We have put our comments in bold text, reviewer's remain in standard text.

The manuscript presents new retrieval statistics for planetary boundary layer (PBL) water vapor from high-spatial resolution spaceborne imaging spectroscopy. The authors focus on a sensitivity analysis based on a coupled forward and inverse modeling in the frame of the Earth Surface Mineral Dust Source Investigation (EMIT) mission. They analyze uncertainties introduced by instrument errors, surface type, and varying solar zenith angle (SZA), and assess the overall potential of upcoming spaceborne high-resolution VSWIR instruments.

The study is really interesting, novel and well written. Especially the presentation of the statistical evaluation is of high quality. If proven robust also for real data, the concept will be of great interest for the atmospheric science community. However, I have a few comments, which follow below.

Thanks for the positive feedback and for your attentive reading. We genuinely appreciate your efforts to follow and critically evaluate this lengthy paper. We tried to balance readability and relevance without going even longer but your perspective has helped us to re-evaluate our choices.

Regarding use of "real" data, we now clearly state in the abstract that this is an observing system simulation experiment, and in the intro that this is a model sensitivity study, we then discuss in more detail the difficulty of observational comparisons (Section 3.3) and mention how this might be tested in future airborne campaigns or be thought about for other missions (Section 5).

General comments

The introduction could benefit from a clearer structure. While the two closing paragraphs including the four research questions are distinct and coherent, the remaining part could be more explicitly separated into literature research describing previous work and theoretical concepts on the one hand, and presenting the novelty and methodologies applied in this study on the other. For instance, lines 7-11 could be moved to the final
We have restructured:

- Decadal survey detail added early on
- Discussion of DESIS, PRISMA, MSI on Sentinel-2 added as new paragraph
- The pg2 lines 7—11 text has been modified and moved to just before the final two paragraphs of the introduction.
- It’s now specified that this is a sensitivity study targeted at EMIT, although many of the principles should apply to other VSWIR instruments.
- The discussion part of Section 3 could be improved by a more detailed comparison with retrieval results from already existing instruments such as MERIS. You are listing several instruments for TCWV retrievals in the introduction and the reader could get a better impression of the retrieval performance from synthetic EMIT data in case some reference values from other datasets are given.

We have added several paragraphs to Section 3.3. We try to emphasise the following points:

- Observational study RMSE includes our bias+spatial variability+retrieval error+differences between LES cases. Our bias+spread is right ball park compared with these other instruments.
- Previously published AVIRIS-NG Isofit results are also consistent, and the derived spatial variability and random error from one of the Thompson et al. (2021) flights is within the range we explore in this paper.

Overall, the manuscript would strongly benefit from an application of the presented methodology to “real” data. You basically agree with this on page 12, lines 26-28, with the statement “Limitations include the use of the same radiative transfer code for forward and inverse simulations...”. For instance, the Italian PRISMA instrument already delivers high-spatial resolution imaging spectroscopy data and could be used for PBL TCWV retrievals in the same manner as EMIT. On the other hand, if this study is intended to serve as a pure sensitivity analysis, this should be clearly mentioned in the introduction.

In the new Section 3.3 we discuss how standard comparisons don’t tell us much about our retrieved $s_x$, since we would need independent measurements of TCWV that are exactly collocated at the same resolution.

We checked the PRISMA data here: http://spazio-news.it/asi-prisma-da-oggi-la-comunita-scientifica-puo-accedere-ai-dati

I’Agenzia Spaziale Italiana wants a detailed licence agreement with description of data use etc. Given the limitations of any comparison that we mention in Section 3.3, we’re unsure of getting anything useful out of such a comparison.

We think the new Section 3.3 text justifies this choice and we added extra text in Section 5 to help point out future ways to address this limitation.

Specific comments

Page 1, lines 24-27: Could you provide a little bit more context why the knowledge about vertical moisture structure of the atmosphere is crucial for weather and climate
applications, and why thermodynamic information is a targeted observable recommended by NASA’s Decadal Survey?

We have added a quotation from the Decadal Survey and touched on what we identify as the three main reasons: PBL-surface coupling, PBL-troposphere coupling, and within-PBL cloud formation. We also only state that we are filling in just one measurement gap, and not fully addressing the goals of the survey, which also include more vertical detail and diurnal sampling. That’s a rabbit hole we avoid since it adds little to our study.

Page 2, line 14: “However, similar capacity is anticipated...”. I would go beyond and replace “similar” with “improved” since SBG and CHIME will most likely be offering even higher spatial-resolution than EMIT.

We changed this to “similar or superior” since we do not know the full specs and in-orbit performance yet, and “capacity” could be interpreted in different ways, e.g. swath size, sampling/revisit time, instrumental noise etc.

Page 3, lines 12-14: The reader could get the impression that the AVIRIS-NG flights were selected for this study. Please try to rephrase and clarify.

Changed to: “Thompson et al. selected these flights...”

Page 3, line 18: Although it is explained later on, it would be good to have a short definition of the “true TCWV” here, e.g., “…, which was used as input for our forward simulations...”.

Change made

Page 6, line 8: Please define the quantity \( \rho_s \).

“surface reflectance” inserted before.

Page 6, line 10: Don’t you miss to list the spherical sky albedo here when mentioning the flux calculations coming from MODTRAN?

This is a good catch, thanks. We changed the ordering of this section a few times before submission and have carefully re-read it. We think all properties are now properly introduced.

Page 6, line 11: I think it would be better to say “spectral response function (SRF)” instead of “line shape (ILS)”. This might be more common in the remote sensing community.

Change made, but we don’t refer back to it so acronym removed.


Citations added, and “for summary see...” removed.

Page 6, lines 14-15: Is the number of DISORT streams of importance for your application? Either remove it or explain why you used 8 streams.

This was inserted on autopilot by someone who’s spent a lot of time doing RT sensitivity tests. This matches the default Isofit configuration and isn’t important
for our application, so we removed it.

Page 6, lines 24-25: You define the used reflectance quantity as the hemispheric-directional distribution function on page 7. However, it would be good to have the definition here, directly after introducing Eq. (1).

The HDRF mention and Schaepman-Strub reference have been cut and pasted directly after the reflectance sentence following Eq. (1).

Page 7, lines 4-6: Did you normalize the surface prior distribution to avoid constraints on the reflectance magnitude as described in Thompson et al. (2018)?

We did not – this allows us to show absolute magnitude of the surface spectra in Figure 4. We have inserted:

“We retrieve absolute $\rho_s$, rather than the normalised value discussed in Thompson et al. (2018), and the...”


Oops – the SI text next to (original) Supplementary Figure 3 (now 4) has “Error! Reference not found”. There was supposed to be a Supplementary Table. We have moved this part of the text after Eq. (2) which describes the emulator, so we can describe performance in terms of emulator parameters:

“Tests with SZA from 14—60° show no significant differences in $a_1$ with SZA, while the standard deviation of $\epsilon$ increases by up to 25 % at SZA=60° relative to SZA=45° (Supplementary Figure 5, Supplementary Table 1). Section 3.1.4 shows how we are able to identify and remove the effect of on derived statistics, so we anticipate that our conclusions will largely apply to SZA up to 60°.”

The Supplementary Figures have been re-ordered to match their introduction in the text following the movement of this sentence.

Page 8, lines 1-2: What about other types of surfaces such as artificial surfaces or snow? Do you plan to extend your analysis to those types as part of future work? If yes, this could be mentioned in the discussion/conclusion of your results.

We felt it make sense to address the artificial surfaces at this point and have added: “The database used to generate the surface model includes artificial surfaces, which are captured in the “mineral” spectra.” This is the default surface model distributed with isofit from github, we think that just mentioning artificial materials’ inclusion is sufficient.

In Section 5 we have added a paragraph on how current development will add snow surfaces, and a quick comment on how its spectral shape might matter.

Page 10, line 8: What does “retrieved well” mean? Give quantities.

We have added:

“Surface $\rho_s$ are retrieved well, with mean bias magnitude equivalent to 0.3—1.6 % of true $\rho_s$ (e.g. for Lambertian $\rho_s=0.1$, the mean bias is 0.00021) and standard deviation of 2—4 % of true $\rho_s$.”

It’s quite fiddly phrasing but we think this provides the necessary information.
We calculated values from the Lambertian surface errors because for the other surface spectra there would be ambiguity between (1) calculating percentage at each wavelength, then mean of those and (2) calculating the mean bias in ρs, and then turning that into a percentage.

Page 10, line 12: Which prior mean and covariance did you use for the TCWV state vector parameter in your ISOFIT setup? And did you use the default first guess estimation based on a heuristic band ratio retrieval? It would be good to provide this information earlier in Section 3.1.1 and to discuss it in a few words as it can influence your retrieval results.

A paragraph has been added to the end of Section 3.1.1. It’s 40.0±7.5 mm in all cases but we originally cut our early sensitivity tests for length. We now show one of them in Supplementary Figure 3, in which we pick an extremely low prior of 7.5±7.5 mm. The effect on retrieved TCWV is minor: no change in gradient so σx is unaffected. A 0.15 mm change in bias, which is ~15% of total bias.

Technical corrections

We appreciate your painstaking reading and have made the suggested corrections, except where noted.

Page 2, line 10: Although “LES” is defined in the abstract, it would be nice to have the full expression here again.

Done.

Page 2, line 26: Rephrase to “…via two demonstrated approaches in order to provide a single value…”.

We rephrased the sentence instead in order to avoid repetition.

Page 3, lines 4-5: “More TCWV leads to increasing depth of H₂O absorption features relative to other wavelengths.”

Done.

Page 3, line 10: “The retrievals…”.

Done.

Page 6, line 8: Rephrase to “Conceptually, it targets ρs and the estimation of TCWV is seen as part of an atmospheric correction.”

Done.

Page 6, line 24: “…the cosine of the solar zenith angle,…”

Done.

Page 6, line 31: “…generated using…”

Done.

References


ADDITIONAL COMMENTS TO BOTH REVIEWERS

Please note that we found and corrected some figure, table and notation errors, these do not affect results.

Figure 5 – removed y ticklabels from (c,f). Added axis labels to edge subplots.

Figure 9 – x-axis label added to panel (c).

Figure 11 – axis labels added.

Table 1 – we accidentally included an old version calculated from bugged code, and have now corrected rows (vii)—(ix). The LES vertical grid definitions differ between simulations (either Arakawa A-grid or C-grid). The biggest issue was that for C-grids our early code smeared upper-LES qv into the reanalysis layer above, resulting in way too much TCWV. This was fixed before submission except in Table 1. For example, RICO TCWV was originally 49.6–49.7 mm in Table 1, but the new ~37 mm agrees with Figure 8. The BOMEX LES only includes ~86% of the total TCWV so P4L17 has been changed from “…show that the LES capture >90% of total TCWV…” to “…show that the LES capture >85% of total TCWV…”.

Equation (4) had a mix of \(r\) and \(\Delta r\) we changed to consistent use of \(\Delta r\) to emphasise it’s a gap between points.

We also had feedback that the error estimation in Sec. 3.1.4 could be confusing. To our knowledge it is new, so we have rephrased some text in Section 3.1.4 and referred to new Supplementary Figures 9—11. These figures show a step-by-step guide to our method, and compare results with a standard spatial filtering method.