable (and the errors are attributed to the dependent atmospheric variables). But still originally, when retrieving the altitude levels as part of the LMO retrieval, they of course also carry some uncertainty even though it is afterwards attributed to the dependent variables. In fact that altitude is a very accurate measurement on its own is one key advantage of radio and microwave occultation, whilst in general (passive) remote sensing techniques accrue significant errors into variables from altitude uncertainties since relying on external information or pressure-derived altitude.

- **Comment to Section 2.2:** *Consider including a figure showing the IR spectrum of relevance.*
  We reconsidered this but prefer not to again include such as figure here since we have exactly this type of figure already in Kirchengast and Schweitzer (2011), which we prominently cite in this section.

- **Comment to Section 3.1:** *It is assumed that there is a one-to-one relation between impact parameter and time. This is, however, not the case when there is atmospheric multipath. I think a short discussion is needed. Presumably atmospheric multipath is less of a challenge for the IR signals since they are almost insensitive to humidity gradients, which generally are considered the source of atmospheric multipath in GRO and LMO. Is atmospheric multipath expected to be absent for the IR frequencies?*
  Yes, the humidity dependence of the IR refractivity is essentially negligible down to 5 km. Also the LMO process providing the basic MW impact parameter profile has its own suitable bending angle and impact parameter retrieval ensuring decent impact parameter values down to 5 km (even in case of multipath useful approximate ones, but most of the multipath also in LMO as in GPS radio occultation occurs in the lower troposphere below 5 km). The IR therefore does not have a separate multipath problem and the approach to derive the IR impact parameter via the MW impact parameter is quite meaningful.

- **Comment to Equation(1) and related text:** *I don't understand why this* *iteration is necessary. I would expect that the relation between z and a is already known from the LMO retrieval. Later, on page 10, it becomes clear that the MW altitude levels corresponding to the MW measurement times are indeed available from the LMO retrieval, but they are not used. I find the arguments for why not, rather weak and unclear. For instance, in line 312: "This will ensure strict consistency of final differences of MW and IR altitudes despite some retrieval errors involved in the LMO retrieval". I don't see why using the MW $z(t)$ levels directly from the LMO retrieval should cause problems? Why would they not be the same as what you get from eq. (1)? What errors are referred to here? Is it a fundamental problem? In line 310: "... same way of using the information is advisable...". It is not clear which information is referred to here. In line 308: "... impact parameters will be naturally related [to time] based on proper geometrical-optical formulation of ray paths...". What is meant by "naturally" and "proper"? As mentioned in my comment above, one cannot generally expect a one-to-one relationship between MW impact pa- rameter (or altitude) and time because of possible atmospheric multipath in the LMO retrieval. Thus, although I understand that the LMO retrieval in the implementation presented here is based on the geometrical-optical formulation, the whole notion of computing $z(t)$ for the MW retrieval is generally and fundamentally flawed. In regions of multipath there will be more than one altitude related to a given time. However, if I understand things correctly, then it should not be necessary to know the MW altitude levels corresponding to the times of the measurements; see next comment.*

Ok, obviously we have to make these sentences more clear in various points. The key why this somewhat subtle approach is relevant is indeed that each retrieval step in LMO also propagates and adds some small (numerical) noise and there is generally some filtering. Therefore, for example, the MW altitude (after the Abel transform) is not entirely consistent and reversible with the MW impact parameter (only up to some small noise). The same applies to the relation of MW refractivity and the individual MW atmospheric profiles of p, T, q. So the point is in order to avoid slight inconsistencies even from this type of small noise it is only formally clean to right start from MW impact parameter, on the one hand, and from p, T, q for both the MW and IR refractivity, on the other hand. In fact if one has done the real implementation of the stuff in code one obviously sees the utility. But its true it is a little difficult to express but it is an important cautionary comment. Also it is true that we assume the $z(t)$ vector that we have from the MW is decent down to 5 km (at least approximately, i.e., in multipath situations with real data one would construct it "smoothed through"; but the key point is to have a good original z-levels grid and we found the one via Eq. (1) the most suitable so far). So we will make the various sentences more clear as follows "...of LMO retrieval this may not be directly related to the time grid..." "...while the impact parameters will be formally related based on geometric-optical formulation of ray paths." "...despite the small extra errors that have been incurred when retrieving p, T, q from MW refractivity." "...as introduced here is better than the direct use of..."

- **Comment to Section 3.3:** *The description of the algorithm to find the ai and zi levels is overly complex and too detailed in my opinion. The description with both i and j levels/grids is a bit confusing and makes it difficult to keep track. The notation leads to trouble in line 364 where $\alpha(a_i)$ is mentioned while referring to eq. (5), which contains a_j , not a_i. I understand it, but it is not mathematically stringent. However, I don't see why it is necessary to know the a_j and z_j levels at all. I believe the approach could be described much simpler by focusing on how to obtain the a_i and z_i levels in a more generic way. I don't think it is necessary to describe every detail of the implementation, just the main things so that it is possible (in principle) to reproduce the results. I see it this way: We have from the LMO retrieval, $p(z)$, $T(z)$, and $q(z)$. At what levels we have these is not important. Equation (2) (without the j subscript) gives $N(z)$. The Abel transform gives $\alpha(a)$. This would be the estimated bending angle as a function of impact parameter corresponding to the IR refractivity (in practice at some arbitrary levels, but it is not important; interpolation will have to be done later on anyways). As I see it, there is no need to involve the MW rays and their levels in the description, and there would be no need for the j subscripts. Geometry gives eq. (6), which could be written "$\alpha_{\mathrm{g}}(a, t_i) = \ldots$". Thus, only subscript i would be necessary to indicate a specific time of measurement, whereas a would be the independent variable in this equation. I think this would be more mathematically correct, since α_{g} in eq. (6) should be considered a function of a, not a value at some specific a_i . The specific a_i for a given t_i is then found as the value of a for which $\alpha(a) = \alpha_{\mathrm{g}}(a, t_i)$. How this is done by iteration using Newton's method or something similar (and including numerical interpolation) does not need to be described in great detail, but could be just mentioned in words. In practice this can be solved in different ways, but the end-result should be that $\alpha(a_i) = \alpha_{\mathrm{g}}(a_i, t_i))$, which is the important message to the reader. Is this a correct account of the approach, or am I missing something? If correct, there would be no need for the j indices, it would simplify the description considerably, reduce the number of equations, and make the approach easier to understand for the general reader.*

  We very carefully worked on this section and had different shorter and longer versions. We finally preferred, for introducing this first time here it is an advantage to do it in detail, including also a specific iteration approach since the given iteration is robust but fairly subtle and shows weak or no convergence if not carefully implemented. Furthermore, while it is basically true that there is no strict need to start exactly with the MW altitude grid that we derived based on Eq. (1), we found this clearly most suitable. If we would drop the j indices (one variant we considered) it becomes too general and many readers will not understand in detail that one always has to start with a certain impact parameter grid that should be as close as possible to the IR impact parameter target grid (the MW grid is ideal since the IR grid becomes to be essentially equivalent to it above about 12 km). In other words, actual reproducability will depend on details for this algorithmic part. However we will like to take into account these concerns by several modifications as follows. On p. 2289, line 4, we expand to "...(interpolated from Eq. 5)..." which avoids any trouble with notation at this point. On p. 2289, lines 9-14, and p. 2290, lines 5 and 12, we will make sure that we have subscript notation also here, so eliminate this current special use of "parantheses notation" for the iteration index k here. On p. 2286, line 24, we will add "In principle also a different altitude grid than the MW grid used here could be employed as starting point but this one was found clearly most suitable for a reliable and fast subsequent derivation of the IR impact parameter and altitude grids."

- **Comments to Equation(2):** *and related text: If I understand correctly, this formula has been derived based on a more elaborate formulation of Bönsch and Potulski (1998). It is noted that the equation follows closely the Bönsch and Potulski formulation for $\lambda > 0.5\mu m$. So $0.5\mu m$ is the lower limit of validity, but what is the upper limit? If equation (2) has not been published in this form before, perhaps it would be worth including an appendix where it is derived and verified against the Bönsch and Potulski formulation. With a rigorous treatment in an appendix, the claim that it is an improvement over the Edlén formula could be well justified.*
The IR refractivity becomes nearly non-dispersive at a wavelength of about $\sim 2\,\mu$m as shown in Schweitzer et al. (2011a) and there is no actual upper limit within the short-wave infrared region of interest here (the original papers also do not quote a clear upper limit). We verify this formula in detail as part of a separate upcoming paper on our fast LIO performance simulation tool ALPS (used for simplified performance estimation by Kirchengast and Schweitzer (2011)) so we prefer not to have it as appendix here.

- **Comments to Equation(5):** *The Abel transform is formally an integration to infinity. Here the integration stops at r_{top}. What is the value of r_{top}, and is anything done to estimate the remaining integral from r_{top} to infinity?*
The r_{top} value is determined at a height of $\sim$80 km as this is the maximum defined simulation height for the MW altitude in our current LIO/LMO setup; above this height the bending angle is in the random noise level as shown by Steiner et al. (1999). The error due to this finite top at our heights of interest below 40 km is <0.01%. We will add on p. 2288, line 8 "...numerical implementation of this Abel integral in EGOPS (setting r_{top} to 80 km, leaving negligible residual error at the altitudes of interest up to 40 km)."

- **Comments to Page 11, line 363:** *Is it correct to refer to the iteration as Newton iteration (or perhaps it should be Newton's method) when you have the relaxation factor η involved? Please check if there is a well-established name for such a scheme.*
Ok, we will refine the sentence to "We use an implementation of Newton's method for the iteration process..."

- **Comments to Page 12, line 377:** *"un-relaxed iteration can lead to convergence to a spurious bi-stable solution… beyond the first bifurcation in the state space…". Can this be supported by a reference?*
There is no good direct reference for this, only general ones for behavior of itera-

tions under nonlinear dynamics. We therefore just prefer to keep it in parentheses as a caution that there can be convergence problems without due care; we will further simplify the comment by deleting the part "of next higher order" that is not strictly needed.

- **Comments to Section 3.4.1:** *I think it would be good to add a short discussion (just a line or two) of the limitations of the defocusing correction, e.g., for a non-spherically symmetrical atmosphere.*
  Ok, we will handle this in amending the sentence on p. 2291, line 20, as follows "...by Schweitzer et al. (2011b), who also address its limitations in non-spherically symmetric atmospheres; residual effects of horizontal gradients only cancel in differential transmissions between neighbor frequencies as formed in Sect. 3.4.2 below."

- **Comments to Page 14, line 452:** *"...is used next to correct...". Should it not be "...is corrected for..."?*
  Ok, will be done.

- **Comments to Page 14, line 458:** *Interactive "...residual foreign species absorptions need correction as well.". Comment Literally, I would understand this as the residual absorptions are not quite correct, and therefore they need correction to become correct. But I suppose the meaning is something like "...residual foreign species absorptions need to be eliminated." Please clarify.*
  Ok, will be done.

- **Comments to Section 3.4.3:** *I don't understand the sentence saying that the log-transmission derivative enters the algorithm (line 499), since this is exactly what seems to be avoided when using the form by Schweitzer et al. (2011b). In my opinion it would be sufficient to only make a reference to the formula (as already done), and omit the discussion starting on line 497: "Besides...". In line 508, filtering is discussed as if it had been introduced earlier (using the words "even more refined filtering...". But only the minimization of the noise amplification by using the specific form of the Abel transform has been mentioned – is that considered filtering? Or is there some additional filtering going on? Please clarify or skip the sentence. Only the information on the vertical resolution seems important.*
  Ok, we will stricken the sentence with "Besides..." and next just say "This type of Abel transform leads to noise amplification by about a factor of 2 to 2.5 (Sofieva and Kyrölä, 2004). The implementation in EGOPS is very robust, however..." In the next paragraph we will change to "Future more special filtering may..."

- **Comments to Equation(16):** *Can a reference be provided?*
  Ok, we will add on p. 2296, line 12 "...fraction to ppmv (e.g., Salby, 1996)."

- **Comments to Page 16, lines 528–531:** *The sentence starting "In this end-to-end simulation..." seems irrelevant. Is it needed?*
  We find it a useful justification that we cite no further derived quantities, but we will simplify it by strickening the part "without loss of generality in this introductory context", and we will clarify "...we can refrain from computing these addtional

profiles..."

- **Comments to Page 19, lines 625–626:** *Mention already here that* ε_m *in eq. (18) should be specified in %. That information is important to be able to understand eqs. (17)-(18).*
  Ok, we will extend to "...express the altitude-dependent errors of the individual VMR profiles (in units %), which determine the..."

- **Comments to Page 19, line 638:** *For completeness, I think the value of the isotopic ratio,* $\delta^{13}\mathrm{C}$, *should be given. Or alternatively, the values of* $\mathrm{a}_{^{12}\mathrm{CO}_2}$ *and* $\mathrm{a}_{^{13}\mathrm{CO}_2}$.
  Ok, we extend right from Eq. (19) to ", where $a_{^{12}\mathrm{CO}_2} = 0.98420$ and $a_{^{13}\mathrm{CO}_2} = 0.01106$ (Rothman et al., 2005). The needed..."

- **Comments to Page 19, line 645:** *AMTD I suggest to write "... experience with [simulated] LIO retrieval performance..." or something similar, since there is no experience with real observations.*
  Ok, we will add "simulated".

- **Comments to Equation(21):** *What is the value of* $\mathrm{a}_{\mathrm{H}_2^{16}\mathrm{O}}$ *?*
  Ok, we extend right from Eq. (21) to ", where $a_{^{12}\mathrm{H}_2\mathrm{O}} = 0.0.997317$ after Rothman et al. (2005). In this case..."

- **Comments to Page 24, line 797–798:** *Interactive Remaining biases are at the order of 0.1%...". How can such a small bias be estimated for an individual profile? Oscillations in the results, presumably originating from the superimposed errors, are a few percent, so it seems to me to be difficult to say anything quantitatively about the bias when/if it is this small.*
  We refer to biases relative to the fully converged profile here. We will clarify this by saying "Remaining biases relative to full convergence are at the order..."

- **Comments to Page 25, line 831/870:** *"In this study we introduced a new retrieval algorithm...". It may be new, but it is also the first and so far only one existing/published, which is better than just "new". The sentence would actually be stronger without the word "new", in my opinion. When including "new" it sounds like an improvement or alternative to already existing algorithms. Also in line 870.*
  Ok, we will stricken the word "new" both on p. 2309, line 13, and on p. 2311, line 2.

- **Comments to Page 26, line 833:** *I would say "... as a function of altitude..." instead of "... and altitude levels...". See also earlier comment on the notion of altitude being the inde- pendent variable, not a retrieved parameter as such.*
  Ok, will be done.

- **Comments to Page 27, line 878:** *I would say "... so that LIO could also [potentially] help...", since it has not actually been applied yet.*
  Ok, will add in "potentially" on p. 2311, line 12.

- **Comments to Fig. 1:** *The geometry can not be correctly understood by the general reader, since the angles between the ray asymptotes and the impact parameters (a_{ir} and a_{mw}) appear to be somewhat off 90° . Please indicate right angles in the figure.*
  Ok, will be done.

Technical corrections:

- **Comment to Page 1, line 13:** *Discussion Paper "Schweitzer et al. (2011b)". Avoid citations in the abstract.*
  Ok, we will stop the sentence with "...(LMO) data."
- **Comment to Page 1, line 19:** *Perhaps "... above 10–15 km... " instead of "from 10 km to 15 km upwards... ". Similarly on page 24, line 813, the text can be misunderstood. Check for other instances.*
  We now say "from about 10 km to 15 km upwards..." (also on p. 2308, line 22).
- **Comment to Page 2, line 47:** *Very long sentence. Could be broken at "... (LIO). This vastly... ".*
  Ok, will be done.
- **Comment to Page 3, line 69:** *Wording: "determining"? Is it needed here?*
  Ok, word will be stricken.
- **Comment to Page 4, line 98:** *Interactive Better to use "such as" instead of "like". Also on page 14, line 440.*
  Ok, will be done.
- **Comment to Page 4, line 100:** *...*
  Ok, will be done.
- **Comment to Page 4, line 103:**
  Ok, will be changed to "other studies".
- **Comment to Page 4, line 125:**
  Ok, will be corrected.
- **Comment to Page 5, line 158:**
  Ok, will be done.
- **Comment to Page 7, line 209:**
  Ok, will be corrected.
- **Comment to Page 7, line 215:**
  Ok, will change "likewise" to "as well".
- **Comment to Page 7, line 216-217:**
  Ok, will be done.

- **Comment to Page 7, line 226:**
  Ok, will be done.
- **Comment to Page 8, line 263:**
  Ok, will be corrected just to “SSR” at all instances.
- **Comment to Page 8, line 269:**
  Ok, yes, will be corrected this way.
- **Comment to Page 10, line 326:**
  Ok, yes, will be done.
- **Comment to Page 11, line 357:**
  Ok, will be done.
- **Comment to Equation(8)-(10):**
  Ok, will be done as mentioned earlier above.
- **Comment to Page 12, line 376:**
  Ok, “only” will be stricken.
- **Comment to Page 12, line 399:**
  Ok, will be done.
- **Comment to Page 14, line 460:**
  Ok, will be done.
- **Comment to Page 15, line 500:**
  Sentence is now deleted, see comment earlier above.
- **Comment to Page 15, line 509:**
  Ok, will be corrected to “reduce”.
- **Comment to Page 16, line 541:**
  Ok, the part of the sentence will be stricken as suggested.
- **Comment to Page 18, line 598:**
  Ok, will be done.
- **Comment to Page 20, line 662:**
  Ok, will be corrected.
- **Comment to Page 20, line 668:**
  Ok, will be improved this way.
- **Comment to Equation(23)-(24):**
  Ok, will be set to upright SNR; also in the line above the equation. We will keep this very widely used symbol really the only one with multi-letter. It appears very confined only in this part of the text so no confusions.
- **Comment to Page 22, line 716:**
  Ok, will be changed to “the altitudes associated with these two...”.

- **Comment to Page 22, line 749:**
  Ok, “its” will be changed to “the”.
- **Comment to Page 24, line 803:**
  Ok, will be done.
- **Comment to Page 24, line 813:**
  Ok, typo will be corrected.
- **Comment to Page 26, line 875:**
  Ok, will be done.
- **Comment to Page 26, line 880:**
  Ok, will be changed to “O_3 signal-to-noise ratio...”.
- **Comment to Page 28, line 930:**
  Ok, will be done.
- **Comment to Page 29, line 982:**
  Ok, will be corrected.
- **Comment to Page 30, line 1029:**
  Ok, typo and filename will be corrected.
- **Comment to Fig. 4, panel d:**
  Ok, we will put it to superscript or correct as you suggest.

References

Harrison, J. J., Bernath, P. F., and Kirchengast G.: Spectroscopic requirements for ACCURATE, a microwave and infrared-laser occultation satellite mission, J. Quant. Spectrosc. Ra., In Press, doi:10.1016/j.jqsrt.2011.06.003, 2011.

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Steiner, A. K., Kirchengast, G., and Ladreiter, H. P.: Inversion, error analysis, and validation of GPS/MET occultation data, Ann. Geophysicae, 17, 122–138, 1999.