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Atmospheric Measurement Techniques
Discussions

Interactive comment on "Addition of a fast GC to SIFT-MS for analyses of individual monoterpenes in mixtures" *by* Michal Lacko et al.

Anonymous Referee #3

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The authors present the use of soft ionization mass spectrometry (SIFT-MS) combined with a fast-GC system in order to achieve separation and identification of different monoterpenes. The capabilities of two different columns are discussed. Furthermore, the potential use of different ionization modes when operating the SIFT-MS in order to better separate the monoterpene mixtures is suggested as a method to improve separation for this type of systems. After following the revisions suggested below, the publication should be suitable for AMT.

Specific comments

In the "abstract" and "summary and conclusions" sections of the manuscript, the achievement of quantitative analysis is suggested. This is not supported though by the main text and is even discussed that it's not the case by the authors on page 17,

line 14. To my understanding, a quantitative analysis would provide ppb values of the individual monoterpenes together with their detection limits. On the contrary, only normalized intensity values are provided throughout the whole manuscript, for a mixture of monoterpenes that are not fully separated in the conditions used except in one case-study where the retention times are high (Fig. S3, 5V, retention time: 500s). It is therefore essential that the abstract and summary are re-written to avoid any misleading suggestion of quantification that overpromotes the presented work. The authors should work towards providing a more representative view of the manuscript that is related to the separation optimization of a monoterpene mixture using a low-resolution fast GC combined with the information obtained from differences in fragmentation patterns when using different ionization in the SIFT-MS.

There is only one point in the manuscript where the authors discuss the detection limits of their technique that are as high as 100 ppb (page 17, line 15). How was that calculated? Did the authors perform calibrations for the individual monoterpenes? Where could this technique be applied with this high detection limits? I would expect that the values used in this study are not applicable to ambient field measurements since they are higher than any ambient observations. Comparison of this technique to other fast GC techniques shows differences in the limit of detection by orders of magnitude (page 17, line 15). As discussed in section 4.5, this technique is, therefore, inferior to others but could still be useful for identifying monoterpenes based on fragmentation. This should be the main part of the abstract and conclusions sections. This should be further discussed in the manuscript, especially since the authors attempt to publish in an atmospheric measurement technique journal.

In order to obtain valuable information, the authors suggest that changing ionization in the SIFT-MS is recommended. This implies that in order to obtain valuable information relative to other techniques the GC-SIFT should run in both ionization modes. What would be the time needed to go through an $H3O+$ and a $NO+$ cycle? How much more is the time compared to other fast GC techniques that only run once and with better resolution (page 17, line 16)? Overall, I would recommend that the value of this work and the comparison of this technique to others should be further discussed and emphasized throughout the manuscript.

Section 2 is hard to read and I would suggest restructuring. In the first sentence of the section the authors introduce Fig. 1 but this is not followed by a discussion of the figure, the instrument parts, and operation. On the contrary, they discuss the column options and operating details and then go through the temperature profiles. I would recommend the following structure: A. A discussion of the parts of the fast GC pre-separation system and the modes of operation with their details that are discussed in section 2.1 and page 4, line 15 to page 5, line 4, B. Operating details together with columns of choice and temperature profiles.

In section 3.1 a short discussion regarding the humidity dependences is presented that is not supported by any figure or graph. Was the humidity of the different samples measured? If so, shouldn't these values be provided in all figures, especially since the effects seem to be substantial? Furthermore, this paragraph and further discussion should be part of the results and discussions and not the section it is now.

Section 4.1 and 4.2 have an overlap of results and discussion that makes these sections hard to follow. I would recommend that the authors work towards restructuring these sections to a clearer presentation of the results that the table and figures promote followed by a detailed discussion, for each graph, for each column, and the comparison of the two columns. A characteristic example of the difficulty of the reader to follow the results and discussion is the title of section 4.2 that has little to do with what is discussed in it. Furthermore, please discuss why NO+ was not tested for the MTX-Volatiles column.

Technical comments

Title and manuscript: change "analyses" to "analysis" Page 1, line 19: change to "...to separate them in less than 180 s...". Page 2, line 15: change to "... which can affect

human health...". Page 2, line 29: correct to "fast GC-PTR-ToF-MS" and in general correct throughout the manuscript "fastGC" to fast GC". Page 2, line 33: change to "we report method development results aimed to...". Page 6, line 27: change to "are given in Table 1, and discussed in section 4". Page 6, line 28: This is hard to follow sentence. Rephrase. Page 6, line 30: Change to "reagent" Page 8, line 2: change to "saturation vapor pressures" Page 17, line 27: change citation style Page 17, line 17: Which results? What are the authors comparing here? Page 18, line 22-23: "... allows analysis of mixtures of monoterpenes in the air in short time periods..." Is that the case for ambient measurements in the detection limits of the system? Isn't this overpromoting the capabilities of the system? Table S1: It will be nice to add the m/z of detection.

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