Comment on amt-2021-85

Anonymous Referee #2

Referee comment on "Application of a mobile laboratory using a selected-ion flow-tube mass spectrometer (SIFT-MS) for characterisation of volatile organic compounds and atmospheric trace gases" by Rebecca L. Wagner et al., Atmos. Meas. Tech. Discuss., https://doi.org/10.5194/amt-2021-85-RC2, 2021

Review of "Application of a mobile laboratory using a Selected-Ion Flow-Tube Mass Spectrometer (SIFT-MS) for characterization of volatile organic compounds and atmospheric trace gases" by Wagner et al., for publication in AMT

This study presents the development of a mobile analytical platform equipped with two analyzers: an Ultraportable Greenhouse Gas Analyzer (UGGA) and a Selected-Ion Flow-Tube Mass Spectrometer (SIFT-MS) measuring carbon dioxide, methane, several VOCs and other trace gases. The authors describe the different techniques used by these instruments and give some details about the calibration of the SIFT-MS. This mobile platform was deployed in the city of York, UK, where it completed a total of 31 surveys of the same route over a 10-day period. The authors present here some preliminary results of these measurements.

Overall, this study has a lot of potential and could be a valuable contribution to the literature as it is important to monitor pollutant emissions and their evolution in urban areas. Mobile measurements of VOCS are very useful especially to characterize and identify different types of sources within a city. However, I was expecting a deeper analysis of the measurements. The development of such a mobile platform represents a lot of work but it is enough to justify a paper. The authors managed to collect an impressive amount of data (especially during a pandemic period), the paper would really benefit from developing the results section, I recommend addressing the following major points before publishing it:

- It is not specified in the article if the authors took into account the time delay between

the sampling inlet at the front of the van and the moment it reaches the instruments. This time delay can induce a shift of the measurements due to the motion of the vehicle and impact the aggregation of the measurements into the 30 metres segment. It is important to give this information when presenting mobile measurements.

- Did the authors look at the wind conditions during the measurements? If the wind was coming from one direction on given day and on the opposite direction on another day, it will likely have an impact on the composition of the sampled air, especially when measurements are performed close to known sources.
- I would have liked more discussions about the calibration approach.
    - First, I would make it clear at the beginning of Section 3.1 that 2 or 3 different calibration approaches were used for different components (AGCU and equation 1 plus calibration of UGGA?).
    - Second, I would explain why the authors chose this seven steps approach? I understand that due to time constraint, it is not possible to measure each step for too long but 3 minutes seem a bit short. Why not measure each step only once but twice as long? Why did the authors only used the right-hand steps of the post-drive calibration? What is the point of the pre-drive calibration? Did the authors observe any drift of the measurements between the first and the last day of the campaign?
    - Third, I would have also been interested in a comparison of the two calibration methods. The authors could have applied both approaches to benzene measurements for example, and shown how the two sets of calibrated measurements compare.

- Reorganize Section 3.2: having only one subsection does not make much sense. I would either add a title to the first part of Section 3.2 or remove "3.2.1 Spatial correlation mapping". Also, I do not understand why the authors presented the distribution maps of only 2 components, I would have liked to see more, especially species that are correlated (benzene, toluene, alkylbenzenes…). I was a bit disappointed at the end of this section when the authors teased the application of the correlation approach to smaller scales for a future study, I was expecting to see that in this paper…
- In the end, I am not sure I am convinced of the benefit of measuring all of these components at the same time. Here are a list of questions I got after reading this paper: What is the dominant source of VOCs of York? Do we really need C2-alkylbenzenes and C3-alkylbenzenes measurements to identify emissions from gasoline evaporation? What are the ratios of these different components for known sources? How do they compare with ratios found in other studies for the same type of sources? Can we differentiate emissions from gasoline fuel and diesel with one of the measured component? What about the other sources mentioned in the paper (dry cleaners, hairdressers…), were you able to detect any emissions from them?

Minor comments:

L1: "The importance of emissions source types…": the authors should specify what type of sources they are referring to (VOCs? GHG? atmospheric pollutants?).

L23-24: Be consistent with the notation throughout the text: choose between "ozone" and "O$_3$" and stick to it. Same for "secondary organic aerosol"/SOA, "limit of detection"/LOD…

L29-30: I would specify that you are talking about static measurements at monitoring sites here. This is developed later but it is not very clear in this sentence.

L50: Replace "targeted" by "targeting"?

L83: "1/2 inch": shouldn't the authors use SI units?

L82-84: How long does it take for the sampled air to go from the inlet in front of the car to the instrument? Is this delay taken into account and corrected on your maps? If not, it will have an impact when you bin your data into 30 meters segments.

L86: Is the wind corrected for the motion of the platform?

Section 2.2: The authors give the precision of the UGGA for methane and carbon dioxide but they do not talk about the precision of the SUFT-MS. What is the precision of the SIFT-MS for the different species? Does it correspond to the limit of detection described in Section 3? What is the limit of detection of the UGGA for methane and carbon dioxide?

L120: How many species does the SIFT-MS actually measures? This is very confusing: Table 2 and Section 2.2.1 state that it measures 13 components but Table 1 states 14 species.

L123-125: I am not sure I correctly understand what is a cycle? Does it correspond to the measurement with one reagent or to the succession of the three reagents?

L134-135: The precision of an instrument should always be stated over a time period.

L154-158: Why do you only use the right-hand steps of the post-drive for the calibration? Did you test several calibration approach with the AGCU? I wonder why you implemented these seven consecutive steps of three minutes instead of only doing four steps but with longer measurements. Also, each step of the calibration last 3 minutes, did you use all the

data within the 3 minutes or did you get rid of the first measurements that are usually influenced by the transition? Why is the agreement between pre- and post-drive calibration not as good for ethanol and methanol?

L161: Delete "instrument" in "The daily instrument ICF was derived…".

L162: Add a space between "2" and "ppm".

L175-178: It would have probably be more intuitive to test the effect of the movement and vibration of the van by comparing measurements when the platform is in motion and when it is parked.

L178: Why is there no mention of the calibration procedure for the UGGA? Did you also calibrated this analyzer before and after each drive with a multi-point calibration approach? This should be discussed here.

L188-190: I do not understand this sentence: why does having more data points in bins than in your limit of detection test confirms the confidence of the SIFT-MS measurements?

Figures 1 and 2: I would combine these two figures.

Figure 6: Change the legend of the benzene plot to better emphasize that the cps are represented by the blue dots (and only the dots) and the mixing ratio are represented by the pink line (without dots).

Figure 8: Replace" No2" and "Hono" by "NO2" and "HONO", respectively.

Figure A1: Replace "No2" by "NO2".

Table 1: The second column most likely indicates the measurements frequency or resolution rather than the response time of the instrument.