

Atmos. Meas. Tech. Discuss., referee comment RC1  
<https://doi.org/10.5194/amt-2022-230-RC1>, 2022  
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## Comment on amt-2022-230

Anonymous Referee #1

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Referee comment on "Optimization of a Picarro L2140-i cavity ring-down spectrometer for routine measurement of triple oxygen isotope ratios in meteoric waters" by Jack A. Hutchings and Bronwen L. Konecky, Atmos. Meas. Tech. Discuss.,  
<https://doi.org/10.5194/amt-2022-230-RC1>, 2022

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The manuscript "Optimization of the Picarro L2140-i Cavity Ring Down Spectrometer for Routine Measurement of Triple Oxygen Isotope Ratios in Meteoric Waters" by JA Hutchings and BL Konecky takes a close look at the way many of us use this instrument and the way we analyze the data. The paper is extremely thorough and takes the time to test many aspects that all users of this model, and really all IRIS and even IRMS instruments, should make note of. The manuscript is well written, well organized, sufficiently referenced and warrants publication in AMT after considering a few minor suggestions described below.

### Specific Comments:

The permeg notation: " $10^6 * \delta$ " is awkward and confusing. I am not familiar with expressing permeg in this way. The authors define a delta value using equation 1 which includes the \*1000 term. To me, then, this means delta values are in permil and have thus had 1000 multiplied by them. So if  $\Delta_{17O}$  is  $10^6 * \delta$ , then it is  $* 10^9$ . I know this is not what the authors mean, but perhaps you can see my point. I suggest simply using "per meg" and removing the " $10^6 * \delta$ " throughout. Equation 3 is sufficient for the authors definition of  $D_{17O}$ .

18O Laser Flag: The 18O Laser Flag seems like a great tool. I would like to see the authors make a short statement about how they came upon the "18O Laser Flag". The authors also need to describe in greater detail how the flag value is calculated, or is it simply the "SD\_18\_18" value from the h5 files? What specific values of the 18O Laser Flag constituted action? That is, what is the threshold value of the 18O Laser flag that, if exceeded, meant organic contamination? Why does this 18O Laser Flag work? Are the authors assuming the alcohol absorption will have a changing baseline from 7190 to 7200 /cm ? It seems to that the 18O Laser Flag is a way of comparing the the two lasers. 18O Laser Flag and  $D_{17O}$  both appear to be good indicators of contamination and both make use of comparing the two disparate absorption bands. I suppose we could also use deuterium excess calculations that use 18O from laser 1 and 18O from laser 2. I wonder then if it is appropriate to extend a generalized statement about the utility and benefit of having two lasers to compare. I realize much of this is musing speculation but it would be

great to have a sentence or two giving the reader insight into the authors thought process around this idea and this flag. As it is, the 18O Laser Flag is just thrown in without any introduction or elaboration. Lastly, and very minor, on line 285, the authors state "referred to hereafter as "18O Laser Flag"" but rarely if ever refer to this metric in that way. I see "18O-Laser Values", "18O Laser", "18O-Laser Metric", "18O-Laser spectral contamination metric".

What is the outcome or course of action after finding an aberrant point such as is shown in Figure S14? Does use of h5 level data allow you to recover without rerunning the water? Given the authors preference for high resolution data over coordinator data, further explaining this process will help their case. Minor comments related to this topic: Fig S14 (a) caption, I think should refer to injections, not vials, not because the statement isn't true as is, but because the authors are showing injection data, not vial data. Also, and again, minor, it may be worth pointing out in the caption of S14 that C and D data do not come from the h5 files referred to thus far in the manuscript, but rather from the very high resolution spectral data. I know the authors already say "spectral readings" but helping the readers who don't use any of the h5 files may be useful.

#### Technical Comments:

- Consider referring to the supplemental figures and tables as appendices. It seems as though AMT uses supplemental information to refer to a text based document and stand-alone figures and tables are appendices.
- Check for delta notation missing superscripts throughout the manuscript, for example line 216.
- Also, on occasion, I see "D-Excess" instead of "d-excess". Change to lowercase "d" throughout.
- Line 39 - "slope of 0.528 calculates values" is awkward. Reword.
- Line 59 - "isotopogues" should be "isotopologue"
- Line 66 - "H2H16O" should be "1H2H16O" with appropriate superscripts, of course.
- Table 1 caption ends prematurely. "...measurements by this study." perhaps?
- Line 154 - "To apply the drift correction, the slope of the drift regression was multiplied by an injection's position and subtracted from the injection's observed delta value." As worded, this sentence suggests that the slope is multiplied and then subtracted. I think the slope is multiplied by the injections position and then the product is subtracted?
- Line 182 - "experienced increased memory experienced", I think, should read "experienced increased memory"
- Line 246 - "account drift" should read "account for drift"
- Line 317 - "term", while correct, is slightly awkward with the two other "-term" uses in that sentence. Perhaps "factor"?
- Line 333 - The word "excess" seems out of place. "exceed" perhaps?
- Line 337 - "as measure" should perhaps read "as a measure"

- Figure 5 - The average of the MSD should be zero, or not different from zero. I am not sure if it is worth showing this in the figure text. It would be like changing your equation 5 to  $x_i - \bar{x}$  instead of  $\hat{x}$ . We expect the sum of  $(x_i - \bar{x}) / n$  to equal zero or not different from zero. Also, and minor, I am not sure you need an additional y-axis label of "Histogram (counts)" since it is in the caption. Furthermore, Table S3 has exactly the same data presented as the text in Figure 5. I feel the same way about the mean MSD in Table S3 and since you have the same data in Fig 5, I suggest deleting Table S3.

- Line 345 - "an average of by" should perhaps read "by an average of"
- Figure 6 caption - "were differenced" should read "were subtracted"
- Line 500 - "sample" should be "samples"
- Line 628 - "only strongly" seem to contradict each other. Seems like "only" should be deleted

- Figure S1 - The order of figures is inconsistent with other figures. All other figures are d18O, d17O, dD, d-excess, D17O.

- The data in Figure S3 seems like it may be better presented as histograms, which are made good use of elsewhere in the manuscript.

- Figure S13 caption - "differenced" should be "subtracted"

- Table S2 - missing peak 1, H218O. Also, consider removing this table entirely and simply cite Steig et al 2014.