

Atmos. Chem. Phys. Discuss., referee comment RC1
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Comment on acp-2020-1294

Anonymous Referee #1

Referee comment on "Measurement report: Online measurement of gas-phase nitrated phenols utilizing a CI-LToF-MS: primary sources and secondary formation" by Kai Song et al., Atmos. Chem. Phys. Discuss., <https://doi.org/10.5194/acp-2020-1294-RC1>, 2021

This paper describes an interesting analysis of the sources and formation of nitrated phenolic compounds in a Mega city. The material presented is original and the topics are well chosen. The paper contains some model-based data analysis parts and a section about source apportionment by NMF. While the latter is quite well done the former has some room for improvements. Actually, the manuscript is in these parts difficult to follow. I think there are two reasons for that. There may be some weaknesses in the language (however, I am not a native speaker myself) and possibly some errors and un-preciseness in relation of the figures and their description in the text. Both together made it difficult to really judge the quality of the scientific content.

Still, in my opinion, the manuscript has valuable information and potentially good science in it. I suggest, to consider the manuscript for publication in ACP after some major revisions and formal improvements along the comments below.

Formal:

I suggest the authors a) check use of present time / past tense; b) check use singular / plural for predicates / verbs; c) check use of single words and notations (in a thesaurus), if they really express what they wanted to say. In addition, it seems that names are mixed up, which makes it difficult and time consuming to understand the results. I indicated some examples below, but not all.

Major comments:

line 126 – 131: The authors note missing “mechanism” for NP formation. But NP from phenol oxidation is in their chemical mechanism, so I would call it missing “sources of phenol”. And that is actually, how they treat the problem, by testing phenol sources with two different source strength.

At the same time, I am wondering what is to be learned from the use of the two suggested emission factors of phenol. The emission ratios phenol/NO_y and phenol/CO look similar, but de facto they lead to an order of magnitude different phenol concentrations, because of the different concentrations of NO_y and CO. Do the authors want to say that linking phenol to CO leads to more realistic phenol concentrations? However, the use of the CO related phenol source leads indeed to about the right level NP concentrations, but the model time series does not really match the time series of observations.

In addition, unfortunately, the most important last lines in Table 1 are messed up. What is the meaning of the number in brackets? I would also suggest, to replace the different references in the last column of Table 1 by numbers or symbols and list them in the captions under the table.

line 195-199: I am sorry, I am not able to recognize the features described in the manuscript for the Figure b and c. E.g. NC and MNC have a different diurnal cycle but are treated together. I can also not identify gentle peaks at 5 pm. To me it looks as if either the descriptions do not express what is intended to say or the explanations and plots maybe mixed up.

It would be also helpful if the time notations in the manuscripts and at the axis of the Figure would be the same and to have minor ticks at the time axis or a grid in the diagram.

Because of all this I cannot really judge conclusions drawn from diurnal cycles.

line 205 – 214: Again, I have difficulties to follow the text along the Figure S3. If DMNP is explained by the xylene emissions the red symbols should indicate that, because this should be covered by the base case, right? I don't see them. On the other hand, MDNP is according Figure 1 a product of toluene, not of xylene, as I think, is claimed in line 213. In

any case, if MDNP can be understood from the VOC then there should be again red symbols showing that? Why do you show the effect of phenol constraints in the lower panels when phenol is not expected to contribute to the formation of DMNP and MDNP? In addition, the symbol style is chosen such, that overlapped curves cannot be seen very well.

And as already mentioned above, even if the model predicts the levels of the observations quite well, the time behavior does not really match.

Line 220-227: NO₃ and OH contribute to C₆H₅O production. In the model phenol + NO₃ and phenol + O have fixed branching ratios into C₆H₅O of 75% and 6%, respectively, and others of which about 80% lead to catechol in the OH case. Now I am wondering, does the green NO₃ section comprise NO₃-produced C₆H₅O or is it subsumed under the turquoise C₆H₅O part? For first case, how can the ratio of C₆H₅O path to catechol path vary since the phenol + OH reaction has a fix branching ratio? For the second case, assuming that NO₃ will dominate C₆H₅O production the path to the other NO₃ products seems to large. Please add a more detailed explanation what you used in detail to achieve the results in Figure 4 and Figure 5.

Line 228-234: I do understand what you wanted to say, but it is somewhat difficult to grab. It might be helpful to show the NP concentrations in Figure 5, too.

Line 241 – 244: What exactly is the Xylenol+NO₂ reaction? The sentence starting with "As for DMNP, the production ..." is unclear. Please rephrase it. Where can I see the loss of DMNP in Figure 6?

In general, I would suggest, to modify the Figures remove overlap of elements. E.g., pie charts are partially in the Figure, partially outside. Formulas are crossing the frame of the diagrams, or in Figure S1 the formulas are too large and overlap the MS peaks.

Minor comments:

line 94f: how can you be sure about the suggested structures? You used MS.

line 100f: you calibrated with only one compound. Can you add something on the range of sensitivity expected for measurement of the addressed compounds by NO₃-CIMS?

line 117: "other necessary packages", if the packages were necessary/important, you should name it otherwise I would skip that phrase.

Figure S2: Why do you observe larger noise/fluctuations for the higher signals?

Typos etc:

line 19f: contribution to production or concentration?

line 34: "gained much concern", I would formulate that differently

line 39: I believe that Beijing is still the capital ...?

line 40: "preserves ... cars" , I would formulate that differently

line 42: NAC is not defined

line 45: either "spectrometry" or "spectrometers" (2x)

line 91: "...time resolution of the measurement..."? and 'The CIMS data processing was "conducted" by...' ?

line 112f: something is wrong with this sentence

line 119: I believe "functioned" is not the right word here.

line 121: I would use present time (you should check the whole manuscript, there are more of these)

line 132: budget

line 137: "total primary NPs 'were' calculated by subtracting", plural (you should check the whole manuscript, there are more like these)

line 188: explanation for what exactly?

line 201f: something is wrong with this sentence

line 244: is hailed the right word?

Figure 1: scenarios (bold red)

Figure 8: I suggest, to use different colors for the grouping boxes

Figure S3: see my major comments, I suggest, to improve the figure such that you can better separate the different cases.

Figure S8: I suggest, to use different colors for the grouping boxes