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Interactive comment on "Introducing the Extended Volatility Range Proton-Transfer-Reaction Mass Spectrometer (EVR PTR-MS)" *by* Felix Piel et al.

Anonymous Referee #1

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Piel et al present the characterization of a new type of inlet for Ionicon PTR-MS instruments, which enhances the sampling of molecules less volatile than typically reported by such instruments. This is a good addition, since PTR has more potential than has been realized in the most commonly deployed instruments, where VOC detection has been the main focus. The paper is for the most part clear and well written, and the topic suitable for AMT. However, I have a few questions and comments to the authors, relating to both clarity and novelty, that need to be addressed before possible publication in AMT.

Major comments:

In the abstract, lines 18-20, the EVR configuration is presented primarily as an improvement by passivating surfaces, with "further improvement" by heating to 120 C.

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Discussion paper

However, as far as I can tell, there is no data presented in the manuscript about how much the passivated surfaces changed the response times. If the authors want to highlight the passivation, this type of information needs to be included in some form. Otherwise, the temperature increase, for which there is clear data (e.g. Fig. 3a), should be presented as the main improvement. And in that case, the novelty of this manuscript (and the EVR inlet) is questionable, as there are a wealth of PTR studies where inlets and inlet lines have been heated in order to improve response times and detection of less volatile species (see e.g. section 2.4.5 in Yuan et al., 2017, Chem. Rev.). The authors need to make very clear what exactly causes the improvement of response times in this manuscript, and how this is different enough from earlier work that it deserves publication in AMT.

Lines 55-58 at the end of the introduction do not even mention the temperature issue, suggesting that the material changes are the main topic of this manuscript. This requires verification.

A related point is the lack of any schematic diagram of the EVR in the manuscript. It may be understandable if the design itself did not change, but rather only materials were exchanged, yet it would still be beneficial for a reader to see a figure showing these changes. As it is, the only reference on PTR in section 2.1 is the Yuan et al (2017) review, which itself doesn't have a schematic of the exact system used in this work. This makes it very laborious for a reader to understand the changes, and consequently to properly assess the novelty of the changes and the manuscript itself.

Specific comments:

1. Lines 28-29: Since these measurements were done using NH4+ adducts, I don't think it should any longer be called "PTR-MS".

2. Lines 69-70. Since T_drift is used later as a parameter, it is important for a reader to have a clear picture of how the drift tube looks. Also here a schematic would be useful.

3. Lines 50-51: “H3O+ ion chemistry thus detects a wider spectrum of analytes than any other chemical ionization method for atmospheric organic carbon.” This is a strong statement and would need a citation. Instruments like the NH4+-CI3-TOF or C3H7NH3+-APi-TOF (Berndt et al., 2018, Angew. Chem. Int. Ed. 2018, 57, 3820 –3824) seem to detect almost all organic compounds (including radicals) except hydrocarbons. Can the authors show references where H3O+ ion chemistry would have detected a broader spectrum than that?

4. Lines 73-75. These two sentences need to be reformulated. “was measured as the time that evolved until” is hard to understand.

5. Fig. S1. The part inside the red dashed box is presumably the inlet and drift tube of the PTR? This needs to be clarified, as it is not easy to read for someone not highly experienced with the system.

6. Lines 108-109: This leaves the reader with the question “why?”.

7. Lines 133-134: This also leaves the reader with the question “why?”.

8. Section 3.2: The discussion is about T_drift, and the text suggests that it is only the drift tube temperature that is changed. But Fig. S1 suggests that the entire inlet is one temperature-controlled entity. Please clarify. This again would be easier to understand if there was a proper schematic included.

9. Lines 138-139: This seems consistent, but Fig. S2 shows that the dependence of tau on C0 is very weak, with compounds of the same C0 easily having an order of magnitude or larger differences in tau. Were these two compounds selected to be shown because they happened to match?

10. Line 144: Why are you now shifting from tau_1/e to tau_90?

11. Line 145: It is unclear which data from this study is used in Fig. 4. This should be made clear, so that a reader would be able to compare responses compound by compound. In addition, there is a nice monotonic trend of tau vs C0 in Fig. 4, which is

hard to understand given the huge spread of points in Fig. S2. One is left wondering how the authors selected the 5 data points shown in Fig. 4 for the EVR.

12. Line 153: C13 ketones are referenced, but I do not know where I should be looking to find this data.

13. Fig. 4: It took me a while to realize that the unit of tau changes between Fig. 2 and Fig. 4, from sec to min. Why not keep them the same? Now both the time unit and the decay reference (1/e vs 90) change, and it makes things much harder to follow. I suggest to make all of these the same, as it would make the reading much smoother and avoid confusion.

14. Fig. 4: If I understand the plot correctly, the non-EVR PTR-TOF from this study seems to work much better than the EVR. All measured response times are on the order of 0.01min, while in the EVR all points are at 0.1 min or higher. Does this mean that the EVR setup has actually made the response times worse compared to the original design (as long as the inlet is heated)?

15. Line 155: The fact that temperature explains the major part of the differences, and this fact is only mentioned in one sentence in the main text, makes Fig. 4 very misleading. For example, one would read from Fig. 4 that the reason the PTR-TOF in this study was 3-4 orders of magnitude better than the PTR-qMS from Pagonis et al is related to the quad vs tof, since that is the only clear difference. Not to mention the comparison to other instruments, which were not run at elevated temperatures. Please put the operating temperatures into the figure legend, since these values are the most critical parameter to understand the major differences in the figure.

16. Lines 171-172: Again, the fast changes are attributed to the materials, and temperature is not mentioned at all. This needs to be clearly validated before making this claim.

17. Conflict of interest statement: Ionicon analytik is said to be “commercializing

(CHARON) PTR-MS”, but they are also advertising directly the EVR setup presented here (https://www.ionicon.com/accessories/details/extended-volatility-range-evr). Why is this not mentioned here?

Technical corrections:

1. Line 97 and line 107: Caption, not legend.

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