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Interactive comment on "Greenhouse gas profiling by infrared-laser and microwave occultation: retrieval algorithm and demonstration results from end-to-end simulations" *by* V. Proschek et al.

Anonymous Referee #2

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General comments:

I think this is a very good and interesting manuscript describing an algorithm for retrieving various species of green-house gases (GHGs) from (hopefully) future LEO-LEO microwave and infrared-laser occultation (LMIO) measurements. The performance of the algorithm is assessed by end-to-end simulations, and the authors have included a number of potential error sources in the assessment. The retrieval approach seems robust and efficient, and the results look very promising. The manuscript is generally well written and well organized, but could be shortened in places. The science is innovative, the algorithm is the first of its kind, and the scientific quality is high.

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I recommend publication in AMT after revision. 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.

I find parts of the algorithm description overly complex and too detailed. In my specific comments I have suggestions to shorten and simplifying the algorithm description and the number of equations.

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.

Below, I refer to the version of the manuscript provided to me for review. Page and line numbers are different from those in the version available on the AMT website.

Specific comments:

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.

Page 2, line 24: I suggest skipping sentence on "Subsequent work...". It doesn't belong in the abstract.

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.

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 demon-

stration been part of establishing the expected performance of LMO? Maybe sentences should be re-arranged.

Page 6, line 168: For completeness, I think the 5 frequencies used for the LMO ought to be mentioned in the parenthesis here.

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.

Section 2.2: Consider including a figure showing the IR spectrum of relevance.

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?

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...".

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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 parameter (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.

Section 3.3: The description of the algorithm to find the a_i and z_i 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 i subscripts. Geometry gives eq. (6), which could be written " $\alpha_{g}(a,t_{i}) = \dots$ ". 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 $\alpha(a) = \alpha_g(a, t_i)$. 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 $\alpha(a_i) = \alpha_g(a_i, t_i)$), 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.

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 0.5μ 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.

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?

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.

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?

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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.

Page 14, line 452: "... is used next to correct...". Should it not be "... is corrected for..."?

Page 14, line 458: "... residual foreign species absorptions need correction as well.". 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.

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.

Equation (16): Can a reference be provided?

Page 16, lines 528–531: The sentence starting "In this end-to-end simulation..." seems irrelevant. Is it needed?

Page 19, line 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).

Page 19, line 638: For completeness, I think the value of the isotopic ratio, δ^{13} C, should

be given. Or alternatively, the values of $a_{12}CO_2$ and $a_{13}CO_2$.

Page 19, line 645: I suggest to write "... experience with [simulated] LIO retrieval performance..." or something similar, since there is no experience with real observations.

Equation (21): What is the value of $a_{H_2^{16}O}$?

Page 24, line 797–798: "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.

Page 25, line 831: "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.

Page 25, 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 independent variable, not a retrieved parameter as such.

Page 26, line 878: I would say "... so that LIO could also [potentially] help...", since it has not actually been applied yet.

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.

Technical corrections:

Page 1, line 13: "Schweitzer et al. (2011b)". Avoid citations in the abstract.

Page 1, line 19: Perhaps "... above 10-15 km..." instead of "from 10 km to 15 km

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upwards...". Similarly on page 24, line 813, the text can be misunderstood. Check for other instances.

Page 2, line 47: Very long sentence. Could be broken at "... (LIO). This vastly...".

Page 3, line 69: Wording: "determining"? Is it needed here?

Page 4, line 98: Better to use "such as" instead of "like". Also on page 14, line 440.

Page 4, line 100: "receive[r]".

Page 4, line 103: "... as discussed by [others] (Emde and ...).

Page 4, line 125: Kirchengast and Ramsauer (2002), not in reference list, but there is a Kirchengast, Fritzer, and Ramsauer (2002) (line 985).

Page 5, line 158: To improve readability I suggest something like "... variables, namely pressure (p), temperature (T), and humidity (q), as well as the concentration..." instead of "... variables pressure p, temperature T, and humidity q and the concentration ...".

Page 7, line 209: I believe it should be "excess" instead of "access".

Page 7, line 215: Wording: "likewise"? Could it be omitted?

Page 7, line 216–217: "LIO SSR parameters" instead of "SSR LIO retrieval parameters".

Page 7, line 226: Perhaps "tie" instead of "allocate".

Page 8, line 263: Wording: "... SSR single species retrievals...". SSR already stands for "single-line trace species retrieval". Also on page 16, line 538 and page 17, lines 552 and 554. Check for other instances.

Page 8, line 269: Do you mean "... that have already..."?

Page 10, line 326: Perhaps "single-equation" instead of "one-equation".

Page 11, line 357: I suggest: "The angle θ_i ...", not to start the sentence with a symbol.

Equation (8)-(10): Iteration index k was earlier a subscript (in Eq. (1)). Here it is in parentheses.

Page 12, line 376: The meaning of "only" here is unclear.

Page 12, line 399: "dark red boxes"? In Fig. 3 caption is says "light red boxes". I see only one red color in my copy of the manuscript. I also see orange, green, light green, and grey boxes. If there are two different reds, they need to be more distinct.

Page 14, line 460: "... for..." instead of "... from...". Two places.

Page 15, line 500: "derivative with respect to" instead of "derivative after".

Page 15, line 509: Typo: "... may slightly reduced this noise...".

Page 16, line 541: Unclear what is meant by "as seen from the first demonstration results of this study". Could it be omitted without changing the meaning of the sentence?

Page 18, line 598: I suggest to insert "The concentrations of" (or similar) before "N $_2$ O and CH $_4$...".

Page 20, line 662: "... the the...".

Page 20, line 668: Perhaps "... unbiased with a standard deviation less than 1%..." instead of "... unbiased and reaching a standard deviation of within 1%...".

Equation (23)-(24): Mix of SNR (italics) and SNR. By the way, SNR is an acronym, not a mathematical variable. Avoid using multi-letter symbols in equations.

Page 22, line 716: "... altitudes just of these two...". Something is wrong here.

Page 22, line 749: "Given its". What does "its" refer to in this sentence?

Page 24, line 803: Perhaps "confirms" instead of "fully shadows".

Page 24, line 813: "s[t]ratospheric".

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Page 26, line 875: I would say "Carbon dioxide" instead of " CO_2 ", to avoid starting the sentence with a chemical symbol.

Page 26, line 880: "signal-to-noise [ratio]".

Page 28, line 930: "ILO" should be in capitals, I suppose.

Page 29, line 982: "Gonzlez", missing a letter.

Page 30, line 1029: "performa[nc]e". I believe the correct filename is: "WCV-SciRep-No34-SSchweitzer-Jun2010.pdf".

Fig. 4, panel d: Maybe use unit 1/m for absorption coefficient, if the plotting tool does not allow to write m^{-1} .

Interactive comment on Atmos. Meas. Tech. Discuss., 4, 2273, 2011.