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Interactive comment on “PTR-QMS vs. PTR-TOF comparison in a region with oil and natural gas extraction industry in the Uintah Basin in 2013” by C. Warneke et al.

Anonymous Referee #1

Received and published: 7 August 2014

Review of PTR-QMS vs. PTR-TOF comparison paper Warneke, et al., AMTD, 2014:

This manuscript reports the comparison of two proton transfer reaction chemical ionization mass spectrometers, where the primary difference between the instruments lies in the mass analyzer – one using the traditional quadrupole mass filter, and the other using a new time of flight mass spectrometer. The ion-reaction portion of both instruments was similar in design and in operational conditions, such that a reasonable characterization of the differences between the mass analyzers was possible.

Overall, this work shows quite clearly that the PTR-QMS and PTR-TOF work in much

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the same fashion for the field observations that were compared, and that, for almost all applications, the PTR-TOF will be the preferred instrument due to 1) its inherent ability to continuously monitor the entire mass range, and 2) its ability to separately quantify certain isobaric ions (given its superior resolution).

Recommendation:

Overall, this paper is clear and well written, and appropriate for publication in AMT, which I recommend after consideration of the following points.

General:

The text could be streamlined somewhat. There are several places where the same information is repeated.

Somewhere it would be good to define the term 'isobaric ions', distinguishing it from 'isomeric ions' arising from isomeric analytes, and point out that the latter are not separable using ToF separation, as they have exactly the same mass.

Specific comments:

P6567 L19: Reference Muller, et al., 2009 also for MS/MS PTRMS

P6559 L27-28: How were the apparent differences between the standards treated in the analysis? Not all of the compound sensitivities 'step' in sync with the tank change, i.e., m73 is different than m42, m33 (Fig2a); What is the reason for this?

P6570 L16: Extraction frequency of 250 kHz seems much too high for this instrument for a mass collection range of ~500 amu. Recommend describing the ADC or TDC which was used.

P6572 L8: Poisson distribution.

P6572 L11-12: Perhaps specify that this occurs for instruments operated in ion counting mode, and the under-counting is related to the ion-count-rate and the ion pulse-

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width (dead time).

P6573: I suppose for the reader to better understand this section it would be good to describe more details of the ToF operations, including the raw signal baseline stability (was the ADC/TDC temperature controlled), threshold level (was this dynamically varied or static?), average single ion peak height relative to threshold and how did this vary over the experiment. Was there a mass dependence to the average single ion peak height for the detector gains used in this experiment? What reagent ion signal is used to normalize the other signals (m/z 19 or m/z 21)?

P6577 L6: Insert 'individually' before 'measurable' Figure 4a: To the extent that these sensitivities are based solely on authentic calibrations, this shows that after correction for the well-known discrimination in the ToF pulser, the remaining mass-dependent discrimination for both the quadrupole and ToF analyzers is very similar. This might be worth some added discussion in the text.

Figure 5: Labels read m_{21} , but counts seem to be for m_{19} ?

Figure 9: This figure might be enhanced if the high resolution ToF peak-fits are added to the lower two panels, and add molecular assignments. What are the units for the ToF data? Counts/extraction/? Can these be made the same as those used for the QMS data?

Technical corrections: P6566 L7: insert 'to charge ratio' after 'mass'.

Figure 2: solid red and solid magenta colors are difficult to distinguish in the print version. Suggest making these symbols more different.

References: Müller, M, Mielke, LH, Breitenlechner, M., McLuckey, SA, Shepson, PB, Wisthaler, A, and Hansel, A: MS/MS studies for the selective detection of isomeric biogenic VOCs using a Townsend Discharge Triple Quadrupole Tandem MS and a PTR-Linear Ion Trap MS, Atmos. Meas. Tech., 2, 703-712, doi:10.5194/amt-2-703-2009, 2009.

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