

Earth Syst. Sci. Data Discuss., referee comment RC1
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Comment on **essd-2022-406**

Anonymous Referee #1

Referee comment on "Two years of volatile organic compound online in situ measurements at the Site Instrumental de Recherche par Télédétection Atmosphérique (Paris region, France) using proton-transfer-reaction mass spectrometry" by Leïla Simon et al., Earth Syst. Sci. Data Discuss., <https://doi.org/10.5194/essd-2022-406-RC1>, 2023

General Comments

Simon and coauthors present a two-year long PTRMS dataset of VOCs in the Paris region. Data was collected across seasons and before and during COVID-19 lockdowns and will be very helpful for models and other interpretations of urban VOC measurements. The authors do a good job of presenting what the dataset is and guide the reader through points of interest and further study in the data set while presenting some of their own conclusions. However, the quality of the dataset is questionable only because a large amount of detail on calibrations and quality control is left out. Major revisions are required to add this detail in and are outlined in the comments below. I have many other minor comments that are needed to communicate some conclusions and for the presentation of this data set.

Specific Comments

Line 137-139: I think the kinetic approach needs a little more justification for your system. It's not clear that this will work for your full range of k . This could be a figure of k^* (transmission) vs. measured sensitivity in the supplement and then you overlay a few species of estimated sensitivity over a broad k range.

Line 149: You should briefly describe the implications of having a higher humidity in the drift tube.

Line 157: It is unclear what "sensibility" is used for here.

Line 159: Explain why it is advantageous to have a cycle of <15 minutes.

Line 171-175: You should include a supplement table for the sensitivities of select species across the different standards. Also do you propagate this uncertainty into your measurements? If not, you should and state how you do it.

Line 174-175: Include the NPL standard species in Table S2.

Line 175-177: It is very unclear what this lab test was. What specifically was done to "infer the repeatability of measurements over 3 days"?

Line 177-179: It is surprising that for a quadrupole PTRMS the sensitivities changed on average by 3% from an RH of 30% to 90%. There should be a supplement figure showing sensitivity vs. RH or the ratio of water dimer to monomer for a few ions to support this claim.

Line 180-181: State what reagent ions you are calibrating to and what the normalization factor is. Also there needs to be more detail on how you applied humidity corrections. Did you gather sensitivity vs. humidity curves and then apply them? Which species did you calibrate for/which standard cylinder did you use and what did you do for a humidity correction for species with no standard calibration? The low humidity influence in general is questionable without supporting figures.

Section 2.3.4: To support the quality of this dataset this section needs a lot more detail. In addition to the above comments, you should state in the main text how many species were directly calibrated for and for what fraction of the measurement period (since you changed standards) had direct calibrations. Since you only calibrate once a month you should state how much the sensitivities are changing and include a supplement time series for select species of the sensitivity vs. time. This would also be a good place to overlay calculated sensitivities when cylinders changed.

Line 186-187: Specifically what measurements are you referring to here? Which ions/metrics are you tracking? Are these ions species you would assume are stable over two years in an air cylinder? Also you mention that you check instrument parameters but do not comment on their stability. There needs to be more detail on these tests.

Line 207: It looks like you could not perform zeros for most of the PTR-ToF measurement time due to lockdowns. Can you show that the zeros are robust over a long period of time? Were you able to calibrate during this time too?

Line 208: There needs to be more discussion on how the PTR-ToF is calibrated if you are going to use it for assigning species fractions to isobaric peaks. Is the internal dilution system the calibration system for the PTR-Q-MS or a different one? How frequent were the calibrations and what was in your calibration standard?

Line 220-221: These guidelines need to be summarized here. The quality of this data cannot be supported without explaining your detection limit and error determination.

Line 223-224: You need to explain what these internal and external quality control checks are.

Line 226: define what Ebas is and include a DOI citation for the dataset in the text.

Table 1: It is unclear what the mean error is and what quality checked by ACTRIS means.

Line 258: This sentence for isoprene is for global BVOC and you are looking at an urban region. Unless you have literature to support this, it is not necessarily expected that isoprene will be very high in this region relative to monoterpenes. You should remove this or reword it.

Line 259: Briefly explain what is meant by this. Are you saying the median monoterpene concentration is high because of a wintertime contribution?

Line 261-270: The purpose of figure 3 needs to be articulated more or figure 3 should be removed. The supporting paragraph preceding figure 3 does not explain what the figure means but rather states the concentrations of some classes in each bin. Is there some takeaway about sourcing at lower or higher concentrations that uses this figure rather than the other sourcing details later in the paper? There is a brief portion on comparison to particles but no data to compare.

Line 290: How many hours back do the back trajectories go? This would be important for estimating chemical and transport lifetimes. Also are these trajectories sourced and stay near the surface for the duration of the trajectory?

Line 308: is the NO_2^+ signal included in your "N-containing" species and if so what fraction does it compose of that class? Since it could be part of reagent ion chemistry I would be cautious of using m/z 46 unless you have a strong calibration and zero to prove that it is not generated in the instrument.

Line 315: How was mixed layer height measured?

Figure 6: This figure needs more detail in the caption explaining what the distributions are and what the lines are. The title (or legend?) should be consistent with the naming convention in the rest of the paper (N containing instead of n_containing).

Figure 8: A suggestion: I think a comparison of diel cycles during different seasons for select species would be very valuable and support your month average plots of Figure 7 and could be included. For example, your differences in monoterpene concentrations in the summer and autumn could be highlighted in the supplement and could add to your claims of changes in lifetime against oxidation and sourcing across the seasons.

SI Line 51-53: What fractions of m/z 69 are isoprene and furan?

Technical Corrections

Line 38: secondary organic aerosols and ozone should not be capitalized.

Line 63-64: non-methane hydrocarbons and oxygenated VOCs should not be capitalized.

Line 97-98: Is "important" here used to describe the frequency and intensity of traffic? If so, I would suggest replacing "important" with "heavy".

Figure 1 caption: Change "South-West" to "southwest"

Line 116: Specify that the AE33 model is an aethalometer. I would just place it in your parenthesis before "Magee Scientific".

Line 186: You should replace instances of "bottle" with "cylinder" if you are referring to a gas standard. Unless it really is a bottle, then my apologies.

Line 198: "While isoprene is an abundant biogenic VOC..."

Line 239: VOC has already been defined. You do not have to define it again here.

Line 262: In general, remove any contractions (e.g., don't) from the text.

Line 263: use a · instead of . in your units.

Figure 3: x axis needs units

Line 290: define h

Line 298: Be consistent in naming conventions. Earlier it is "oceanic 1" but here it is "Oceanic 1".

Line 302: "...Figure 5b." You should use this notation for other instances.

Line 326: "... to the temperature..."

Line 361: This variable is defined as B_{ff} earlier on. Stay consistent with names.

Figure 9: define NR-PM1

Line 445: remove "seem to have"

Figure 10: Replace "During" and "Lockdown_2" with "Spring Lockdown" and "Autumn Lockdown", respectively. This is consistent with you caption and text. Also use subscripts with your BC variables to be consistent.

Should "CRedit" in the authorship statement be "Credit"?