A reply to https://doi.org/10.5194/amt-2022-208-RC1

Original referee comments in blue, with author response in black.

This paper presents a new compact packing system for a commercial cavity ring-down laser spectrometer that is intended for in-situ deployments in harsh (here cold, polar) environments. The manuscript also presents a few additional modules such as a cold trap module and a profiling arm. While I find the paper well-written and very interesting to read, I have a few fundamental critiques in particular with respect to the structure and focus of the paper that the authors should reflect upon and address before acceptance of the manuscript.

1) Technical innovation and significance: While I really like the level of technical detail and completeness of the description of the ISE-CUBE, I do not fully understand why it stands in the center of a paper publication. Dozens of previous scientific investigations have been conducted in different in-situ installations of cavity ring-down spectrometers in containers, cars, ULM, ventilated aluminum housings, tents or aircraft racks. All these deployments were done in such a way as to address the scientific question at hand in the best possible way. The ISE-CUBE seems a useful packing method for exactly the chosen deployment: namely near-surface profiling of stable water isotope gradients in cold environments. But already in the midlatitudes and especially in the tropics the chosen setup would not work due to overheating. In my view the technically relevant and innovative part of this study is not the CUBE but the profiling arm, which however is only very sparsely addressed. Therefore, in my view the profiling arm should stand in the center of the story framing. The full use of the compact packing provided by the ISE-CUBE only becomes obvious, when combined with the profiling arm. The authors should seriously reconsider their storyline, provide a better literature-overview of existing studies with different in-situ deployments, and justify why such a detailed presentation of a very specific packing is useful to the community. To me the fact that the system is not autonomous in terms of power use is a big drawback and doesn't make the system so much more flexible than a sheltered installation with a long inlet-line.

We agree that a reframing of the manuscript as you propose would be very beneficial. Therefore, in the revised manuscript, rather than present our work as a "field **deployment** system" with the focus on the primary modules (analyzer and pump), we will shift the focus to an entire "field **profiling** system", where the profiling modules feature on an equal level as the primary modules. We maintain the equal importance of all three of these modules. As will be addressed in a comment below, the cold trapping module will remain as an optional expansion module. We will also expand our description to include an alternate profiling arm frame that we used to make profiles at the fjord. A possible revised title would be "*A modular field system for vertical profiling of in-situ vapor in harsh environments using cavity ring-down spectroscopy*"

2) Motivation for a profiling system of the near-surface profiles within 2 m above the surface:

- As mentioned above I really like the profiling arm and think that this is a clear innovation and add-on to the current state of the art in the isotope literature. It also has in my view clear potential for scientifically relevant investigations. The authors should mention these in the introduction more explicitly: why is it important to measure near-surface humidity/isotope and potential other trace gas gradients up to 2 m height?

The primary science aim driving the development and construction of the system was on the near-surface interaction and exchange between the surface and overlying air during processes such as evaporation and condensation. Our ultimate goal is to use this system to better understand the isotopic fractionation across the surface-atmosphere interface in these situations from profile measurements. We will better communicate this motivation in the introduction, since as the manuscript now stands, this is only briefly mentioned.

- Normally bulk fluxes are computed using measurements over about 10 m depth near the surface, why are the authors interested in the lowest 2 m?

Scalar surface fluxes can be measured at 2 m (Foken, 2008), and a lower measuring height produces a more localized footprint for our observations. As our focus is on the surface exchanges and given the generally very stable stratification in the Arctic surface layer during spring, we determined 2 m to be sufficient for our science aims mentioned above.

- The authors should highlight more clearly in the introduction why in a polar environment it is of utmost importance to have short inlet lines (due to strong interactions with the tubing walls at low concentrations, longer response times, lower precision at low concentrations).

We will make sure to clarify this point in the revised manuscript, especially as it directly ties to our design motivation for the analyzer and pump modules

- What makes a profiling arm with free choice of sampling height more valuable than a setup with a manifold and inlets at discrete heights? This is an essential argument for the profiling arm and should come very early in the manuscript. It is now mentioned only at the very end at L. 465.

We briefly touch upon the additional advantage that the arm has over tidal waters in L.483, but we will expand upon both points earlier in the manuscript.

3) Section 4.1 & 4.2: this section is much too detailed: 7 pages to state that the measurements were essentially unaffected by the harsh environmental conditions seems exaggerated to me. I am conscious of the effort that the authors put into the data analysis to come to that conclusion (stated at L. 374-376) and I fully acknowledge that this effort is worthwhile. Figures 5 to 7 with respective tables and shortened text would make an excellent supplement. But the information given in the paper should be succinct. The DAS temperature is not that relevant for the measurements, much rather the cavity temperature and pressure should be kept stable (this can be summarized in a few sentences). The WLM discussion in Section 4.1.3 remains inconclusive to me. The importance of the air prewarming by using the exhaust of the pump module can be mentioned in the methods section. A maximum 1-page summary of these results putting forward mainly the results of Section 4.2 (L. 399-402) with Fig. 10 should be sufficient to describe the main results and keep the reader's attention focused.

We appreciate the recognition of the time and effort gone into our analysis of the CRDS performance, though we ultimately agree that these sections are too intricately (and exhaustively) presented. In accordance with your previous suggestion, and our proposed reframing of the manuscript as a field profiling system, the main focus will be on the integrity and reliability of the profiles, from which the performance of the CRDS naturally follows. We will significantly shorten these sections to better respect the attention of the reader.

4) Cold trap module: This is an interesting adaptation of the Peters & Yakir 2010 system. However, if no data from this system is shown and compared to the CRDS data, then this part should be left away. Currently, this part of the paper is difficult to assess without data.

While our cold trap samples are not quantitatively compared to the CRDS isotope data, we do assert that our qualitative assessment of the setup (ie. the need for a different type of collection vial) is sufficient grounds for inclusion. We've taken a system proven by Peters and Yakir (2010), and attempted to apply it to a much different environment than they tested in. In the revised manuscript, we will present some data for an initial assessment of the system performance.

5) Field calibration expansion module: I do not understand why a calibration module is useful for such a deployment, which needs manual handling of the system anyways. Recent studies have shown that CRDS systems operate reliably over the timescale of several days with minimal drift (without calibration), such that a calibration every few days (1-3) is entirely sufficient and can be done in shielded temperature regulated conditions. See also the statement of the authors themselves at L. 220.

In the context of our particular profiling deployment, we agree that the necessity of a field calibration unit is limited, hence why we deemed it sufficient to calibrate in the lab before and after deployment. However, in the larger context of our presentation as a deployment system that might be used for longer periods, we thought it important to emphasise the necessity of proper calibrations. In this regard, we will remove Section 2.6, as it is not relevant to our particular deployment. Though we will keep our mention of it in the Outlook section, as anyone considering to deploy for longer periods of time should incorporate a calibration system into the setup.

6) Profiling module performance: as mentioned above, I think that the real innovation of this paper is this profiling arm, which also makes the need for a low-footprint and modular box clear to keep the length of the inlet line at a minimum. Unfortunately, the authors put much more effort in sections 4.1 and 4.2 than in the key sections 4.4 and 4.5.

- I recommend restructuring these sections and showing more results on this essential part. In my view L. 421 to 428 should be in the methods.

These will be moved to the methods section.

- The response time of the system & precision at the encountered concentration should inform about the ideal length of the measurement periods at a given height. This point should be discussed. Is 30 s averaging ideal also from a signal-to-noise ratio perspective? Or should it be longer?

In our revised manuscript, we will discuss the inlet response time in more detail. And as we will be discussing the profiling capabilities in more detail, we will discuss our findings on the minimum time left at each height.

- The temperature sensor calibration is a good thing to do, but a Supplement figure would be sufficient.

Figure 11 is not a calibration, but a comparison with the nearby AWI station. However we will consider moving it to an Appendix.

- Fig. 12 is (one of) the most interesting figures (together with the very nice technical drawings in Figs. 1-3) but it is difficult to read because it is shown as a time series (and too small with many panels). A profiling arm allows to measure profiles, so why not show profiles? When looking at Figure 12 and considering the main aim of the paper (providing a modular system that is able to measure near-surface isotope and trace gas profiles in cold environments) then I wonder: can the proposed setup resolve the vertical gradients given the uncertainty of the measurements at these low concentrations? The authors should show the vertical profiles under different conditions including the total uncertainty of the measurements and discuss this very important question. Also, in addition to the isotope, temperature and wind information they should add the water vapour mixing ratio and dexcess.

We agree with your suggestions. Especially in regards to your last point, we will re-make Figure 12. As we've explained previously, under our original manuscript structure, presenting the measurements from both the Analyser and the Profiling module as a time series made the most sense, as both data streams are fundamentally just that. In the new framing, we will present the measurements from the CRDS as vertical profiles. We will also change the day that is presented from 28 Feb to 9 Mar, which is more suitable to illustrate the profiling operation.

Detailed comments:

I refrain from a detailed list of language and technical comments here, given my advice above for fundamental reorganization of the paper. I however chose to list a few points that need clarification in the text:can the proposed setup resolve the

vertical gradients given the uncertainty of the measurements at these low

concentrations?

- L. 15: which processes? Those relating to fluxes?

This should read "these processes", referring to the exchange processes of the previous sentence.

- L. 17: during stable stratification -> really only then? I can imagine many situations in which the stratification is not stable and in which near-surface measurements would be very useful.

This will be changed to "Near surface (<2m) gradients over the snowpack can be strengthened significantly due to the stable stratification that often occurs in these regions, and ultimately govern the fluxes of …"

- L. 20: "disentangling water vapor of different origin and undergoing different" processes -> do you want to disentangle the water vapor? Or the different sources of the water vapour?

The isotopic composition can be used to disentangle the moisture origin. We will clarify this in our revisions.

- L. 23: did Steen-Larsen et al. 2013 investigate moisture sources? Or airmass origin? Maybe choose a different reference here. Also Sodemann 2017 is a proposal that is not accessible online and not a document that I would expect to be referenced in a peer-review paper. Maybe Sodemann et al. 2017 is meant?

True, Steen-Larson et al. 2013 looked into arimass origin, and a different reference would likely stand better.

Yes, thank you and well spotted. This was likely from a mixup between Sodemann2017**a** and Sodemann2017**b** in the citation software.

- L. 26: remove "or so" (spoken language)

We will change this to "Over the last few decades…"

- L. 30: what is the advantage of an in-situ system such as ISE-CUBE-profiling-arm over a line with a manifold? Please be more explicit. This touches upon the key innovation of this work.

The arm can be set at any height in an observational range (~2 m), and can therefore generate a profile observed across a multitude of levels (N). These multiple levels better capture the near-surface profile, which may have a non-linear shape. Any similar approach with a manifold system would involve N-times the amount of inlet lines. Additionally, the flexibility and the distance sensing capabilities of the arm enables us to observe over a changing reference level (i.e. tidal waters). We will be sure to expand upon these advantages in the revised manuscript.

- L. 51: Wall effects -> indeed very important and how is that addressed? How long are the response times of the system? This is important for the profiling strategy (i.e. how long does the arm stay at a given elevation)

Our efforts to mitigate the wall effects (stainless steel tubing, heated lines, minimal length) are brought up in Section 2.5, albeit insufficiently given our proposed focus change. Response times will be elaborated upon in Section 4.4.

- L. 101: stand-alone field operation -> no power (how much in total?) is needed

Stand-alone refers to the fact these two modules (Analyser and Pump) can stand on their own, apart from the other two modules, not stand-alone from grid power. The sentence will be clarified.

- L. 169: I would say this is a typical example of an unstable situation at least over the open ocean.

Agreed. When referring to stable conditions/startifications in the manuscript, it pertains to the conditions over the snow.

- L. 190: An overview … is given.

We will change accordingly.

- L. 204: if that is a central tool to this publication it should be made available online along with the data

We will expand our description of the routine to further detail the processing that the script does.

- Section 3.4: I have difficulty assessing if the comparison dataset from the lab is an adequate one to use. Is the amount of data (sample size) and sampling frequency comparable to what was used in the field? The description is a bit vague in this respect.

Our lab benchmark is approximately 5 times larger than the field dataset. In the lab, the analyser sampled at 1 Hz, while in the field the analyser had a sampling rate of 4 Hz. However the comparisons done between the two environments are both at 1 Hz.

- L. 387: the fact that the vials have to be manually changed in the cold trap module should be mentioned in the methods.

We will include this detail in the revised manuscript.

- L. 353: I cannot follow the argument why the only slightly larger RS at low water vapour mixing ratios in the field necessarily implies less accurate measurements in the Field.

As per Johnson and Rella (2017), the residual represents the difference between modelled spectrum and the observed, best-fit spectrum measured by the analyser. The best-fit routine makes adjustments to free parameters such as the amount of the various isotopologues to the observed spectrum, in order to minimize this residual. With a larger residual at a particular humidity level, measurements can be considered as less precise. See our comment below for more details on our proposed revisions for Section 4.1.3 and Fig 8.

- L. 360-362: so then why such a detailed discussion of these metrics?

In our revised manuscript, we will introduce the Zeppelin Observatory dataset in Section 3, as its own reference period for the WLM. Therefore, we will forego the discussion of the Laboratory WLM metrics; Fig 8 will essentially be replaced by Fig D1. This will also work towards shortening the manuscript.

- L. 416-419: I don't understand why the authors introduce the cold trap module if they don't use its data. That makes it difficult to assess if the system is fulfilling its purpose.

As mentioned above, we will be including cold trap analysis of select samples in the revised manuscript.

- Fig. 11 should go to the supplement.

We will move this figure to the Appendix

- L. 424: how were these response times estimated, to me the averaging intervals are also a key factor for optimizing the signal-to-noise ratio and obtaining the best possible precision.

We will discuss the inlet response time in more detail in our revised manuscript.

- L. 449: "strongly stable", this is even an inversion

Yes, other nearby instrumentation documented a persistent near-surface inversion throughout much of the time at Snow. However, this profiling example will change in the revised manuscript.

- L. 454: which isotope gradients do you mean here?

$\delta^{18}O$ and δD. We will state this in the text.

- L. 458: we captured d18O and dD (leave away "isotope signatures" of, that is a repetition)

We will change accordingly

- L. 462: what does "the temperature gradient… converged" mean here?

The temperature gradient between lowermost and mid levels weakened and approached the value of the gradient between mid and uppermost. In Fig 12e, the black dotted line converged towards the black dashed line.

- L. 463: not shown -> but that would be very interesting!

We are currently preparing a manuscript for Earth System Science Data.

- L. 463: this is very important and should be mentioned in the introduction as a motivation for the ISE-CUBE with profiling arm system.

We will ensure that we emphasize this strength in the revised manuscript.

- L. 483: "Flexibility of the measurement's height… with strong tides" interesting, but I missed that argument in the results part of the manuscript

As mentioned above, we will introduce this design consideration earlier in the manuscript.

- L. 486-491: the authors should compare the cold trap sampling to the CRDS measurements or leave it away.

As mentioned above, we will consider including comparative data from our cold trap sample analysis in the manuscript.

- L. 492-498: As mentioned above, I do not understand why this is needed, as long as no autonomous operation over months is targeted.

Agreed, though we will keep mention of this potential module here in the Outlook. We feel that we would be remiss to not mention the importance of proper calibrations, for which an in-situ unit would be necessary in deployments approaching 3+ weeks (Leroy-Dos Santos, 2021).

- Fig. 12 is very small and difficult to read. Also, the information would be much more accessible (and interesting) in the form of vertical profiles instead of timeseries.

Yes, we will be changing Fig 12 to show profiles alongside the timeseries. The text of the figure will also be larger.

In summary, I very much like the profiling system presented by the authors and strongly encourage them to focus on this aspect, presenting its performance and limitations in an accessible way to the readers and the community. I think that the paper will gain in attraction, if shorter and more focused on the vertical profiling capability.

References

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