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Comment on acp-2021-666

Anonymous Referee #1

Referee comment on "Are reactive oxygen species (ROS) a suitable metric to predict toxicity of carbonaceous aerosol particles?" by Zhi-Hui Zhang et al., Atmos. Chem. Phys. Discuss., https://doi.org/10.5194/acp-2021-666-RC1, 2021

Summary

This study measured the reactive oxygen species (ROS) and oxidation potential (OP) of two different types of SOA that was produced from the oxidation of naphthalene and beta-pinene. To mimic the urban environment, soot particles were used as preexisting organic matter. The authors measured ROS by using an online technique coupled with DCFH/HRP assay and compared it to the offline measurement using the same assay. They also compare the results to the measurement of OP by using DTT assay and the results from cell exposure. A significant amount of work was performed in this study to understand the toxicity of two different types of SOA and to evaluate the chemical assays for better representing cellular response. The authors concluded that naphthalene SOA, in general, has higher toxicity compared to beta-pinene SOA. They also concluded that ROS quantification could be a feasible method to represent aerosol toxicity. This manuscript is suitable to be published in ACP after minor revision by considering the comments as listed below.

Major comments:

- Page 1, line 29, "The SOA mass was condensed onto soot particles …". What is the major purpose to use soot particles? Will the soot particles also cause OP or cellular response? It would also be better to briefly introduce how soot particles are connected to SOA and OP in the abstract.
- Page 5, line 134. It would be better to provide a simple explanation to calculate the carbon oxidation state of aerosol. The brief description of the post-process of AMS data would also be helpful.
- L163: The different precursor produces the different ROS which can have varying physicochemical properties. Naphthalene SOA and b-pinene SOA may have different solubility in water. Can Milli-Q water thoroughly extract the organic products on the filter?
- Page 9, line 254. In order to show that the ROS is caused mainly by the SOA coated on the soot particle but not the soot only, it would be valuable to add the ROS control for soot particle only in Figure 2.
- Page 9, line 263-265. Is there any evidence during the experiments about hygroscopic

aerosol growth when RH increased from 40% to 70%? Both naphthalene SOA and beta-pinene SOA are relatively less polar in general (Chhabra et al., 2010; Chen et al., 2015). If water is less partitioned onto aerosols, the impact of humidity on the aerosol phase reaction will be little, and humidity will have a small impact on aerosols. However, for other types of SOA, such as isoprene oxygenated products, it is relatively polar, and their SOA formation, as well as OP, could be potentially impacted by RH. Can the authors conclude the the humidity effect on the SOA by using less polar organic matter ?

- Page 11, line 313-319. Figure 3 shows that the carbon oxidation state for terpene SOA is different between the experiments under 40% RH and that under 70% RH (the highest number is 3 times different). Please provide the explanation for the higher carbon oxidation at the higher RH ? Is it due to the high OH radical concentration at the higher RH ? (high ozone production at the high RH). However, their observed ROS is very similar. It seems that the correlation between ROS and carbon oxidation state is only valid within the type of precursor but it is not sensitive to experimental conditions within the same precursor (i.e., SOA from different RH). This needs to be explained.
- Page 12, line 333-line343. The filter samples were stored at -20^{o}C for about 6 months. Can the short-lived ROS decay during this period and cause the uncertainties in the analysis? If SOA products are semi-volatile compounds, how can the one understand whether these species are reduced due to decay or by evaporation? There is no clear definition between short-live and long-live species in this manuscript. What is the expected lifetime of short-live species? Is it in second or minutes magnitude? The comparison of the samples between real-time samples and samples after 6 months is too much long time gap.
- Page 15, line 378. When were OP determined by suing the filter samples? Were these samples measured right after sampling or stored for 6 months before analysis?
- Page 15, line 382. What is the possible reason for the higher OP at 40% RH than that at 70% RH? Does this observation happen in NAP SOA but not in terpene SOA?
- Section 3.4. The cell studies were performed with the filter extractions. Then, were the most ROS species used for cell studies long-live products? Can the cell studies using filter extraction be same with the results of online ROS measurement?
- Page 23, line 527. Will the ROS products slowly decay in the cell medium in the absence of cell cultures? It may also be useful to test how SOA products decay in the cell culture buffer without cells within 24 hrs.
- Table 1: Author increased the concentration of both soot particles and VOC, and Table 1 shows the changes in the oxidative characteristics of particles generated form the different concentration of soot particles and VOC. If there is a change in the concentration of VOC or soot particle only, are those oxidative characteristics influenced? Which one mainly cause this difference in oxidative characteristics?
- Table 1: Carbon oxidation state of particle from SOA_{bpin}-SP are negative values. What does the negative values of carbon oxidation state of particle mean?
- Is there possible impact of vapor-wall loss on the oxidative characteristics of particles produced in the reactor or sampling lines?
- QC/QA: How many data points were used for the QC/QA? This information can improve the reliability of the QC/QA.
- Figure 2, Figure 4, Figure 5, Figure 6, Figure 8, and Figure 9: Please explain the calculation of the error bars?

Minor Comments:

- Page 9, line 276. What is "photothermal aging"? Should it be "photochemical aging"?
- Page 9, line 277, "highest ROS formation" -> "the highest ROS formation".
- Figure 3 and 7. It would be better to add order number (e.g., a, b, c, and d) for each

sub figures.

- It would be also useful for readers to organize the experimental conditions in a Table (in main content or SI) for the experiments described in Section 3.1-3.3.

Reference

Chen, Qi, et al. "Elemental composition of organic aerosol: The gap between ambient and laboratory measurements." Geophysical Research Letters 42.10 (2015): 4182-4189.

Chhabra, P. S., R. C. Flagan, and J. H. Seinfeld. "Elemental analysis of chamber organic aerosol using an aerodyne high-resolution aerosol mass spectrometer." Atmospheric Chemistry and Physics 10.9 (2010): 4111-4131.