

Atmos. Meas. Tech. Discuss., referee comment RC1
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Comment on amt-2021-186

Anonymous Referee #1

Referee comment on "Fragment ion-functional group relationships in organic aerosols using aerosol mass spectrometry and mid-infrared spectroscopy" by Amir Yazdani et al., Atmos. Meas. Tech. Discuss., <https://doi.org/10.5194/amt-2021-186-RC1>, 2021

General comments

This article presents a comparison of chamber SOA interrogated with IR spectroscopic and aerosol mass spectrometry, in an effort to use the strengths of each to build something greater than the sum of its parts. The key drawbacks to each approach (temporal resolution for IR spectroscopy and functional group accuracy for mass spec) are clear, and the authors have taken advantage of multi-variate regression and other analytical techniques to bridge the obvious gaps in the data each method presents. This makes the article both relevant and novel, and the use of their multi-variate approach is novel as well. Further, mechanisms of aging can be interrogated by the comparison of these two methods - that is, there is value in their differences as well. The authors have certainly achieved this goal, and have communicated the results fairly clearly.

The results indicate a potential for this approach to provide greater insight in future studies as well as some words of caution about using tracer fragments from AMS. These conclusions are well-supported by the data they present as well as the references cited.

One small criticism is the readability of the manuscript, and I provide some very minor suggestions to improve this. The nature of this work is that the results are tedious to report, so this is not a major criticism. Overall the paper is suitable for publication with some minor improvements.

Specific comments

Section 3.1.3 (but possibly earlier) - the authors are using CC for coal combustion and

WB for wood burning. It took me quite some time to internalize those acronyms while reading the analysis, where many other acronyms are used. Because they are not very commonly used acronyms (unlike SOA or OM), it adds confusion to use these instead of the full terms. I appreciate that the terms are used many times in the analysis, and that spelling out the phrases will make for longer sentences. However, I'd have to read the paper at least twice to be comfortable with them. I leave it to the authors to decide how to proceed on this point, but I felt it was worth sharing. Given how dense the manuscript is, having uncommon acronyms interfered with my ability to process the information.

Likewise, when using NaCO (as in line 295), it would be very helpful to have "non-acid carbonyl" written as well.

Line 296 - It appears that the offset between AMS and MIR in estimated H:C is in the opposite direction for wood burning and coal combustion particles. It's worth the authors pointing this out to readers, and perhaps speculating on why this might be. A different offset, but in the same direction, is easier to understand than a similar magnitude offset in the opposite direction.

Table 1 would be more readable if functional groups had their names.

Line 272 (discussion of Figures 4a and 4b) - I wasn't sure, until much later, that 4a and 4b represent replicate experiments, and not experiments with slightly different conditions. This became clear at the very end of the manuscript. It would be useful to note this in the caption for Figure 4 as well as in the text (especially since there are varying numbers of replicate results for each combination presented in Figure 4).

Figure 5 has two similar shades of green used for COOH and NaCO and it is very challenging to distinguish them. Similar for Figure 6 and Figure 8.

Line 382 - Are the authors referring to the normal subtraction of gas phase mass spectra in "compensation" or some special treatment of the data?

Line 390 - The authors note that different aerosol source will benefit from different fragments being used as tracers for (for example) alkane. Do the authors have suggestions or are they simply commenting that this fragment was not the expected one, or maybe one that is not commonly used in other studies, but was the winner for the VIP analysis?

Technical corrections

Figure is missing the y-axis label.

Line 277 - the sentence would read better if "low" and "lower" became "small" and "smaller"

Line 290 - The sentence "The high H:C ratios before aging support the low amount of aromatics to aliphatic CH observed from MIR spectra" is awkward. I suggest, "The high H:C ratios before aging are consistent with the high ratio of aliphatic CH to aromatic carbon observed in MIR spectra."

Line 343 - insert "also" before "known" to read "fragment is also known"

Line 383 - is "carbonyl CO" the same thing as NaCO ?

Further Reviewer Questions:

- Are substantial conclusions reached? Yes
- Are the scientific methods and assumptions valid and clearly outlined? Yes, clearly so.
- Are the results sufficient to support the interpretations and conclusions? Yes.
- Is the description of experiments and calculations sufficiently complete and precise to allow their reproduction by fellow scientists (traceability of results)? Yes, very clear descriptions are provided.
- Do the authors give proper credit to related work and clearly indicate their own new/original contribution? Yes.
- Does the title clearly reflect the contents of the paper? Yes.
- Does the abstract provide a concise and complete summary? Yes.
- Is the overall presentation well structured and clear? Yes.
- Is the language fluent and precise? Yes.
- Are mathematical formulae, symbols, abbreviations, and units correctly defined and used? Yes.
- Should any parts of the paper (text, formulae, figures, tables) be clarified, reduced, combined, or eliminated? I have made small suggestions above.

- Are the number and quality of references appropriate? Yes.
- Is the amount and quality of supplementary material appropriate? Yes.