

Comment on **essd-2022-406**

Anonymous Referee #2

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-RC2>, 2023

This work shows a two year long PTRMS data set in SIRTA, and it is very valuable to the community, particularly modelling community, as it captures COVID 19 lock down as well as other very interesting and contrasting atmospheric chemistry periods. I think it is well written and the paper should be published, but, much more information needs to be provided on data methodology and analysis. Therefore I suggest major revisions mostly on methodological process.

2.1.2. I would remove this section or put it later as this is not your main objective and the data is only for comparison purposes.

I also do not see information on temperature, pressure and par measurements which you use for concentration calculations and show it on graphs. I need info on sensors and methodology.

2.3.1.

Line 126: Please state the period of PTRMS measurements

Line 134: from where do you get the clean air, how clean is this?

Lines 137-139: the transmission calculation needs to be better explained. How is the transmission curve? How did you calculate it? How often did you calculate it? How do you

interpolate transmission curves over time? Please state k rates for each compound. Why 3 instead of 2 for unknown k rates? Can you provide a reference for this? Which standards you use for transmission, how did you take into account fragmentation of compounds. But to me the most critical thing is to see if you have calculated several transmission curves or only one (the latter would not be correct then).

2.3. I need a longer explanation on inlet set up. How it is? A picture would be very explanatory. Is the line isolated? How are you heating the line? How tall is the SIRTAs station, because 6 m for 15 m above ground is confusing. What is the OD and ID of the PFA lines. How this may be affecting compounds such as dichlorobenzene for stickiness? What is a Valco valve? Explain more on what is this and which material is done, how many connections you have.. etc..

2.3.2.

You say t_{drift} is 60°C in the text but it says 40°C in table S1

What do you mean by regularly adjusted... How is this done, how often, do you calibrate for each change? You need to state better how calibrations are done, but we will get there.

2.3.3.

Did you have equal dwell time for all compounds? It is not the same to measure acetone and sesquiterpenes for instance, and a dwell time of 10 s for compounds such as acetone, seems too long... although not necessarily wrong. But let me get this straight, you only get a value per compounds every 15 minutes? This may decrease the power of online measurements... but again not necessarily wrong. I understand calibrations were done with the exact dwell time of measurements, right?

How this lower sensitivity with 5 s has been observed? Can you explain in time when changes were done? Also can you show this decrease in sensitivity?

Also can you explain why a resolution of 15m is better than 22m?

Line 160: Can you show your scan mode measurements? Which previous studies you used?

Line 166-168: This lines seem to contradict what you say in 156-159. Please rephrase and make it consistent.

I suggest including a table with all monitored masses, compound assignment, possible fragmentation, k rates, calibration factors, LOD and uncertainty..... (basically an updated table 1)

2.3.4.

This is the most critical part to me

How did you perform blanks with the gas calibration unit. Did you have n₂? Synthetic air, catalytic converter? If the latter at which temperature? Also how is your blank for compounds such as acetic acid?

Did you find a drift in your calfactors over time? Somehow it may seem one month per doing calibrations is too long. I would like to see a list of calibrations and how these change when ptr parameters are changed.

Please show cal factors (ncps/ppbv) per each compound and how they drift with time and with cal gas. This also adds to the comment on transmission. Add the NPL cal gas, and please show how did you account for the variations in calgas. This is very important for the compounds used to calculate the transmission curve. Please also state which compounds are those.

Line 175-179: please rephrase.... This is very confusing. When did you do these tests?

About humidity in calibrations, did you perform humid calibrations or not? How did you apply this effect?

How did you interpolate sensitivities? Did you interpolate humidity effect over time? Also I guess the impact of humidity is totally different depending the compounds. Please show.

2.4.1.

What is stable ambient air? Can you please rephrase this part? What do you mean check the stability?

2.4.2.

Line 205: please state inner diameter, as this is the same residence time as expressed in line 143, however with a different flow. Thus Both ptr system sample from different lines? Please restate to make it clear.

Line 206 ohh so here is the catalytic converter. Only performed once per two days? This is too long, it changes with time.. even 13hrs may be too long.....

Line 209: how are these calibrations done with the internal standard?

2.4.3.

S3 text

If you cant calibrate for formaldehyde, drop it...

The main source for acetaldehyde is not biomass burning (or not only). There is photochemistry and even biogenic. Please rephrase and show references.

m/z 46 how can you calibrate for them two with transmission only?the same goes for m57

you say corresponds when I think the word here is we have assigned this mass to this compound. Please change.

2.4.4.

Please state how did you calculate the statistical error, the systematic error, and how did you use the theory of error propagation. This information is totally missing. Also how did you calculate the LOD.

I think you cant cite ACTRIS guidelines, because they are not ready yet. On the other hand please state which are those guidelines.

Line 223 what do you mean by internal quality check by carefully verifying? How is the quality check by ACTRIS, please state. What is ebas database, please state.

3.1 I suggest using statistics (like correlations or heatmap) to group compounds, as in the city you have many different sources, and perhaps what is expected may not be the reality. And also have you considered doing a positive matrix factorization? This could really help on source identification.

Line 242: this statement about methanol and acetone is inconsistence with Figure 4, oxygenated compounds have even higher yaxis.

Line 246. I really do not understand why you pass to concentrations when comparing ppb across other literature could be valuable. The only thing I need to know is that you indeed use real temp and atm pressure data to calculate this, per point. Correct?

Line 258: you keep saying isoprene is the most important biogenic compound, and this is not true. It may be the most copiously emitted, but there are species who do not emit isoprene. So rephrase these statements.

Why are monoterpene concentrations important during winter? And why only in winter, if it is a source from the city, (i.e. perfumery, or cleaning products industry) wouldn't it be all over the year?

Despite im not really happy with a figure 2 because it does not give you much info as it is averaged over summer and winter and day and night, so I expect a huge variability, I do not know what is the purpose of figure 3. Please rephrase the purpose of the figure or remove.

3.2.

Are the trajectories more dominant in particular seasons? Please also state this.

3.3

Line 381: where does the 77% comes from?

4.

Explain what flags are