Atmospheric Measurement Techniques Discussions

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Comment on amt-2022-228

Anonymous Referee #2

Referee comment on "Chemical ionization mass spectrometry utilizing ammonium ions (NH_4^+ CIMS) for measurements of organic compounds in the atmosphere" by Lu Xu et al., Atmos. Meas. Tech. Discuss., https://doi.org/10.5194/amt-2022-228-RC2, 2022

Review of: ***A Chemical Ionization Mass Spectrometry Utilizing Ammonium Ions (NH_4^+ CIMS) for Measurements of Organic Compounds in the Atmosphere***

This paper describes the optimization and calibration of a commercially available Chemical Ionization Time of Flight Mass Spectrometer for the measurement of a suite of organic compounds in the atmosphere. Field data from the instrument and comparisons to other instrumentation are also presented. The instrument utilizes NH_4^+ reagent ions and a relatively new (less than 5 year old design) Focusing Ion Molecule Reactor (FIMR). The authors present the advantages and limitations of using NH_4^+ chemistry. The paper is very detailed (more on this later) providing more than enough information for other groups to reproduce the results presented here. It is well suited for publication in AMT and will be of great value to the community. That said, I do have a few comments and suggestions below.

General Comments:

As mentioned above the paper is very detailed. While this is a good thing, there are times this borders on overwhelming and does make the paper quite long. At times I wondered if could be split in two, with the field measurements and instrument intercomparisons being their own paper. The sheer number of species quantified (or estimated using voltage scanning) by the instrument also makes some of the figures difficult to digest. Figure 3 is an example of this. While I understand what the authors are trying to show, the sheer number of traces makes it almost impossible pick out individual species. Anyone suffering

color blindness would have no clue what they are looking at. At times, I also found it difficult follow through the jumping around of formulas in the modelling of the reagent ion distribution. Again, I appreciate the level of detail the authors have provided the readers of this paper, I simply feel it should be tightened up in places and presented in a more digestible way.

Specific Comments

Title: I assume the authors meant "*A Chemical Ionization Mass Spectrometer Utilizing…..*" or *"Chemical Ionization Mass Spectrometry Utilizing….."*

P3 L66: Tofwerk Vocus

P11 Figure 2: A plot of the model results showing the final optimal conditions would be nice to see here somewhere.

P13 Figure 3: As mentioned above this is a very busy plot. I'm wondering if there's a way the species could be grouped or if the authors could split the plot into panels so that if would be easier to see what is going on. Right now it kind of looks like a mess.

P14 L281: We have performed……..and measured……

P15 L308: oxygenated aromatics have a…….

P16 L333: …..k have less uncertainty than TE.

P16 L333: You really should not start a sentence with a lower case variable. Perhaps "The value of k……"

P17 L343: This has been mentioned elsewhere and is an opportunity to tighten up the manuscript.

P21 Figure 5: I’m finding it difficult to wrap my head around the sensitivity comparisons between the instruments without taking into account the change in reagent ion signal (sensitivities are cps/ppb not ncps/ppbv). Fluctuations in reagent ions will surely occur. The authors even mention the example of day vs night. I realize this is difficult in the VOCUS instrument since proper counting of the reagent ions puts significant wear on the MCP detectors, but I'm wondering if there is some other way to account for this.

P22 L476: should be “produce”

P22 L489: Absence?

P23 L516: ….throughout the day.

Supplement

P3 L58: “Further, the dipole moment…..”

P4 Figure S2: Same comments as Figure 3.