Review of Voliotis et al. 2021 “Exploring the composition and volatility of secondary organic aerosols in mixed anthropogenic and biogenic precursor systems”

Summary

The authors investigated the composition and particle volatility of secondary organic aerosol systems from a-pinene (biogenic volatile organic compound, bVOC), o-cresol (anthropogenic VOC, aVOC), and a mixture of the two. As the two precursors are structurally very different (bicyclic monoterpene vs aromatic compound), the resulting SOA systems exhibit distinct chemical composition profiles, SOA mass yields, and particle volatility. In the mixed SOA system, a unique group of compounds appears in the “moderate” to “less” volatility range. This shows that, already in a binary mixture, complex interactions between the different oxidation processes can occur and these will impact the volatility distribution of the resulting SOA.

This work falls into the scope of ACP as it furthers our understanding of the interaction of different precursor groups (here aromatic and terpenoid compounds) and how this interactions impact SOA particle formation and properties. I recommend this work for publication after a few mayor concerns and many minor issues have been addressed. In several places, the manuscript is unnecessarily difficult to understand due to some poorly phrased sentences. I recommend that the native English speakers in the author team should have a more careful look at the overall language of the manuscript when submitting the revised verion.

Major Comments

1) The study suggests that the interaction of intermediate oxidation products (among them RO_2) is very important when more than one precursor is present. The chosen experiment conditions have a realistic OH concentration level (order of 10^6 cm^{-3}) The VOC/NOx ratio is also in an atmospherically relevant range. But the VOC and NOx concentrations are orders of magnitude higher than could be expected in most regions with strong bVOC emissions. The fate of RO_2 (e.g. which termination products are formed or how many autooxidation steps occur) strongly depends on the balance between the consecutive reactions with NO_2, HO_2, and RO_2. The experiment conditions may favour the NO_2 and RO_2 paths over auto-oxidation and HO_2 reactions. How well will such experiments represent the actual atmosphere?
2) I disagree with how the authors decided to treat the elevated signal levels at the start of some thermograms (“instrument background”, described in lines 254ff). From the example in Fig S1b, this looks like a carry-over from the preceding gas phase measurement (exponential-like decrease after switching). The gas phase zeros also show a delay in the decrease/increase of the signal indicating that this is a “sticky” compound. Another option is that semi/intermediate volatility gaseous compounds were adsorbed on the filter and quickly evaporate when the flow is switched to pure N_2.

This will occur already at room temperature. The driver is switching from a high concentration gas flow (= sampling) to the pure N_2 for desorption.

However, for the given example, the value decreases to close to 0 before the actual desorption peak starts at ~36min. I.e. the carry-over/artefact does not impact the region of interest. Note how the signal level before and after the desorption peak are the same and close to 0. The authors used the average value from 30 – 60 seconds as the “instrument background” and subtracted it from the whole ion thermograms. I indicated the value for the given example below (derived “by eye”). Subtracting the value of the red line will remove more than half of the signal from this peak. This will lead to systematic bias in the data. “Sticky” ions with high enough concentrations in the gas phase will be underestimated using this procedure. To avoid this bias, the authors could either remove the first X seconds from the integration for every ion (or equivalently set a minimum temperature from which to start the integration). Or they could fit an exponential (or other suitable) function to the 15-60 sec data and then use that as the gas-phase carry-over background value.

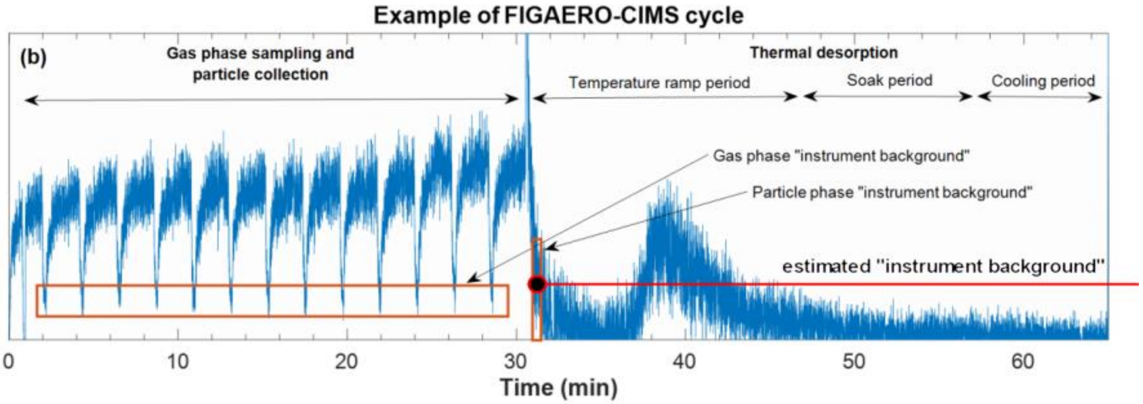

Figure 1: Copy of Figure S1b with added estimated “instrument background” level as red line.

3) I find the presentation of the FIGAERO-CIMS composition results in Figure 1 only useful for part of the discussion. The logarithmic scale is good to show the small, but important contributions from C>10 compounds (or C>7 for o-cresol) which would be probably invisible on a linear scale. But the eye is misguided by the seemingly large bars. E.g., the unique in mixture compounds seem to be predominantly present at C>10. But the majority of these compounds really falls into the C4-C8 range where the contribution is dwarfed by the large a-pinene compound bars. Also, this Figure reduces the composition information to the carbon number. While this is an important property to investigate, the degree of oxidation (OSc) as a measure of functionality (and somewhat Mw) is equally important - especially when discussing volatility.

I therefore recommend that the authors add a different depiction of their mass spectra results to the manuscript. One option is to plot the OSc value for each ion (calculated from the sum formula) vs the carbon number and then use marker size to indicate signal intensity (using a logarithmic spacing). The colour of the marker can be used to indicate the compound category. Examples for this type of figure can be found as Figure 5 in Faiola et al. (2019), Figure 8 in Ylisirniö et al.(2020), or Figure 1 in Isaacman-VanWertz et al. (2017). This type of figure can be helpful when investigating why the fraction of C>10 is not significantly different between the gas and particle phase for the mixture. It would directly show if the degree of oxidation is different for the compounds grouped by their carbon number (see specific comment about line 308ff). It will also be helpful for the discussion in section 4.1.

I am aware that there is a degree of uncertainty for the calculation of OSc for N containing compounds (Priestley et al., 2021). However, for plotting purposes this may be neglected.

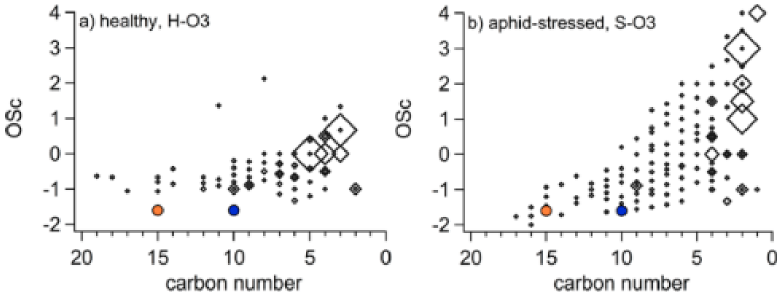

Figure 5. Ozonolysis oxidation products measured in the chamber during the last 30 min of the experiment plotted on a 2-D axis of oxidation state (OSc) and carbon number for the (a) healthy plant emissions and (b) aphid-stressed emissions. Each diamond marker denotes one peak identified in the acetate-CIMS, and the size of the marker indicates intensity of the signal. Filled circles indicate the location of dominant SOA precursor species in the ozonolysis experiments with (solid orange circles) for sesquiterpenes and (solid blue circles) for monoterpenes.

Figure 2: Example for OSC vs C number plot from (Faiola et al., 2019)

4) Determining the particle phase volatility is an integral part of this study. Using volatility categories to simplify the complex FIGAERO-CIMS data is a valid approach. But unfortunately, the authors do not explain how the volatility categories were derived for the FIGAERO-CIMS measurements. They define three categories with rather hand-wavy terms (more, moderately, and less volatile) instead of using the established categories of semi-, low-, and extremely low volatile. There may be reasons to use these broader categories (however, no reasons are given). But it is surprising that the authors do not even mention a T_{max}-> p_{sat}/C* calibration using compounds with known p_{sat} values here when one of the co-authors published about the necessity of a robust calibration (Bannan et al., 2019) and three more from the author list also participated in that publication. Also, the authors are aware of a more comprehensive study on FIGAERO-CIMS T_{max} -> p_{sat} calibration methods (Ylisirniö et al., 2021) as they cite this study in a different context. When they introduce their volatility categories, they instead refer to a non-relevant paper (Saha and Grieshop, 2016) using a thermodenuder method (the desorption temperature categories cannot be directly compared to FIGAERO desorption temperature) and a study (D'Ambro et al., 2019) which has two example ions which exhibit peaks a t 55 °C and 90 °C (and uses these to explain how there can be compounds with different volatility appearing at the same sum formula). Lopez-Hilfiker et al. (2014) does contain a T_{max} -> p_{sat} calibration curve, however model calculations (Schobesberger et al., 2018) and

experiment by Ylisirniö et al. (2021) have shown that such calibration lines are instrument specific and cannot be easily transferred.

The authors have to clearly explain

- a. why they chose these desorption temperatures as category borders
- b. how these relate to the established S/L/ELVOC classification system
- c. what calibration was used for the FIGAERO-CIMS
- d. If they did not perform the necessary T_{max}->p_{sat} calibrations for this data set, they need to mention this and clearly state what other method to relate desorption temperature and volatility they use.

5) Following up on the previous comment. It is commendable that two independent methods were applied to derive particle volatility. But the authors have not clearly explained how the volatility categories from FIGAERO-CIMS measurements relate to the VBS distribution. It is important to stress that compounds detected at a desorption temperature of 50 °C in the FIGAERO-CIMS do not necessarily have the same volatility as the fraction that evaporates during 30 sec in the thermodenuder at 50 °C.

6) Section 4.1 contains the main part of the interpretation of the observed data. The authors try to link the observed composition and particle volatility to the SOA formation processes. But unfortunately, this whole section is very hard to follow for multiple reasons:

- a. It is not clear when the authors are talking about processes/measurements of the gas phase are solely about the particle phase. Does "FIGAERO-CIMS measurements" imply only particle phase data (e.g. in line 474f)?
- b. They use fraction of contribution for different compound groups defined by carbon number. But this quantity is not easy to visualise from Figure 1 as it is in log scale. It may help to create some additional graphs/table in the supplement to help the reader follow this discussion. I understood that the authors are looking at three groups: oligomers with C > precursor (precursor =10 or 7), monomers with moderate fragmentation leading to precursor-x< C< precursor, significant fragmentation C< precursor -x. x is 5 for a-pinene and the mixture.
- c. The fraction of contribution of compound groups are then linked to the fractional contributions in the volatility distribution. But carbon number is not the only factor for volatility. That Mw may be the more direct measure that correlates with volatility. It should be easy to verify this by looking at the sum thermogram for each compound group (e.g. summing up all C>10 compound thermograms)?
- d. It is hard to follow how the authors determine what is comparable to the subgroups of the "unique to the mixture" compounds. Should not the properties of the C>10 compounds from the single precursor experiments be compared the properties of the C>10 in the unique to mixture category when investigating if the interactions in the mixture lead to more or less volatile compounds in that carbon number range?

I recommend that the authors carefully evaluate what they really want to express in this section and clarify their message.

Specific comments

1) Line 26: "…compounds with saturation concentration less or equal than 0.01ug m^{-3}…" This isolated value of 0.01 ug m^{-3} is not very reader friendly. It is better to give the volatility class that this refers to (so LVOC ?).
2) Line 60ff: "A number of studies…" This sentence is generally difficult to understand. It is also an oversimplification. "Functionality" is usually associated with a larger number of functional groups (e.g. -OH or -C=O). Adding more functional groups to a molecule typically will reduce the vapour pressure as intermolecular forces become stronger and the molecular weight (Mw) increases. But a larger carbon backbone may have an even stronger impact on the volatility of a compound, e.g. when comparing monomer and dimer compounds which have same relative functionality (functional groups per carbon backbone). Li et al. (2016) show that volatility had a strong correlation with Mw for a wide range of functionalities.
3) Line 102: "aromatic oxidation" This term can be misunderstood as the oxidation being of aromatic character. Better use the term "oxidation of aromatic compounds"
4) Line 128: "electronic capture device grade nitrogen" ECD is not a specific enough purity identifier. A quick google search gave 3 different purity grades (between N4.8 and N6.0) depending on the supplier. Replace this by something specific.
5) Line 132: "…during the final fill cycle…" the description of the chamber operation does not specify any filling cycles. It rather suggests that there is a continuous flushing of the chamber before and after the experiments ("cleaning cycle")
6) Line 150ff: How much O_3 was formed during the experiments? This may have relevance as non-aromatic products from o-cresol may react with O_3.
7) Line 162: "…established by stabilising the chamber with clean air…" What is meant by "stabilising"?
8) Line 170ff: While I agree with using the "high O_3" cleaning procedure in general, the authors should not be so general in their statement here. The aromatic compounds (like $C_7H_8O_2$, the dominant product from o-cresol) will not react with O_3 even at this high concentration. So, this will not help with "oxidising any remaining gas-phase organic species".
9) Line 195ff: Was the assumption of minimal changes in the aerosol composition for this time period verified with the available instrumentation (AMS, FIGAERO-CIMS)?
10) Line 195ff: Which instrument was used for the MFR calculations? AMS total mass? AMS organic mass? SMPS total mass?
11) Line 205: Was the FIGAERO from Aerodyne or custom build? This should be stated as different instrument designs are currently in use.
12) Line 209: "high purity N_2" This is now the third purity grade for N_2 (after ECD and UHP). Where 3 different types of N_2 used?
13) Line 210 (and below): "0.635 cm OD" Is that a ¼ inch tube? While I strongly favour using metric units wherever possible, it feels odd to not use the precise description of the tubing.

14) Line 250f: "… were subtracted from the measured values in each cycle by linear interpolation." This is not clear. What was linearly interpolated? How does subtraction by interpolation work?

15) Line 250f: It is not clear if the authors are speaking about the gas phase part of the data or everything. Was the "instrument background" and the "chamber background" subtracted only for gas-phase data or also from the particle phase?

16) Line 253ff: "…high initial particle phase signal was observed…" Did the authors scale the signals to the primary ions (I-species)?

17) Line 266-275: This whole paragraph is unnecessarily difficult to understand. See next three comments.

18) Line 268f: "…products with assigned formulae which were common among all systems and CIMS is unable to resolve (i.e., isomers)…" This means to me that the "common" category consists mainly of isomeric compounds, i.e., that there are even less true common compounds between a-pinene and o-cresol. Is that what the authors want to imply?

19) Line 270ff: "…we compared the resultant products categorised as unique to the mixture with the Master Chemical Mechanism." What is compared to the MCM? The compounds grouped into "common"? What are they compared to? MCM using a-pinene as input? o-cresol? A mixture?

20) Line 270ff: Why would a single precursor product expected from MCM calculations not show up in the single precursor experiments but only in the mixture experiment?

21) Line 277-288: This is another example where the authors do not clearly state what they did: Which data was used for the MFR and volatility model calculations? The mass concentration from AMS or SMPS? If AMS was used, what CE&RIE were used? How well did AMS and SMPS total mass agree?

22) Line 277-288: What is the uncertainty of the derived volatility distribution for this specific setup?

23) Line 291: "Figure 1 shows the average distribution…." What was averaged? The authors have the reader guessing if the averaged multiple FIGAERO samples from one experiment. Or did they combine data from multiple experiments?

24) Line 294: "…unidentified fraction (se Section 2.4)" Section 2.4.1 states that more than 80% of the total fitted signal was assigned (Line 245). But there is no explanation about the unidentified fraction. Why is it unidentified? is there no reasonable formula possible? Is it outside of the trusted m/z range?

25) Line 301f: The two main products for o-cresol oxidation are $C_7H_8O_2$ and $C_7H_7NO_4$. These are formally a H abstraction and OH addition or H abstraction and O&NO_2 addition. This seems to suggest that very little oxidation occurs for this precursor system. How does this compare to the expectation stated in Lines 102ff. Could this behaviour be linked to high VOC and NOx concentration in relation to OH (see mayor comment 1)?

26) Line 308f: The contribution of C>10 compounds is not significantly different between the gas and particle phase of the mixture. But are these really the same compounds? Are the compounds in the particle phase more oxidised? What is the volatility of the particle phase compounds (derived from Tmax of their ion thermograms)? Are they expected to be semi-volatile and thus show contribution in both gas and particle phase?

27) Line 311ff: Are $C_7H_8O_2$ and $C_7H_7NO_4$ still the dominant species for the o-cresol group? I.e. what fraction of the o-cresol group is attributed to these two compounds. Is this similar to what was seen for the single precursor experiment.

28) Line 323: I do not understand this sentence. I guess this is supposed to be an interpretation of O:C ratio?

29) Line 326 ff: The O:C(AMS) is smaller than the FIGAERO value for a-pinene SOA but larger for o-cresol SOA. For mixed SOA the effect seems to be cancelled. Could this change in trend be caused by the AMS using a parameterisation optimised for ambient data?

30) Line 328 – 331: Again, an example for unclear language. The main challenges for FIGAERO-CIMS are the sensitivity effects, while the AMS mostly struggles with the fragmentation (i.e. detecting organo-nitrates mostly as NO^+ or NO_2^+). But the sentence structure implies that both problems apply to both instruments. This does not impact the overall message, but this sloppy style may be misleading for a novice to AMS and FIGAERO-CIMS while annoying the expert.

31) Line 339ff: What is meant by "…provides an indirect measure of the volatility as a function of the FIGAERO-CIMS total particle phase signal"? Is this supposed to describe the meaning of the sum thermogram (sum of all ion signals as a function of desorption temperature)? "Volatility as a function of the total particle phase signal" means something else to me.

32) Line 342: "average sum thermogram for each system" Again, what was averaged? All FIGAERO samples from one experiment? All samples from all experiments? How many samples are part of the averaging? (see also comment 34)

33) Line 342: For the average values used before ±1σ was used. Why is ±2σ used here?

34) Line 345: "characteristic experiment" why were these experiments chosen as characteristic? The authors should clearly state (best in the methods part):

    a. what were the averages they used (averaged over one experiment or multiple experiments?)
    b. how many FIGAERO samples where averaged?
    c. why certain experiments were chosen as representative for a SOA system.
    d. mark the "characteristic experiments in Table 1.

35) Line 360 "modest volatilities" modest is the wrong word here. "moderate" is probably more fitting.

36) Line 373: Unidentified ions was not clearly introduced. Was it just not possible to assign a sum formula? Are these the same masses as the unidentified in the a-pinene and o-cresol case?

37) Figure 5: How different were the total aerosol mass concentrations ("c_{OA}") in the three experiment types? How much will these different loadings impact the observed volatility distribution of the SOA particles?

38) Line 406: What does "large size of the molecules" refer to? High Mw? Higher carbon number?

39) Line 407: what does "close to unity" mean in this context. The values were close to 1? The values from the two different systems were almost the same?

40) Lines 413-427: What are the uncertainties of the O:C enhancement ratio? It looks like that it is possible to pick one out of the two experiments for each category and get almost overlapping slopes. I.e. the highest points from a-pinene and the lowest points from o-cresol almost overlap.

41) Line 414: "O:C enchantment" = enhancement?

42) Line 415: The term “BP line” was not introduced. Is that the bypass line for the thermodenuder? By now I am a bit tired of having to guess what the authors are trying to say.

43) Line 425: “…whereas that of the mixed system was approximately between.” What doe you mean by approximately between? The values for the mixed system a definitively between the values for the single precursor systems? Is this supposed to be “approximately half-way between”?

44) Line 426f: “…the less volatile SOA particles from the o-cresol system are considerably more oxygenated compared to the average than those of the α-pinene system.” What is compared to what here? What is the “average”?

45) Line 436: The variable “maximum desorption temperature” was not properly introduced anywhere. This term can be misleading to a non- FIGAERO expert. As described in other comments, the authors should clearly introduce the relationship of T_{max} (desorption temperature of the maximum of the ion/sum thermogram) and volatility.

46) Line 440: “This broad consistency…” If the authors want to express that the two volatility distributions roughly agree, then “broad” is not the right word here.

47) Line 447-467: Do the general statements of the authors about fragmentation include the initial oxidation step? Or are they looking at the fate of RO/RO_2 radicals?

48) Line 447-467: For the general fragmentation vs functionalisation discussion, the authors should point out the fundamental difference in the precursor structures. a-pinene is a bicycle molecule. I.e. two C-C bonds can be broken without actually loosing a C. o-cresol is a C6 aromatic compound. I.e. the aromatic ring will be very stabile against oxidation (e.g. no ozonolysis reaction. But once the aromaticity is broken, fragmentation reactions will create two very small molecules.

49) Line 460ff: The statement about the sensitivity of I^- CIMS with regard to volatility classes is misleading in this context. It is correct that in “gas-phase mode” CIMS mostly detects I- and SVOCs. But the particle phase mode of FIGAEO-I^--CIMS detects SVOC to ELVOC compounds equivalent to C* $10^4 – 10^{-6}$ ug m^3 or even lower. (Isaacman-VanWertz et al., 2017). 60% of the particle phase signal appears at desorption temperatures >90 °C. Even with all the differences between different FIGAERO instruments, that is in the LVOC range.

50) Line 476f: The conclusion that dimers are not relevant because the observed fraction of C>10 compounds is low is not correct. Many dimers are thermally labile and will be detected as thermal decomposition products with sum formulas similar to the corresponding monomer composition. A clear example is shown by D’Ambro et al. (2019) for $C_5H_{12}O_4$ which shows two distinct peaks (at 55°C and 90°C). More examples can be found in a recent overview on FIGAERO-CIMS (Thornton et al., 2020). The authors need to adjust this statement to reflect the importance of thermal decomposition for oligomers.

51) Line 480: “…with 7 or more carbon numbers”. this should be either “with 7 or more carbon atoms” or “with a carbon number of 7 or more”

52) Line 492: Fig S2 is not the right figure reference. Is this refereeing to Figure 1?

53) Line 498ff: The authors compare the volatility of unique to mixture products to the rest of compounds in the mixed SOA particles with the same carbon numbers and attribute the observed differences to the change in O:C. But is the determining factor really the increase in oxidation or is it the increase in Mw?

54) Line 504f: "The vast majority of those products were found to be common between all experiments…" This is confusing. This is supposedly about the "unique to mixture" compounds. How can they be found in all experiments? Is it not by definition that these compounds only occur in the mixture experiments?

55) Line 501-514: The most important indication if these C<5 compounds are likely from thermal decomposition should not be their O:C value but rather the thermogram data (Figure 7). Are compounds with a volatility equivalent to an average $T_{max} > 100$ °C expected to have a significant fraction in the gas phase?

56) Line 504ff: It is not clear what the comparison of O:C is aiming at. The unique to mixture C<5 compounds have higher O:C than the other C<5 compounds? Or the particle phase compounds compared with the gas phase compounds?

57) Line 537ff: "…to assess the potential role of product interactions in altering the SOA particle volatility" This sentence suggests that conducting FIGAERO-CIMS measurements with a precursor mixture would be enough to achieve this. As I understand the identification method described in this manuscript, the key to assigning the compounds to the different categories (common/unique to mixture etc.) is the combination of chamber experiments with single precursors and the mixture. The authors need to clarify what they mean in this sentence.

58) Lines 543-558: I disagree with the interpretation of the decreasing T_{max} values with increasing filter loading. To my knowledge and according to the modelling framework presented by Schobesberger et al. (2018) artefacts related to increases in filter loading will always lead to a shift to higher T_{max} values. Previous studies have shown that the largest T_{max} shifts when filter loadings where <200 ng to <2.5ug and with loading >~2.5 ug, T_{max} changes were minor (Huang et al., 2018; Wang and Hildebrandt Ruiz, 2018).

The change in the ion thermogram of $C_{10}H_{16}O_4$ (Figure S5) looks more like a change in volatility distribution for that specific sum formula. I.e., there are two or more isomers with different volatility and the more volatile one is not there for the lower mass loading sample. If this is the case, this is not an artefact but a real feature of the data. Without the information about the evolution of the mass concentration in the chamber, there are three possible explanations:

   a. The lower mass loading on the filter corresponds to a lower particle mass concentration in the chamber. Hence, the partitioning is affected and the volatile isomer with T_{max}~40 °C does not partition into the particle phase
   b. There is ongoing chemistry in the chamber and the mass concentration reflects the evolution. At the time when the low loadings were sampled the more volatile isomer did not exist in sufficient quantities. Either because it had not formed yet or because it had reacted away.
   c. If the lower mass loadings are "later" in the experiments, the more volatile isomer may react in the particle phase to form something else, possibly a dimer. Such a dimer will either show up at the dimer formula, at

the same formula at higher desorption temperature or at a different sum formula if the thermal decomposition is more complex.

To verify this explanation, the authors should check their data. Does the T_{max} decrease occur only for T_{max} values in the SVOC range?

59) Line 569: "…as few as 10 products" This suggests that 1 sum formula is just 1 compound is not strictly true. The authors should formulate this more carefully.

References

Bannan, T. J., Le Breton, M., Priestley, M., Worrall, S. D., Bacak, A., Marsden, N. A., Mehra, A., Hammes, J., Hallquist, M., Alfarra, M. R., Krieger, U. K., Reid, J. P., Jayne, J., Robinson, W., McFiggans, G., Coe, H., Percival, C. J. and Topping, D.: A method for extracting calibrated volatility information from the FIGAERO-HR-ToF-CIMS and its experimental application, Atmos. Meas. Tech., 12(3), 1429–1439, doi:10.5194/amt-12-1429-2019, 2019.

D'Ambro, E. L., Schobesberger, S., Gaston, C. J., Lopez-Hilfiker, F. D., Lee, B. H., Liu, J., Zelenyuk, A., Bell, D., Cappa, C. D., Helgestad, T., Li, Z., Guenther, A., Wang, J., Wise, M., Caylor, R., Surratt, J. D., Riedel, T., Hyttinen, N., Salo, V.-T., Hasan, G., Kurtén, T., Shilling, J. E. and Thornton, J. A.: Chamber-based insights into the factors controlling IEPOX SOA yield, composition, and volatility, Atmos. Chem. Phys. Discuss., (August), 1–20, doi:10.5194/acp-2019-271, 2019.

Faiola, C. L., Pullinen, I., Buchholz, A., Khalaj, F., Ylisirniö, A., Kari, E., Miettinen, P., Holopainen, J. K., Kivimäenpää, M., Schobesberger, S., Yli-Juuti, T. and Virtanen, A.: Secondary Organic Aerosol Formation from Healthy and Aphid-Stressed Scots Pine Emissions, ACS Earth Sp. Chem., doi:10.1021/acsearthspacechem.9b00118, 2019.

Huang, W., Saathoff, H., Pajunoja, A., Shen, X., Naumann, K. H., Wagner, R., Virtanen, A., Leisner, T. and Mohr, C.: α-Pinene secondary organic aerosol at low temperature: Chemical composition and implications for particle viscosity, Atmos. Chem. Phys., 18(4), 2883–2898, doi:10.5194/acp-18-2883-2018, 2018.

Isaacman-VanWertz, G., Massoli, P., O'Brien, R. E., Nowak, J. B., Canagaratna, M. R., Jayne, J. T., Worsnop, D. R., Su, L., Knopf, D. A., Misztal, P. K., Arata, C., Goldstein, A. H. and Kroll, J. H.: Using advanced mass spectrometry techniques to fully characterize atmospheric organic carbon: Current capabilities and remaining gaps, Faraday Discuss., 200, 579–598, doi:10.1039/c7fd00021a, 2017.

Li, Y., Pöschl, U. and Shiraiwa, M.: Molecular corridors and parameterizations of volatility in the chemical evolution of organic aerosols, Atmos. Chem. Phys., 16(5), 3327–3344, doi:10.5194/acp-16-3327-2016, 2016.

Lopez-Hilfiker, F. D., Mohr, C., Ehn, M., Rubach, F., Kleist, E., Wildt, J., Mentel, T. F., Lutz, A., Hallquist, M., Worsnop, D. and Thornton, J. A.: A novel method for online analysis of gas and particle composition: description and evaluation of a Filter Inlet for Gases and AEROsols (FIGAERO), Atmos. Meas. Tech., 7, 983–1001, doi:10.5194/amt-7-983-2014, 2014.

Priestley, M., Bannan, T. J., Le Breton, M., Worrall, S. D., Kang, S., Pullinen, I., Schmitt, S., Tillmann, R., Kleist, E., Zhao, D., Wildt, J., Garmash, O., Mehra, A., Bacak, A., Shallcross, D. E., Kiendler-Scharr, A., Hallquist, Å. M., Ehn, M., Coe, H., Percival, C. J., Hallquist, M., Mentel, T. F. and McFiggans, G.: Chemical characterisation of benzene oxidation products under high- And low-NOx conditions using chemical ionisation mass spectrometry, Atmos. Chem. Phys., 21(5), 3473–3490, doi:10.5194/acp-21-3473-2021, 2021.

Saha, P. K. and Grieshop, A. P.: Exploring Divergent Volatility Properties from Yield and Thermodenuder Measurements of Secondary Organic Aerosol from α-Pinene Ozonolysis, Environ. Sci. Technol., 50(11), 5740–5749, doi:10.1021/acs.est.6b00303, 2016.

Schobesberger, S., D'Ambro, E. L., Lopez-Hilfiker, F. D., Mohr, C. and Thornton, J. A.: A model framework to retrieve thermodynamic and kinetic properties of organic aerosol from composition-resolved thermal desorption measurements, Atmos. Chem. Phys., 18(20), 14757–14785, doi:10.5194/acp-18-14757-2018, 2018.

Thornton, J. A., Mohr, C., Schobesberger, S., D'Ambro, E. L., Lee, B. H. and Lopez-Hilfiker, F. D.: Evaluating Organic Aerosol Sources and Evolution with a Combined Molecular Composition and Volatility Framework Using the Filter Inlet for Gases and Aerosols (FIGAERO), Acc. Chem. Res., 53(8), 1415–1426, doi:10.1021/acs.accounts.0c00259, 2020.

Wang, D. S. and Hildebrandt Ruiz, L.: Chlorine-initiated oxidation of alkanes under high-NO conditions: Insights into secondary organic aerosol composition and volatility using a FIGAERO-CIMS, Atmos. Chem. Phys., 18(21), 15535–15553, doi:10.5194/acp-18-15535-2018, 2018.

Ylisirniö, A., Buchholz, A., Mohr, C., Li, Z., Barreira, L., Lambe, A., Faiola, C., Kari, E., Yli-Juuti, T., Nizkorodov, S. A., Worsnop, D. R., Virtanen, A. and Schobesberger, S.: Composition and volatility of secondary organic aerosol (SOA) formed from oxidation of real tree emissions compared to simplified volatile organic compound (VOC) systems, Atmos. Chem. Phys., 20(9), 5629–5644, doi:10.5194/acp-20-5629-2020, 2020.

Ylisirniö, A., Barreira, L. M. F., Pullinen, I., Buchholz, A., Jayne, J., Krechmer, J. E., Worsnop, D. R., Virtanen, A. and Schobesberger, S.: On the calibration of FIGAERO-ToF-CIMS: Importance and impact of calibrant delivery for the particle-phase calibration, Atmos. Meas. Tech., 14(1), 355–367, doi:10.5194/amt-14-355-2021, 2021.