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Comment

Interactive comment on “Positive matrix factorization of PM_{2.5} – eliminating the effects of gas/particle partitioning of semivolatile organic compounds” by M. Xie et al.

Anonymous Referee #2

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General comments:

The paper investigates the effects of gas/particle partitioning of semivolatile organic compounds (SVOC) on source apportioning by PMF that incorporates SVOC as input species. SVOCs data in PM_{2.5} are increasingly used as PMF inputs to apportion organic aerosol sources. The use of particle-only SVOC data in PMF apparently causes complications arising from the strong dependence of their gas/particle partitioning on meteorological conditions (e.g., temperature) and existing particle chemical composition. The paper examines this issue by comparing PMF solutions obtained from particle-only data with those from gas+particle SVOC data. The authors are innovative

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in deriving the total (i.e., gas+particle) SVOC data from the measured particle-phase concentration by applying G/P partitioning theory. The paper is well-written. The results from this work contribute to improved source identification and apportionment for PM_{2.5}.

I list below a number of issues that the authors need to address in their revision.

Major comments:

1. Uncertainty in deriving the gas-phase SVOCs: The authors estimated gas-phase SVOCs using Pankow's absorption partitioning theory. There are studies indicating that adsorption onto solid-like particle surface (e.g., soot surface) also contributes to partitioning of SVOCs (such as PAHs) in particles (e.g., Venkataraman, 1999; Yu and Yu, 2012). Some discussion is needed to address the uncertainty introduced by assuming absorption only partitioning.

2. OC1 fraction is excluded for PMF analysis on the ground that this fraction of OC is semivolatile and the gas-phase concentration of OC1 could not be estimated. It is not clear to me why the authors do not use the entire filter OC as PMF input so that the whole filter OC could be apportioned to sources (or "factors") resolved by PMF. Breaking OC into OC1, OC2, OC3, OC4, and PC and inclusion of the sub-fractions of OC (i.e., OC2 and OC3) do not appear to facilitate source identification by PMF, as shown in Fig. S1. At a minimum, discussion is needed on the PMF solution if the whole OC is used as PMF input instead.

3. A few unique source tracers, such as cholesterol for meat cooking and methoxyphe-nols for wood burning, are measured but are not included in PMF source analysis (see Table S2). Why are they excluded? Would not their inclusion help to apportion the bulk carbon factor?

4. The PMF solutions are represented as n-alkane, sterane, light SVOC, and PAH factors, instead of pollution sources that these tracers track (e.g., fossil fuel evaporation,

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vehicular exhaust, etc). Apart from a brief mentioning that the light SVOC factor is associated with fossil fuel evaporation and biogenic emissions, there is no discussion about what are the underlying pollution sources for the other organic marker factors. Although this work focuses on the effects of using particle-only SVOC vs total SVOC data on PMF solutions, the ultimate objective of PMF analysis is to apportion PM_{2.5} mass or PM_{2.5} OC into pollution sources, the information that can guide formulation of control strategies. Some elaboration of the associated pollution sources is needed.

5. Dominance of odd alkanes (e.g., C₃₁, C₃₃) in the relatively higher n-alkane range is characteristics of vegetative detritus organic aerosol source (Rogge et al., 1993). No odd-carbon dominance is discernible in the n-alkane factor resolved by PMF. Can the authors comment on whether this implies that this n-alkane factor is associated fossil fuel-related sources? Similarly, what are the source implications regarding the strong presence of smaller n-alkanes, oxy-PAHs and C₁₂, C₁₆, and C₁₈ fatty acids in the light SVOC factor?

6. Assuming the PMF solution using total SVOCs as input species are correct, how much does the particle-only PMF solution overestimate/underestimate the individual sources? This information can be extracted in Fig.3, but it is good to describe in words in the text for readers to better comprehend the importance of considering G/P partitioning when SVOCs are used in PMF.

Minor comments:

1. Page 5212: Please clarify whether “straight OC” includes OC₁ and OC₄, which were excluded for PMF analysis.
2. Conclusion (Page 5218): Can the authors be more specific in their suggestion for gas-phase OC data? What type of gaseous OC, total or speciated SVOCs or other?
3. Table 1: The last value of MW_{om} should be “300”, not “30”.
4. Tables S1-S4: Please specify whether concentrations of the organic molecular mark-

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ers are from filter measurements or the sum of measured filter concentration and derived gas-phase concentration.

5. For figures in supporting document, please do readers a service to include figure captions with their respective figures on the same page for easy reading.

References:

Rogge, W. F., L. M. Hildemann, M. A. Mazurek, G. R. Cass, and B. R. T. Simoneit (1993), Sources of fine organic aerosol. 4. Particulate abrasion products from leaf surfaces of urban plants, *Environ. Sci. Technol.*, 27(13), 2700–2711.

Venkataraman, C., Thomas, S., Kulkarni, P., 1999. Size distributions of polycyclic aromatic hydrocarbons: gas/particle partitioning to urban aerosols. *J. Aerosol Sci.* 30 (6), 759-770.

Yu, H. and Yu, J. Z., 2011. Polycyclic aromatic hydrocarbons in urban atmosphere of Guangzhou, China: Size distribution characteristics and size-resolved gas-particle partitioning. *Atmos. Environ.* 54, 194-200.

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