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Atmospheric Measurement Techniques Discussions

Interactive comment on "Performance of SIFT-MS and PTR-MS in the measurement of volatile organic compounds at different humidities" *by* Ann-Sophie Lehnert et al.

Anonymous Referee #1

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General comments:

This paper details a set of modifications to a commercial SIFT-MS instrument that improved the LODs, backgrounds, and sensitivities. The authors have also completed an expansive set of experiments characterizing the modified SIFT instrument's operational parameters and performance. While the work is thematically simple, I think rigorous instrument characterization papers like this are useful to those in the community who measure VOCs with SIFT or other atmospheric chemical ionization mass spectrometers. I recommend this work be published after significant contextual and written issues with the paper are addressed.

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Discussion paper

Particularly, the PTR comparison portion of the work is afterthought and has numerous problems. Instead, I suggest refocusing the paper around the modified SIFT instrument.

My issues with the PTR portion of this work are thus:

1) The authors portray a very old quadrupole PTR-MS as a generic PTR instrument representative of all PTR-MS instruments. There are many different PTR-MS instruments with different performance levels. Importantly, almost all of them have higher performance characteristics than the PTR-QMS 500, which has not been state-of-the-art for a long time.

Lately, newer models such as the PTR Qi-TOF (Sulzer et al. 2014), PTR6000 X2, PTR3 (Breitenlechner et al.), and Vocus (Krechmer, Lopez-Hilfiker, et al.) have much higher sensitivity and much lower LODs. The PTR-MS sensitivities in Figure 4 are poor relative to those of the PTR3, which have been demonstrated to be three orders of magnitude larger. And very relevant to this work, the Vocus PTR-MS has been shown to have no quantitative humidity dependence, making the broad statement on P10 L39 no longer true.

The PTR-MS field has largely moved to time-of-flight mass analyzers that offer much higher mass resolution (as opposed to the quadrupole demonstrated here), fast full-spectrum acquisitions, high sensitivity, and low backgrounds.

While the authors are fair and unbiased in their comparisons here, I fear that measuring a highly modified SIFT against a much older PTR is not representative, nor does it offer useful information to the field. As they acknowledge, SIFT/PTR intercomparisons have been published before for other applications. I do not think there is enough different about the proposed application here that warrants another intercomparison.

2) There is little-to-no mention of “current” PTR literature or instrumental developments to put this paper in context. For example, the improvements made to the SIFT instru-

ment in this work seem to be similar in spirit to those made to the PTR QMS in Deming et al. 2018. Indeed, additional information about the SIFT-MS's time dependence from an experiment similar to Deming et al. would be useful in this paper.

Separately, I believe the authors left far too much information in the SI. Many of the SI plots are important to understanding the SIFT's performance characteristics and are referenced several times. They also clearly involved a lot of work and would be useful to many users. I think it would be a shame if they remained hidden. I would suggest cleaning some of them up and moving them back to the main paper. There is, after all, no length limit in AMT.

In summary, I recommend that this paper be published but suggest that the authors reframe the narrative of the paper around improving and characterizing the SIFT instrument, deemphasize the comparison with the PTR instrument, and bring a large portion of the impressive SI work into the main paper.

Specific comments:

Section 3.1 seems to repeat a large amount of the material in Section 2.2. A description of the SIFT improvements should be in one or the other, but not both.

P3 L7: "...usually a quadrupole MS". Do the authors have evidence of this? For SIFT this is true, but TOF has been the dominant technique for PTR for almost a decade now. This is not trivial, as the issues with how the authors characterize PTR are serious throughout the work.

P4 L16-18: The authors judge the success of their instrument modifications here by evaluating the background. Did they also evaluate response time, which is a critical parameter for ambient atmospheric measurements? PEEK may have a higher background, but its response time has been shown to be significantly better than stainless steel (coated and non). (Deming et al., 2018)

P10 L17: Mass-to-charge ratios should have a label as such everywhere in the paper.

e.g. m/z 19 or m/Q 75

Technical corrections: P4 L33: This is the methods section. Are the authors referring to a different methods section? P5 L20: should be “it more strongly punishes a larger number of parameters” P6 L25: “workdaily” I’m not familiar with this word.

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