**Atmospheric
Chemistry
and Physics**
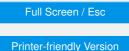Open Access
Discussions

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Interactive comment on "Mapping gas-phase organic reactivity and concomitant secondary organic aerosol formation: chemometric dimension reduction techniques for the deconvolution of complex atmospheric datasets" *by* K. P. Wyche et al.

Anonymous Referee #1

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The manuscript of Wyche et al. represents an exciting step forward in the analysis of complex data sets, relevant to the formation of secondary organic aerosol (SOA). The authors use three statistical analysis approaches (PCA, HCA, and PLS-DA) for dimension reduction. The methods are applied to data obtained from a number of chamber studies involving different precursors grouped into four categories; application of the methods reproducibly resulted in successful classification of the gas- and particle-

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phase composition spectra by precursor category. While the authors suggested the potential for such approaches in ambient data mining, the results were not overstated and potential limitations were acknowledged. The paper was well written and the methodology was easy to follow. This paper should be of great interest to ACP readers involved in acquisition and interpretation of such data sets, as well as to readers interested in improving model representation of SOA.

Content

Studies have shown that limonene for example typically has higher SOA yields than other cyclic monoterpenes (Lee et al., 2006, JGR 111 D17305; Fry et al., 2014, ES&T 48: 11944-11953). Though the oxidation products of the two cyclic monoterpenes were separable from the other categories by the statistical approaches, did the results also suggest differences between the two precursors that may help explain such observations? Along the same lines, within a category, does the spread/distance of clusters/specificity indicate dependence on VOC/NO levels, RH, or other factors thought to influence SOA formation?

Lee et al. reported a number of m/z fragments for oxidation products of isoprene, monoterpenes, and a sesquiterpene detected by PTR-MS. It would be interesting to know if the same conclusions could be ascertained from the reported m/z fragments in Lee et al.; namely that there are significant relationships between the fragments of "like" precursors. There may not be enough data to perform a full analysis as was done in the subject manuscript, but the authors may think about whether their results are similar/supported by Lee et al.

It is suggested that the authors carefully review their citations. There are several places in which widely cited previous work is omitted in favor of self-citations. One example can be found on p. 1655, line 22, regarding the importance of findings from chamber studies over the past decade. The authors do not cite the work coming out of the Caltech chamber (as early as the late 1990's); the parameters from Hoffman et al.,

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1997 and Griffin et al., 1999 still are widely used in chemical transport models (see also papers by Cocker, D.). Restricted to the last 10 years, lead authors on Caltech chamber publications include: Ng., N.; Kroll, J.; Surratt, J. and others. Much influential work has also been conducted over the last 10 years in the Carnegie Mellon chamber; lead authors include: Presto, A., Hildebrandt, L., Grieshop, A., and others.

Editorial

p 1655, line 18: "Atmospheric chemistry" as a system is awkward. One suggestion: "The chemistry of the atmospheric system is highly nonlinear..."

p 1656, line 9: The "CIR-TOF-MS" abbreviation can be introduced on line 4 and used exclusively here.

p. 1658, section 2 heading: The adjective "Experimental " needs a verb, or needs to be changed to a noun.

p. 1661, line 8: Remove "/" prior to photolytic

p. 1666, line 19: Change "caryophyllon" to "caryophyllene"

p. 1667, line 26: It is not clear what is meant by "oxidized atmospheres".

p. 1669, line 10-13: It is suggested the sentence be reworded to more clearly indicate that data are available for only two experiments per each of the two noncyclic monoterpenes. As written the focus is on "only two types of precursor", which is the same as the cyclic monoterpenes. In summary, it is the number of experiments, not the number of precursors that is likely affecting the result.

Can the panel and text sizes be increased for Figs. 7 and 8? They are hard to read (even w/significant expansion-175%)?

The authors may consider more clearly indicating the difference between Figs. 7 and 8 in the figure panels (e.g., just adding a AMS and LC-MS header).

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The authors may consider using consistent colors for the different categories in each of the plots (generally the same in PCA plots, but not in dendorgrams).

Caption Figure 10: Remove "/" after abundance

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