Review: Insights into 3D cloud radiative transfer for OCO-2

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1 Principal criteria

- **Scientific significance:** Does the manuscript represent a substantial contribution to scientific progress within the scope of Atmospheric Measurement Techniques (substantial new concepts, ideas, methods, or data)?
  FAIR
- **Scientific quality:** Are the scientific approach and applied methods valid? Are the results discussed in an appropriate and balanced way (consideration of related work, including appropriate references)? Note that papers do not necessarily need to be long to be scientifically sound.
  GOOD
- **Presentation quality:** Are the scientific results and conclusions presented in a clear, concise, and well-structured way (number and quality of figures/tables, appropriate use of English language)?
  FAIR
- **Reviewer recommendation:** **ACCEPT WITH MAJOR REVISIONS**

2 Review summary

This paper provides an evaluation of the effects of three dimensional (3D) radiative transfer (RT) on the spectra measured by NASA's Orbiting Carbon Observatory -2 (OCO-2) due to clouds within close proximity (several to tens of kilometers) of the ground footprints. Clouds impose a 3D effect that increases as the distance to the nearest cloud decreases. The 3D effect is currently unaccounted for in the full physics retrieval algorithm that is used to derive estimates of total column carbon dioxide (XCO2) from the measured radiances. Using simulations of 1D and 3D radiances (from the SHDOM RT model) for realistic OCO-2 scenes, the authors demonstrate that 3D perturbations to the radiances are of the same order (or greater) than reasonable perturbations to other key retrieval state vector elements, such as surface pressure and aerosol loading. The effect is shown to be significant relative to the precision requirements of the mission on the order of 1 part per million (ppm). It is therefore important to characterize and quantify the 3D effect in order to continue improving the XCO2 estimates in future versions of the data products. **Overall, the paper is well organized and written in fluent English, with appropriate figures to describe the results of the analysis. However, due to a couple of significant concerns, I have to recommend that major revisions be performed.** My primary constructive comments are itemized below, approximately in order of importance.

- **It seems to me that the current work is very similar in nature to the work presented in [Massie, AMT, 2021].** The only clear difference I can determine is that the current work utilizes "bar cloud" calculations, which were not present in the 2021 manuscript. The authors need to make it explicitly clear how the implementation of bar clouds in the current research leads to either substantially different results compared to [Massie, AMT, 2021], or corroborates the previous results. Otherwise, I do not really understand the purpose of the current publication. Is it fair to say that the current research refines the 2021 research, and demonstrates the 3D effect using more first principle physics (or something like that)? In general, the previous publication did clear up some of my questions related to the current research. For example, the description of Fig. 2 in [Massie, AMT, 2021] is more clear than the description of Fig. 5 in the current research. In effect, the figures are the same.
- **The overall conclusions drawn from the analysis are not clear or strong enough.** I'd prefer the conclusions section to be more succinct and void of the analysis details (which should appear in Sections 3 through 6). The authors effectively demonstrate the high frequency of occurrence of the cloud 3D effect on the OCO-2 measurements (40% of all OCO-2 measurements are within 4 km of a cloud!). They effectively demonstrate that the average 3D perturbations will cause errors in the XCO2 estimates on the order of 0.5 ppm, which is highly significant to the scientific goals of the OCO-2 project. However, they also effectively demonstrate, by

analysis of both good (QF=0) and bad (QF=1) data, that the current operational OCO-2 quality filtering routinely identifies the scenes with larger 3D contamination, which would thereby have larger XCO2 errors. **The main criticism is that no real conclusion or recommendation is drawn about the potential for correcting or improving future versions of the OCO-2 XCO2 product based on the results presented in this analysis.** This work seems to be an important stepping stone towards a robust solution, but that thought is never expressed. Ideally, in the future, some methodology could be put into place to "save" the "bad" quality flagged (QF=1) data, or to minimize the size of the dp bias correction term necessary to correct the raw XCO2, but the authors never really say that directly. As it currently stands, one could make the argument that the operational QF/BC is already doing a pretty good job of accounting for the 3D cloud effect, so why should additional effort/resources be put into mitigating it using (closer to) first principles physics? I recommend that the authors address this issue, at least in theory, and discuss proposed future work. Furthermore, I recommend reducing the verbiage in the Conclusions section itself. Many of the sentences there are very detailed and seem misplaced, as if they should belong in the technical discussion in the main body of the text. I have a number of specific recommendations in the technical corrections below.

- **Any new conclusive thoughts should also be amplified in the Abstract to bring the message home quickly to the casual reader.** I feel like in general, the abstract is a bit too detailed and could use more focus on the "big picture" of why the work is important, how/why it is a difficult problem to address, and what the possible solutions might be.
- **Interpretation of Fig 5. and the discussion of the results in Sec. 3.3 (radiance perturbation sensitivity) are of paramount importance to this work, but unfortunately, as currently written they are quite confusing.** I wonder if both the figure and the discussion could be reorganized, or at least better explained, to aid the reader. After a while I think I determined that the x-axis is the 17 values of the Total Vertical Gas Optical Depth (TVGOD) that is described on Line 217. That point needs to be made explicit, as I got stuck thinking that these were iterations of aerosol optical depth in the retrieval for sensitivity testing. But when I read the analysis of the results in Sec 3.3 I cant really follow along in the figure. For example: Lines 312-316 suggest that there will be an increase in radiance if surface reflectance or AOD are increased. What am I supposed to see in the figure that suggest that, because I cannot see it. Are the results in Fig. 5 due to a single perturbation of each variable? If so, then are the results robust to further perturbations? If the figure already somehow contains results for multiple perturbations of state vector values, then I dont understand how that is displayed. That to me would suggest that the TVGOD on the x-axis is not in fact a proxy for channel/wavelength. My impression is that the graph is meant to demonstrate that the 3D effect is much larger than the effect due to perturbing the state variables, seen by the fact that the 3D curve is far away from zero for most TVGOD, while most of the other variables are close to zero at all TVGOD. The exception being Refl.
- Some discussion should be given (might be very brief) as to why the 3D effect cannot be accounted for in the L2FP retrieval simply by embedding the SHDOM RT model to calculate it directly due to the massive computation cost, plus difficulty in parameterizing 3D cloud effects. I'm not sure that this is ever mentioned explicitly (?).
- In Sec. 4 (Amazon and Ocean Glint scenes), a large number of lines (about 40, 6% of total paper) are used to describe the details of the calculation for determining the fraction of cloud shadowing scenes compared to the fraction of cloud brightening. It felt like a bit of a distraction since the conclusion is that cloud shadowing only occurs for on the order of 1-4% of the converged retrievals. I wonder if the details of the cloud shadowing determination would be better moved to a technical appendix. Or, perhaps the authors could work to shorten the description if they prefer to leave it in the main body of the document.
- In general, throughout the text, I found the mathematical notation unwieldy. I would recommend making improvements to aid the readers ability to interpret. Specific examples are given below in the Technical errors/corrections section.
- For all of the results presented in the various sections, it seems like a number of important assumptions were made. I have a feeling that these were all well thought out, but there is no indication as to the robustness of the results for different sets of assumptions. Specific examples are given below in the Technical errors/corrections section.
- The scope of the research is limited to the Amazon for land observations, as well as ocean observations. I un-

derstand the interest and the fact that the cloud morphology is such that the 3D effect is highly relevant. But have other regions been examined? Are the results robust? I'm thinking that regions with brighter surfaces will likely have additional complications of multiple scattering effects, perhaps yielding different 3D contributions (potentially even in sign)? Please state clearly what you have and haven't studied in this work, and that only Amazon forest oceans have been examined, and potentially also mention this as future work, as characterizing 3D effects over different surfaces is an important follow-on.

- Most of the figures would benefit from the use of sub panel lettering, e.g., (a), (b), (c).
- The title and all of the analysis/discussion is focused on OCO-2. But the general principles are applicable to OCO-3. Might we worth mentioning in some form or fashion to broaden the utility. (I'm aware that the "distance to nearest cloud" data does not exist for OCO-3, making actual analysis difficult/impossible.)
- I wonder if there is a tie-in to the results presented in Emily Bell's swath-bias paper (https://doi.org/10.5194/amt-16-109-2023)? Although that work was specific to biases in XCO2 for OCO-3 Snapshot Area Maps, statements, such as;

  "These simulation studies reveal that SB is primarily and intimately connected to the presence of aerosols and the interplay of their optical properties with the solar and instrument viewing geometries. We now have a better understanding of the types of scenes that are likely to suffer from SB – those with high aerosol depths, or aerosols that are lofted higher in the atmospheric column, and in geometries with broader ranges of observation and solar zenith angles. Future work may involve a more detailed study of how the physics of aerosol optical properties with viewing and solar geometries combine to produce an SB response."

  seem highly relevant to your cloud 3D work. Just something to consider.

3 Technical errors/corrections

- Title: might be useful to insert the word "effects" between "transfer" and "for".
- Abstract: Line 33 provides summary result for ocean glint, but does not mention land results.
- Introduction: Line 39 mentions XCO2 measurement accuracy of 0.25% ($\approx$ 1 ppm). Note that although this is the formal project requirement, I think the science is suggesting that biases on the order of 1 ppm would actually be much to large for source/sink inversion work, e.g., [Chevallier, GRL, 2014, Toward robust and consistent regional CO2 flux estimates from in situ and spaceborne measurements of atmospheric CO2]
- Line 44: "The OCO-2 experiment" could/should be "The OCO-2 satellite".
- Introduction: would be good to add a sentence or phrase in the satellite description (near line 50) that mentions sun-sychronous polar orbit moving from SE to NW. That seems relavant to some of the figures and discussions of the sun/sensor geometries.
- Line 51: mention ACOS version (v10).
- Line 52: This sentence uses "XCO2" where I think "CO2" is the appropriate term. XCO2 is a calculated quantity and is not directly measured in the WCO2 and SCO2 as suggested. And I'm not sure that XCO2 was defined?
- Line 53: someone recently informed me that the Rodgers 2000 citation should be replaced with Rodgers 2004, which was a reprint that corrected a lot of typos (small thing). @bookRodgers:2004:InverseMethods, address = 5 Toh Tuck Link, Singapore 596224, author = Clive D. Rodgers, edition = Reprint, isbn = 981022740X, isbn-13 = 9789810227401, keywords = Atmospheric Science, pages = 238, publisher = World Scientific Publishing Co. Pte. Ltd., title = Inverse Methods for Atmospheric Sounding: Theory and Practice, year = 2004
- Line 56: mention which version of the ABSCO files (v5.1) are used in the ACOS v10 retrieval.
- Lines 56-58: Seems like the sentence describing the specific advances in ABSCO v5.1 is unnecessary. Is this information used anywhere else in the paper directly?
- Line 62: check spelling for TCCON Wunch citation!

- Line 69: Equation (1) seems unnecessary. Is this information used anywhere else in the paper directly?
- Lines 64-72 describes in some detail the various individual bias correction parameters. I'm not sure if this is really needed? For the most part these terms are not used again, with the definite exception of dp. I would recommend either remove the descriptions if they are not needed, or alternatively, discuss somewhere in the paper how they may relate to the 3D cloud effect.
- Line 72: The description of the bias correction increasing XCO2 by 2 ppm is misleading. It sounds like just a single global offset. There are a number of parameters (you described just above), a footprint correction term and global land/ocean values. You would probably be best off to just point to the details in the OCO-2 v10 Data User's Guide, which I dont think you currently cite. Alternatively, as mentioned above, you could flesh out more in the results discussion how the 3D effect may (or may not) influence the necessary bias correction and whether mitigation of the 3D effect could in theory mitigate the bias correction. That could be interesting since great effort is spent to achieve small improvements in the successive versions of the XCO2 product.
- Line 74: Could be useful to cite some of the UQ publications at the end of this discussion, e.g., Connor, AMT, 2016, 10.5194/amt-9-5227-2016 and/or Hobbs, JUQ, 2017, 10.1137/16M1060765.
- Line 81: "Of the [approximately one] million…collected by OCO-2, [only] about 25%…passed into the operational retrieval [due to prescreening for scenes contaminated by clouds and heavy aerosol loadings]."
- Line 83: replace "radiances" with "soundings"
- Line 83: The sentence "A quick determination…" should be preceded with "One preprocessor, uses only the O2 A-band to provide a computationally quick…".
- Line 85: Replace "A second quick algorithm…" with "The second preprocessor performs single band retrievals of XCO2 using both the WCO2 and SCO2 bands independently".
- Line 87: Add sentence: "This often identifies scenes with aerosol contamination due to the spectral dependence of aerosol absorption."
- Line 88: Here you mention that the 3D effect is not included in the operational retrieval. Here, and/or elsewhere, I feel like it is relevant to drive this point home. And also to comment on why SHDOM cannot effectively be used as a direct solution in the retrieval due to computation cost, and difficulty in parameterizing 3D cloud effects in the state vector.
- Line 91: Here or somewhere you should mention approximate footprint size of OCO-2 and note that the effective footprint size is not fixed but increases/decreases with viewing geometry. I think Crisp's 2017 AMT paper 10.5194/amt-10-59-2017 has the best description.
- Line 101: It's a bit awkward for Fig. 6 to be the first figure referenced.
- Line 110: "OCO-2 type spectra"?…do you mean "OCO-2 like spectra"? That sounds awkward too. Same comment about "OCO-2 type retrievals".
- Lines 114-116. This is the first example of what I find to be awkward/confusing in-line mathematical notation that I mentioned in my summary comments. I'm not sure if you want to break these out as numerically labeled equations (like you have for the current Eq. (1)). At any rate, if you are using Latex, the notation could be made more elegant by using subscripts and other formatting tricks. If you are using MS Word or some other "low level" editor, then well, I guess you're stuck!
- Line 116. Recommend replacing "zero" with "0.0".
- Line 186: Mention of "3D Stokes radiation field" needs to be fleshed out with a bit more description.
- Line 195: Either mention ABSCO v5.1 here, or since it was already discussed earlier, maybe this whole sentence is unnecassary.
- Line 202-203: Regarding "windspeed specified from the Lite file data". These estimates were erroneous in ACOS L2FP v10, were they not? Aronne would know. May or may not be relevant to your work.
- Line 206: Are the assumptions for cloud and aerosol particle radii fairly robust? Is it a safe assumption that your overall results are pretty robust to reasonable perturbations of those parameters? Is there any way to

easily defend? In reality these values vary, especially by aerosol type, right?

- Line 207: insert “up” between “km” and ”to”.
- Line 209. Missing period at end of sentence. Also, what is this assumption based on besides convenience? Is it defensible and/or do you know if results are robust to perturbations?
- Line 215: “sulfate aerosol”. Why? What is this assumption based on? For Amazon scenes I would think organic carbon would be a better aerosol type assumption, while for ocean glint it would seem sea salt would be best assumption. Furthermore, ACOS L2FP uses 2 aerosol types per soundings. Any comments? Not sure how relevant any of that is to the overall results.
- Line 216: “Stokes field”. Needs ellaboration. See previous comment. May be able to get away with just citing the relevant section in the L2FP ATBD (?). Later I see this is done at Line 226! Maybe move citation earlier?
- Line 216-219: “for 17 total vertical gas optical depths”. It took me some time to realize that total vertical gas optical depth (TVGOD, haha) is a proxy for the wavelength/channel dimension, where, as you say “the lowest gas optical depth is each band corresponds to the band continuum”. And by extension, the highest TVGOD corresponds to deep absorption lines. Is that right? I think this is also part of my confusion with trying to interpret the results presented in Fig. 5. I suggest that this point be made a bit more clear. I just wonder how many readers familiar with OCO, but maybe not so familiar with RT theory, may get a bit confused like me, or worse. Since discussion of radiances is an integral part of this work, I also wonder if it might be instructive to generate a new 3 panel figure plotting example OCO-2 spectra for each band, with the 17 selected TVGOD points highlighted. To me that one simple figure would alleviate much of th confusion about this dimension. Again, this pertains directly to my confusion in initial interpretation of Fig. 5!
- Line 226: Would it be instructive to make detailed comparisons of observed and simulated SHDOM spectra as spectral residuals? Not sure? Or what about plots of the simulated 1D vs 3D spectra? Seems like that could be a valuable lead-in to sensitivity discussion in Sec. 3.3. Again, not sure how useful it really would be. Looking ahead to Line 250, I can visualize a plot of 1D and 3D spectra plotted against the left ordinate for an example scene, with the ratio plotted against the right ordinate (and wavelength or TVGOD plotted on the abscissa).
- Line 234: Again, a bit odd to reference Fig. 6 when we have not yet gotten to Fig. 1. But maybe okay.
- Line 265: “...the ratio decreases [slightly] as the cloud distance...then increases [drastically] as distance D...”
- Line 267: Might be helpful to indicate the value that the ratio actually increases to.
- Line 302 and 305-306: Another example of somewhat unwieldy in-line mathematical notation.
- Line 325: where does the “2 to 4%” come from? I dont see anything in Fig. 5 that matches this description. I see the 3D curve ranging from 0 to 4% in the A-band as a function of TVGOD, 1-3% in the WCO2 band, and 0 to 2% in the SCO2 band. I must be misinterpreting the figure. See previous comments.
- Line 337: The sentence “Fig. 5 illustrates the zero-order physics...” seems like it would be better placed near the opening of the section. Again, I feel like Fig. 5 either needs to be reformed somehow to be more intuitive, or at least the orientation of it in the text needs to be more upfront. Walk the reader through the interpretation of a single variable for instance, and then the reader can extrapolate that knowledge to the other variables and spectral bands.
- Line 343-346: The last sentence in this section is very awkward. I think I know what you are saying, but recommend that it be reworded to be more concise and clear.
- Line 350: “detailed SHDOM calculation”. I’m pretty sure that this is a typo and should be MODIS radiance fields, as is correctly given in the figure caption.
- Line 353: “atmosphere [used in simulations] is derived from the...”
- Line 367: typo: change “point that those” to “points than those”
- Lines 379-420: As mentioned in my summary, I feel that this discussion is overly long in context of it’s importance to the overall results and relative to the overall length of the paper. I recommend either moving most of the details to a technical appendix (if you feel like it is important to preserve the details for someone to reproduce) or just shorten the discussion to get to the main point that cloud brightening events heavily dominant

cloud shadowing events. It's an important point, but probably does not need to take up so much space and kind of derail the reader.

- Line 419-420: what's the split between QF0/QF1 for the cloud darkening scenes? Similar to or different than the cloud brightening scenes?
- Line 423: change "data points" to "soundings".
- Line 435: typo? Should "Fig. 6" be "Fig 7"?
- Line 439: recommend replacing "can reach" with " are significant".
- Line 445: Table 3 - is it necessary? Doesn't add much useful information to me.
- Line 451: "presents [results for] individual…".
- Line 453: "…for the smallest gas optical depth) [versus the nearest cloud distance taken from the 3D metric file…".
- Line 458: "In the [operational OCO-2] bias correction…".
- Line 459: Instead of citing O'Dell, AMT, 2018 for the v8 data, it would be better to cite here the OCO-2 v10 DUG which contains the tables of variables and thresholds used for filtering and bias correction.
- Line 470 area: need to refer to the lettering labels for individual subplots, e.g., "panel (a) of Fig. x…". See comment in Summary section.
- Line 503: typo? Remove "a" after "Table 1".
- Line 506: The phrase "are amply sufficient to add sufficient 3D radiances to bring forward model and observed radiances into agreement" is super awkward. Recommend rewording.
- Line 508-509: It's likely that the ACOS v10 land/ocean dp terms have different thresholds. You could check the DUG tables.
- Line 510: "Figure 12 displays [the Amazon] land glint data."
- Line 528: " approximately 4km [on average] from clouds…"
- Line 536: Awkward to first discuss panels (e) and (f) of the Fig. 14. Either rearrange the figure to put ocean glint panels at the top row, or rearrange the text.
- Line 541: "displayed in Fig. 15 [for year 2016]".
- Line 553: "by approximately [2.2] ppm per year"
- Line 556: "as a function of nearest cloud distance". I don't see this metric in Fig 16?
- Line 557: "raw XCO2" Typo? Should that be "dp"?
- Line 555-562: What is the conclusion from Fig. 16? Is it just as it relates to the analysis of the results presented in Fig. 17? (line 574).
- Line 564: "as a function of nearest cloud distance". Again, I don't understand how that metric appears in this figure. It seems like you mean that the rawXCO2 is a function of nearest cloud distance, so maybe the phrase is just misplaced.
- "toss out" should be "identify".
- Line 579: Recommend "between clouds" should perhaps be "in the vacinity of clouds".
- Line 586: Recommend "But cloud…" should be "However, cloud…"
- Line 592: Recommend putting "ratios greater than unity" and "ratios less than unity" in (parenthesis).
- Line 594-603: All of this detailed discussion would be better in Sec 5 rather than the Conclusions.
- Line 610-617: All of this detail might be better in the analysis sections.
- Line 623-631: Most of this paragraph belongs in analysis section. Or reword each of these multi-sentence paragraphs down into a single conclusive sentence.

- Line 632-640: This paragraph should be earlier in the Conclusions. This is good "high level" discussion that sets the tone for why the work is important. But I would avoid citation and analysis of individual Figures in the conclusions, but that maybe personal taste.
- Line 641-647: This paragraph also should come at the outset of the Conclusions, but in a general way without referring directly to the figures.
- Table 1: I cannot tell from the discussion if the simulations were a single iteration of each state parameter by the perturbation amount listed in the table. Or were there multiple iterations of the perturbations to state vector elements? This point needs to be clarified here and in the main text.
- Table 2: I dont love using footnotes in the table. Might be better to describe in the caption? Personal taste?
- Table 3: Is this table actually helpful in anyway? I feel like it is fairly irrelevant to the analysis. Not sure.
- Table 4: For sure the footnote should just be in the table caption.
- Figure 2: abscissa label should include "[km]". My interpretation of this figure is that as the observation is made closer to the cloud, the 1D radiances (as modeled by SHDOM) become an increasingly smaller fraction of the SHDOM 3D radiances. This implies that the L2FP modeled 1D radiances would underestimate the true measured radiances if all of the retrieval physics were included and setup correctly. But since that is not the case, the L2FP must modify ancillary parameters such as surface albedo and aerosol in order for the modeled radiances to match the measurements. Presumably, a brightening of the surface, coupled with a lofting and/or loading of the aerosol would be required. If that interpretation is correct, it might be helpful to state that more explicitly in Sec. 3.2 when Fig. 2 is discussed (or elsewhere where relevant). This might help readers with the physical interpretation of how the L2FP retrieval is sensitive to the 3D cloud effect.
- Figure 5: I already have made a number of comments about interpretation of this figure above. A couple of more technical comments here: the contrast between the white background and the yellow Refl curve is very poor. Recommend changing to another color. Is there any concern about dependence among the state variables as each seems to have been perturbed individually? I still dont understand if this figure reflects a single perturbation of each state vector element, or if multiple perturbations are somehow wrapped in this figure. If the former, then it seems like a logical question to ask if the results are robust to further perturbations. If the latter, then I'm afraid that I'm lost.
- Figure 6: caption says MODIS radiance, while text discussion says SHDOM. I think the latter is in error.
- Figures 6+7 and 8+9: The utility of these figures would be increased if they were combined into two two panel plots (or even a single 4 panel plot?). Figs 7+9 would be more useful if they displayed the exact same X-Y range, presumably in lat/lon space. This would make them much more comparable. Plus add the OCO individual sounding points (the Xs and Os) to Figs 7+9.
- Figures 10-15: All of these figures would benefit from subpanel lettering, e.g., (a), (b), (c), which could be directly referenced in the text (rather than using awkward phrases like "the middle right panel in figure X" for example. In fact, I'm pretty sure that subpanel lettering is a requirement for AMT.
- Figures 10-12: These graphs take up a lot of space, and what are they showing besides that the operational QF procedure works?
- Figures 13-15: Might be good to utilize color to aid in interpretation. Not strictly necessary.
- Figure 16-17: The yellow curve does not show up well against the white background.