Atmos. Chem. Phys. Discuss.,
https://doi.org/10.5194/acp-2020-648-RC1, 2020

Atmospheric Chemistry and Physics Discussions

Interactive comment on "Source identification of atmospheric organic vapors in two European pine forests: Results from Vocus PTR-TOF observations" *by* Haiyan Li et al.

Anonymous Referee #1

Received and published: 30 July 2020

This article reports the first time the binPMF algorithm has been applied to VOCUS PTR-MS data, as applied to forested environments. There would be a strong interest in this type of broad-base work to try to generalise biogenic emissions, as these can have a profound effect on atmospheric chemistry. While I would say this certainly fits thematically within ACP's scope, right now the paper currently feels unfinished as a research article because while it demonstrates the instrument and algorithm 'working', it currently fails to identify what new understanding this confers to atmospheric science, beyond a running commentary of the authors' interpretations of the factors. I therefore recommend that this paper be published after major revisions. This could take the form of either a research article that is more focused on the atmospheric science arising

Printer-friendly version

Discussion paper

from the work, or a technical note that explores the technicalities in more detail (I have queries regarding the methodology, see below). While it could in theory present a 'measurement report' based on this work, I feel that this may not be in the spirit of what the authors intended.

Comments:

The manuscript currently presents the results very systematically, but it is difficult to see what the reader is supposed to get from these. The authors provide a commentary on their interpretation of the factors, but I am not sure I learned anything new or significant about atmospheric chemistry on reading these. If this is to be presented as a research article, the paper needs to be refocused towards the new scientific insight or a testable hypothesis.

A certain amount of work in this paper goes into arriving at factorisations that aren't simply dominated by the big signals. This is probably to be expected because the gas phase VOC ensemble is likely to have many more degrees of freedom than can be accurately represented by the PMF and furthermore, many peaks will have isomers that won't be resolved using PTR. This is done by removing the main monoterpene signal and separating the mass spectrum into different regions. However, this comes across as a little subjective and prevents a direct association between the peaks in the two regions. Did the authors attempt a more conventional approach, such as applying a 'model error' parameter to downweight the larger peaks? More attention should be paid to demonstrating what the effects of not following these procedures in either case, perhaps shown in the supplement.

One might expect that given the number of degrees of freedom available, there will be a level of rotational ambiguity in the solution sets. This certainly would appear to be the case in figure 11, where all of the factors appear to contain traces of siloxane. Was the amount of rotational freedom available explored?

The observation that reaction products did not contribute as much to the mass budget

is perhaps expected because of their chemical lifetime. However, can the authors be sure the these (presumably more polar) molecules were being detected with equal efficiency? Have the authors tried comparing with a mechanistic model like the MCM or GECKO-A?

Interactive comment on Atmos. Chem. Phys. Discuss., https://doi.org/10.5194/acp-2020-648, 2020.