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Interactive comment on “Identification of particulate organosulfates in three megacities at the middle and lower reaches of the Yangtze River” by X. K. Wang et al.

X. K. Wang et al.

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RE: A point-to-point response to referee #5's comments

“Identification of Particulate Organosulfates in Three Megacities at the Middle and Lower Reaches of the Yangtze River” (acp-2015-393) by X. K. Wang , S. Rossignol , Y. Ma, L. Yao, M. Y. Wang, J. M. Chen , C. George, and L. Wang

We are grateful to the helpful comments from anonymous referee #5, and have carefully revised our manuscript accordingly. A point-to-point response to the reviewers' comments is given below.

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General comments:

In my opinion the manuscript is not suitable for publication in its present shape for at least two reasons.

Reply: We revised our manuscript thoroughly according to comments from all referees. We believe that our approach and data are convincing enough to warrant publication in ACP.

1. A substantial lack of the analytical data The authors intend to present the data from a few field campaigns in three megacities at the middle and lower reaches of the Yangtze River. A key tool they use is hyphenated mass spectrometry. Here is my first concern: the manuscript (including the supporting info) is lacking of the chromatographic and mass spectrometric data. I am utterly aware of a great number of raw data. However, the most relevant/major LC peaks should be discussed or at least briefly defined. The authors should consider a table as a tool to summarize the most ample organosulfates that contribute to the organic fraction.

Reply: We do share with the referee, his/her concern about the practical aspects of adding too many chromatograms. However, as recommended we have added extracted ion chromatograms of major m/z in the main text and in the supplement and now start our discussion around those. A table was added in the supplement (new Table S4) summarizing the most ample organosulfates presented in Figure 2 (now Figure 3). In addition, retention times, potential precursors, and corresponding references for observed OSs have been included in the supplement (new Table S3).

2. A misleading title The title "Identification of particulate organosulfates in three megacities at the middle and lower reaches of the Yangtze" suggests the authors are willing to make a thorough analysis to confirm molecular entities of detected organosulfates in the ambient SOA samples. As an analytical chemist I can not allow for the misuse of the term "identification" by showing only an elemental formula of the detected organosulfate. The elemental formula is a relevant, though not sufficient parameter for

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the structural elucidation of any organic compound. A term ‘identification’ should be reserved for a compound that is positively identified from the comparison to an authentic standard compound.

Reply: In this study, the formulas were tentatively determined by applying a number of restrictions to the detected exact m/z values. We do agree with referee #5 that all molecular formulas are only tentatively assigned and not positively identified. We revised our title into “Molecular Characterization of Atmospheric Particulate Organosulfates in Three Megacities at the Middle and Lower Reaches of the Yangtze River”. In addition, we now state in our revised manuscript (Page 4, Line 85-86) that “Recently, ultra-high-resolution mass spectrometry has been applied for tentative determination of the molecular formulas of OSs in atmospheric aerosols samples” to avoid any misinterpretation of the term “identification”.

3. Constrained data for seasonal variation The authors make an effort to discuss the seasonal and diurnal variations. However, it is not clear for me how the authors are able to achieve this goal from such a limited number of samples.

Reply: Our point of view was not to infer any general conclusion about seasonal or diurnal trends of OSs in China but more to describe our observations and suggest some explanations. Nevertheless, we agree that seasonal/diurnal comparisons from average values in Table 1 are not so relevant and should come along with moderate conclusions. For the Shanghai samples and corresponding manuscript section, even if we do agree that no definitive conclusion can be made about seasonal/diurnal trends with such a small dataset, we think that describing our results this way is informative and could help future more complete field campaign to identify specific points to clarify, as the presence of nitrooxy-OSs during daytime or the importance of the precursors’ seasonality in different locations. The manuscript will nevertheless be thoroughly edited to limit the conclusions about seasonal trends, preferentially highlighting the nature/variety of the detected OSs rather than their seasonal/diurnal trends. For example, new section 3.5 is now titled with “Comparison of OSs in the SH samples” (Page 17, Line 460).

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4. Difficulty in reading The manuscript is written in the unpleasant way for the reader. I found the text difficult to follow, possibly owing to the fact of the data oversaturation. Thus, I would suggest the authors looking for a language editing service to make sure that the manuscript can be read smoothly. Just an example, page 21429 onwards about KMD and/or V K diagrams: I find this section very weird to read and get information out of it.

Reply: The manuscript was lightened and clarified as much as possible and reviewed by a language editing service.

5. Moreover, there are some errors in terminology. An example, Th' and 'm/z' are used simultaneously. Both are a unit of mass-to-charge ratio, and it is redundant here. I would advise on using "m/z" as recommended by IUPAC provisions. Another example, page 21426 line 27-29 and throughout manuscript: Is it a nitrate group or nitrooxy group? How do the authors know without CID (collision induced dissociation) experiments?

Reply: Only "m/z" is used in the revised manuscript. Organonitrates (RONO₂) are compounds bearing nitrooxy group(s), also called "nitrate group". Both denominations refer to the same functionality. See for instance "Volatile organic compounds in the atmosphere" from Ralph Koppmann (2007, Blackwell Publishing Ltd) p 283-284. However, it is true that MS_n experiments were not performed in our study, and hence we cannot exclude other possibilities such as heterocyclic compounds, nitrophenolic compounds, etc. We now state (Page 8, Line 205-209) that "Compounds that satisfy these criteria and present a number of oxygen atoms greater than or equal to $4s+3n$ ($4s+3n \leq o$) were tentatively regarded as OSs or nitrooxy-OSs. However, other S- and N-containing compounds, such as sulfonates or compounds bearing nitro groups, may also be involved (e.g., Riva et al., 2015b; El Haddad et al., 2013)". Other errors in terminology have also been revised.

Interactive comment on Atmos. Chem. Phys. Discuss., 15, 21415, 2015.

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