

Dear Dr. Janssen,

Thanks for the detailed review of our manuscript – your suggestions definitely improve readability and technical clarity. Please see below for our responses to your suggestions. We have included the full text of your review with our responses bulleted.

Best,

Jack Hutchings

Dear authors,

Thank you for your detailed responses to the reviewers' requests, which have been fully addressed. In addition to the specific comments of the reviewers, I have some mostly formal remarks that I believe will improve readability of the manuscript, especially for readers who are not so familiar with the CRDS instrument that you are characterising. Please consider my remarks that are listed below.

I also had difficulties to access the supplementary information and I need to ask the editorial office for these files. Did you make the latest version of these files available ?

- Our supplement is hosted by Open Science Framework under the following URL, as indicated in section 7: osf.io/hgn8k. This link appears to us to be publicly accessible. Please let us know if we are mistaken.

With kind regards,

Christof JANSSEN

1. The title should start with "Optimization of a Picarro" since the work has been undertaken using only a single instrument

- Agreed. We have adjusted the title accordingly.

2. The first phrase of the abstract is clumsy to read due to the repetitive use of the word 'measurement'. Please consider to change into 'Until the recent development of commercially available infrared-laser analyzers, the measurement of triple oxygen measurements in water has been restricted to dual-inlet mass spectrometry due to demanding precision requirements.', or similar.

- Agreed. We have replaced the first 'measurements' with 'analyses'.

3. L13. Introduce the acronym CRDS here as cavity ring down spectrometry is mentioned here for the first time.

- Are you sure this is ideal? We have added the acronym CRDS, but we are not sure about the convention of introducing acronyms within the abstract for use in the rest of the manuscript. We note the D17O in the first line of the abstract because D17O is used throughout the abstract, whereas no further use of 'CRDS' is found in the abstract. We are fine either way, of course, but perhaps edit this in or out depending on best convention.

4. L58. I suppose that you mean integrated absorbance values ...

- Yes – we adjusted the text to fit this (L59). We also edited that sentence to hopefully improve clarity.

5. L67. Normal Mode 170 Mode etc. Please use same capitalization and spelling throughout the manuscript. There are occurrences of MCM 170 Long Pulse Mode, 170 Mode, 170 mode, 170-mode, for example.

Also, please, specify the signification of each mode upon the first mentioning.

- We have added additional text between lines 65 and 85 to help clarify. We also edited text throughout to harmonize usage of the terms with consistent capitalization, hyphenation, etc.

6. L68. Each isotopologues -> each isotopologues

- Fixed.

7. L72. are achieving -> are achieved

- Fixed.

8. L78. the L2140 -> a L2140

- Fixed.

9. Table 1: Use superscript 17 in tablenote b

- Fixed.

10. L125. Please check with the editorial office if v/v is an accepted way of indicating a volume fraction. Use consistent notation, because later in the text v:v is used instead of v/v. At other instances, the mass concentration (in g/L) is given instead of the volume fraction. It would be helpful to use either of the two quantities to specify the alcohol concentration. If for some reason original data are specified differently (eg for different commercial products or data sheet values), please select one of the two quantities to be always indicated (for example, give the mass concentration in addition to v/v). This facilitates the comparison of the different concentrations.

- We converted this first instance (now L128) to mass fraction. We left in the v:v notation in the results (section 3.3) where we also specify the mass fraction in mg / L.

11. L173,L210. Please explain Picarro slang to the reader. Is the data format the only difference between coordinator and HDF format ? Explain differences already here, especially the information that you are making use of in the postprocessing.

- We initially omitted details here as they were previously described by Schauer et al., 2016. However, we added some additional information so that a reader can understand our approach without necessary reference to the Schauer paper.

12. L. 177. What are private data ? The presentation of coordinator data vs high resolution data is somewhat unsatisfactory. What is the temporal resolution of the coordinator data, etc ? It seems that a description of what data are provided in the coordinator files is missing in the first place.

- Again, we definitely oversimplified our handling of this. We believe our expanded text in this section should satisfy your questions.

13. L.209. For comparison, ... The logic of this phrase is not clear. Why has the R script been modified, which script has been modified ? What needs to be compared ? Please rephrase.

- Rephrased to help clarify.

14. L.212. Consider citing tidyverse using the recommended source :

<https://joss.theoj.org/papers/10.21105/joss.01686>

- Fixed, thanks.

15. L. 290. Please clarify whether the two delta18O values also depend on independently measured 16O-water peaks.

- Clarified (they use the same 16O-peak) and added some rationale.

16. L. 292. Use of 5.5 and 0.5 is potentially preferable over 11/2 and 1/2 as the former could eventually be misread as 1 1/2 or 1.5.

- Good catch – these were very poorly formatted ratios of different spectral peaks. We clarify this in the next now without use of the forward-slash.

17. L. 339. 'When using the regression coefficients from Fig. S5 ...': Supplementary material should support/supplement statements made in the manuscript, but the manuscript should be complete in itself and without the supplementary material. This is not the case here, where material from the supplementary material is employed for the reasoning in the main text. Please change the paragraph accordingly.

- Fair... we simply removed this sentence as the estimate (18 months) doesn't have much real meaning given how little effect storage length apparently had on replicate precision.

18. L. 364. 'To compare these...'. Please consider writing 'To compare the two approaches ...', as 'these' is seems being associated with 'corrections' in the phrase before.

- Fixed, thanks.

19. L. 366. Please replace the word 'improve'. It seems be chosen wrongly as hdf is already your standard approach.

- Edited this sentence to hopefully improve clarity.

20. L. 376. 'avoid needing these corrections'. Please consider removal of the word 'needing'.

- Removed.

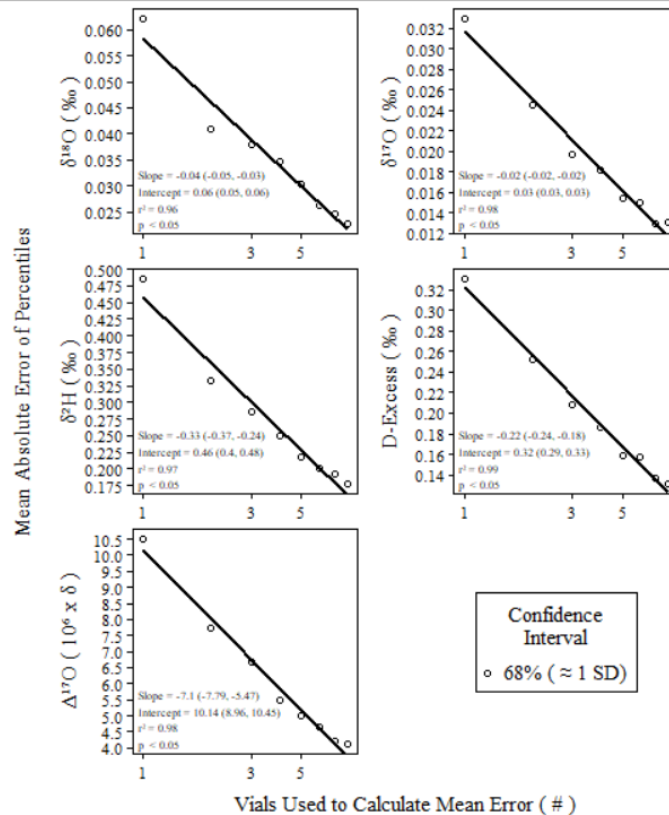
21. L. 369. 'In contrast ...'. Why is that ? This is somewhat unexpected and deserves explanation. Is the missing information provided later on in the manuscript ?

- Edited this line for clarity. The “in contrast” is simply meant to indicate that, although we see improvements in short-term precision, we don’t find similar improvements in the final accuracy metric (RMSE) of the analysis.

22. L. 477. The 'to' seems to be superficial. Please delete.

- Correct, thanks.

23. Fig. 6. You should consider a log scale for the abscissa, on which the SD should yield a slope -1/2 line for white (or gaussian) noise dominated errors. On that logarithmic scale it would be interesting to show the 7th and 8th vial (if available).



- See a log₁₀-transformed x-axis of that plot above with minor edits so everything is visible. That being said, our intended purpose of Fig. 6 is to provide the reader with an easily actionable plan as per the required number of analyses to reach a desired level of confidence in an unknown sample. With that intention in mind, we have opted to keep the current format of that figure for ease of useability.

24. L. 490. 'two lasers'. This is the first time that you mention that the instrument is operating with two different lasers. Indeed, it is unclear whether there are two lasers in the instrument and which spectral range they span. As of reading section on the 18O-Laser flag (~ L292) one might also get the impression that there is just one laser that, however, sweeps a wider range and covers two different 18O-containing water absorption lines. Please clarify.

- We briefly note the second laser in the introduction (L50-55), however we expanded the text in the 18O-Laser Flag section to clarify. We left the text you noted initially alone with the thought that the added text in the 18O-Laser Flag section is sufficient.

25. L. 607. '(see Sect 2.3 for details on output files)'. Actually it seems that some of these details are missing in Sect 2.3, see earlier remarks on the coordinator output.

- Our added text from the previous comment should satisfy this, too.

26. L. 610. and elsewhere. Reference is made to h5. It seems this is a short name for HDF v5. If this is so, please harmonize the notation. Otherwise, please introduce the variable h5 when it is used first.

- You are correct. The extension the Picarro uses is simply h5, but as we noted, it is indeed HDF v5. We have altered text referring to 'h5' to simply be 'HDF'.

27. L. 643. Please consider to delete 'that'.

- Agreed.

28. L. 667-672. This short conclusion refers to three different instances in the supplementary data section. If improved precision is noteworthy in the conclusion, it is preferable that the associated figures (S10, S11) which demonstrate the superior performance appear in the main text.

- We have removed the mention of precision (as this is quite small/negligible) and removed the reference to S11 as we make clear the improvement in d2H at the end of the discussion.

29. Reference section: Please check typography and notation. It seems that sub- and superscripts, as well as delta-symbols in article titles are not always displayed correctly.

- Thanks - we've resolved these typographical issues.