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Atmospheric Chemistry and Physics Discussions

Interactive comment on "A model framework to retrieve thermodynamic and kinetic properties of organic aerosol from composition-resolved thermal desorption measurements" *by* Siegfried Schobesberger et al.

Anonymous Referee #2

Received and published: 13 June 2018

The authors present a detailed approach to modeling thermal desorption from a PTFE filter as is found in the FIGAERO CIMS inlet. This model is itself useful in the field, as that instrument is seeing wide use, and the authors further go on to explore properties of SOA, particularly with respect to volatility, kinetics, and potential thermal decomposition. The manuscript is well written and thorough, and represents a clear advance of knowledge. I recommend publication after addressing the comments below, which are largely minor and technical in nature.

Broader comments:

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I appreciate the explicit discussion of what is (and is not) meant by "oligomerization" throughout this manuscript. Quite often this term is thought of (perhaps incorrectly, but nevertheless) as implying covalent homo-oligomers, such as dimers and trimers, while there is some evidence and reason to believe that SOA is substantially more complicated than that (e.g. methods able to measure dimers often do not see enough to explain partitioning). While the term is used throughout, this clarity is not brought forward until page 10. I recomment that to address the above conceptions the discussion of "oligomer" be brought forward to the introduction. It is also the reason I tend to prefer "accretion products" as the more universal term, but understand if the authors prefer to stick with the more common term "oligomers".

Throughout the manuscript, the authors sometimes mention the possibility that an ion may represent multiple isomers, but its not always clear to me to what extent this is being considered. Figure 11 demonstrates that there are many possible ways to fit each thermogram, and one could imagine for instance an ion consisting of monomers with a range of volatilies, and each also formed from one or two different oligomers. Panel B shows such an example a case in which two isomers are invoked to describe the thermogram, one which is pure and another comprised of low- and high-volatility components. While captured here, it may be a case existing in many of the observed ions, but to which the model is blind given its large number of free parameters. It seems here that in most cases there is a simplifying assumption that each ion can be treated as one compound (except in the case of 11B), which may or may not be a robust assumption. Trying to tackle this question may go beyond the scope of this manuscript, but it should probably be discussed more explicitly and added to the list of "challenges" in Section 5.

Technical comments:

Page 3 line 10: A word seems to be missing in "Other methods by"

Page 3 line 17: What do the author's mean by the "compositions of these molecules"?

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I presume they mean molecular formulas?

Page 10 lines 18-22:

Page 10 line 27: The use of "compound" here and throughough is 'iffy', as for most practical FIGAERO applications a given ion may represent a mixture of multiple compounds. See comment above.

Page 11 line 18: It's not clear to me how k_g,0/(k_g,0+k_d,0) is calculated before each model run

Page 12 line 7-9: My understanding of both cited references is that FIGAERO CIMS saw half the mass, but also assumed equal sensitivity. However, when Isaacman-VanWertz et al. (Nature Chemistry, 2018, doi:10.1038/s41557-018-0002-2) applied the calibration approaches developed in those references, they found that FIGAERO I-CIMS agreed well with AMS-measured mass. It may be worth nothing that assumption (a) is therefore not only probably negligible (per the next lines), but reasonably well supported.

Page 17 line 30: What does "attempt frequency" mean?

Page 23 line 1: missing "are"

Page 23 line 16: Sentence has a typo, not sure exactly what was intended

Caption Figure 4: I think this all refers to Figure 3 panel D, not panel C as stated. Also the descriptions of panels B and C seem to be reversed

Figure 7: Panels C and D are reversed of their descriptions.

Caption Figure 9: typos in lines 1 and 2

Figure 13: I find this figure just generally difficult to interpret, and the plots are very busy with subtly differences between lines. It could uses some re-design.

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