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Atmospheric
Chemistry
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Discussions

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 #1

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This work examines the PMF solutions for a partitioning-corrected SVOC data set in which total (gas + particle) concentrations calculated from aerosol-phase measurements are used for the input matrix, rather than the aerosol-phase measurements. This procedure is intended to (partially) remove the temperature dependence of the observations, leading to a more consistent estimation of PMF factors across seasons or periods with large variations in temperature. This is a well-written manuscript with important consequences for source apportionment for the atmospheric chemistry community and is therefore recommended for publication in ACP. However, the following issues should be addressed beforehand.

Major comments

Section 2.3: It seems that the solutions are artificially restricted to the original (base-case) solutions; possibly limiting the usefulness of the total PMF approach. Were the solutions that were thrown out (not matched) correspond to the extreme values of the sampled distributions, or not necessarily? Were they physically plausible to be considered, even though they did not match? Also, are the factors classified according to profile or strengths, or both (what is the input to the classification model)? In either case, it seems counter-intuitive to classify new solutions to old solutions you are trying to differentiate these solutions from, unless the inter-factor variability is much greater than the variability between G/P partitioning-corrected and uncorrected solutions, in which case the added value of G/P partitioning corrections is seems diminished.

Section 3.4: Is the factor that you were additionally able to resolve with the total PMF significant to your interpretation of sources in the region (disregarding the loss of two factors in comparison to the base-case PMF)?

Figs. 3 and 4: Assuming that the total PMF solution is the correct one, how much might you overestimate your average contribution from each corresponding source factor (in terms of OM) if you only used particle-phase measurements with the PMF without the vapor concentration corrections (the base case)? In the base case, is the mass apportioned to its own factor, incorrectly apportioned to another factor, or remains unapportioned?

Given the uncertainties mentioned in the estimation of the total concentrations, there are improvements observed in the consistency of sub-data PMF solutions. The authors state this but in a less direct way, but is the conclusion of the manuscript that an uncertain G/P correction is better than no correction?

Just a comment regarding one of the additional, unconsidered dependencies that the authors raise, but to a first order, the temperature-dependence of the kinetics of VOC oxidation is smaller than G/P partitioning according to Pathak et al. (2007; J. Geophys.

Res.), but a) they only considered dark ozonolysis and not the full possibility of photochemistry, b) PMF separation may still be sensitive to the relative variations among compounds for its separation.

Minor comments

Fig. 1: why are there lines connecting the species? This should be a barplot instead to show that the chemical species are not connected together in series.

Fig. 3: "filter-based" should possibly be renamed as "original" or "particle only" or something else as the total SVOC-based analysis is also based on filter measurement. Also in the text, the labels "original" and "base-case" are used alongside "filter-based". It would be better to define this label up front and use it throughout (but "filter-based" is discouraged as it is not discriminating enough).

Interactive comment on Atmos. Chem. Phys. Discuss., 13, 5199, 2013.