Reply to interactive comments on preprint egusphere-2025-2743

Anonymous Referee #1

General comments:

This study reports the formation of oxygenated and small organosulfates from aqueous-phase oxidation of an a-pinene-derived organosulfate (apOS-249), some of which have been detected in ambient aerosols but with unclassified precursors or formation pathways. The authors systematically investigated the kinetics and the reaction products and demonstrated that aqueous OH oxidation can serve as an important sink for the model organosulfate (apOS-249) under relevant atmospheric cloud conditions. Overall, this manuscript is well-written, and the conclusions are clearly supported by the results. Some questions and suggestions are listed below for the authors' consideration.

We thank the reviewer for his/her thoughtful comments. The referee's comments are below in *italics* followed by our responses in normal font. Possible text changes or new text is given in blue.

1. *pH has been shown to greatly impact reactivity in particles and droplets, while the pH of cloud droplets may range somewhere from 3 to 7. Could the authors provide some explanations about why a buffer solution of pH 4.5 was selected for this study and how would the range of pH observed in the atmosphere affect the breakdown of apOS-249? The authors also mentioned that the pH of the reaction mixtures were monitored (page 5, Lines 15-17). Did the pH values change at all or remain constant throughout the experiments, given the formation of inorganic sulfate and many different organosulfates that potentially have different pKa values?*

Responses

We thank reviewer for these valuable comments. The pH values of the solution mixture for kinetic and product-capture experiments were measured to be 4.5 ± 0.2 and 5.4 ± 0.2, respectively. All solutions were freshly prepared and measured directly without any adjustments (**Table R1**). We agree with the reviewer's comment that pH can be an important factor affecting the kinetics of aqueous-phase $^{\bullet}$OH oxidation. This phenomenon can be attributed to the pH-dependent speciation of organic compounds, which exist in different ionic forms (protonated, partially deprotonated, and deprotonated), depending on the acidity of the solution. These different states can alter reaction mechanisms, potentially modifying electron transfer pathways or electronic effects, thereby influencing the overall oxidative kinetics (Chu et al., 2023). In our study, according to the dissociation constants ($pK_{a1} = -3.5$ and $pK_{a2} = 12.2$) of αpOS-249 and its corresponding species distribution (**Figure R1**) (Pan et al., 2021), *α*pOS-249 predominantly exists in anionic form across the pH range from −1 to 10. This implies that its reaction kinetics are likely pH-independent under typical atmospheric conditions (Tilgner et al., 2021). Furthermore, a recent laboratory study has investigated the aqueous-phase ${}^{\bullet}OH$ oxidation of five atmospherically relevant OSs (methyl sulfate, ethyl sulfate, propyl sulfate, hydroxyacetone sulfate and phenyl sulfate) as a function of pH (Gweme and Styler, 2024). It was reported that the rate constants were not sensitive to pH, remaining identical within experimental error under both acidic (pH = 2) and basic (pH = 9) conditions. This consistency is attributed to the fact that all the investigated OSs existed exclusively in their anionic form in the aqueous phase at these pH levels (Gweme and Styler, 2024).

In our study, as shown in **Table R1**, the pH values remained at 4.5 throughout the kinetic experiment due to the buffering effect of the reference compound (i.e., benzoic acid, BA). In contrast, during the product-capture experiment, the pH values decreased from 5.4 before oxidation to approximately 4.3 after oxidation. This drop is likely attributable to the formation of more acidic products than *α*pOS-249, such as inorganic sulfates. In particular, bisulfate (HSO_4^-) can dissociate to release H^+ ions, thereby increasing the solution acidity.

Table R1. Summary of pH values in a series of aqueous-phase experiments.

Experimental Details		**Control experiments**		**Kinetic experiment**	**Product-capture experiment**
Reactions		***α*pOS-249 + H_2O_2**	***α*pOS-249 + UV**	***α*pOS-249 + BA + ${}^{\bullet}OH$**	***α*pOS-249 + ${}^{\bullet}OH$**
Measured pH values	**Before oxidation**	5.4 ± 0.2	5.3 ± 0.3	4.5 ± 0.2	5.4 ± 0.2
	After oxidation	5.3 ± 0.3	5.2 ± 0.3	4.5 ± 0.1	4.3 ± 0.2

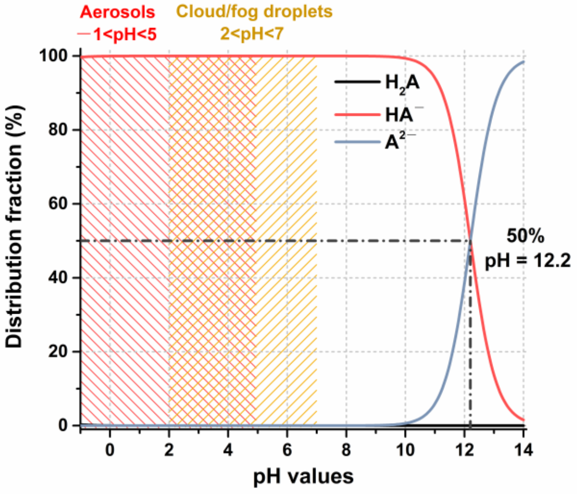


Figure R1. Fractions of H_2A ($C_{10}H_{16}(OH)SO_4H$), HA^- ($C_{10}H_{16}(OH)SO_4^-$) and A^{2-} ($C_{10}H_{16}$ $(O^-)SO_4^-$) in *α*pOS-249 solution as a function of pH values. The shaded areas represent typical atmospheric conditions, with aerosols having pH values ranging from

−1 to 5 and cloud/fog droplets ranging from 2 to 7 (Tilgner et al., 2021). (The dissociation constants of αpOS-249 are $pK_{a1} = -3.5$ and $pK_{a2} = 12.2$. At pH > −1, the fraction of H_2A is zero).

We have added the following information in the revised manuscript:

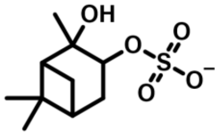
Page 7, Line 28: "Furthermore, as discussed in **Section S5**, the aqueous-phase $^{\bullet}$OH oxidation kinetics of αpOS-249 is likely insensitive to solution pH under typical atmospheric conditions."

The following information was also added in the supporting information:

Page 8, Line 74: "We acknowledge that pH can be an important factor affecting the kinetics of aqueous-phase $^{\bullet}$OH oxidation. This phenomenon can be attributed to the pH-dependent speciation of organic compounds, which exist in different ionic forms (protonated, partially deprotonated, and deprotonated), depending on the solution acidity. These different states can alter the reaction mechanisms, potentially modifying electron transfer pathways or electronic effects, thereby influencing the overall oxidative kinetics (Chu et al., 2023). In our study, the dissociation constants ($pK_{a1} = -3.5$ and $pK_{a2} = 12.2$) of αpOS-249 (Pan et al., 2021) indicate that it predominantly exists in its singly deprotonated form across the pH range from −1 to 10. The reaction kinetics is likely not sensitive to the solution pH (Tilgner et al., 2021). Furthermore, a recent laboratory study has investigated the aqueous-phase $^{\bullet}$OH oxidation of five atmospherically relevant OSs (methyl sulfate, ethyl sulfate, propyl sulfate, hydroxyacetone sulfate and phenyl sulfate) as a function of pH (Gweme and Styler, 2024). It was reported that the rate constants were not sensitive to pH, remaining identical within experimental error under both acidic (pH = 2) and basic (pH = 9) conditions. This stability is attributed to the fact that all the investigated OSs existed exclusively in their anionic form in the aqueous phase at these pH levels (Gweme and Styler, 2024). Taken together, the cumulative evidence suggests that the reaction kinetics of aqueous-phase $^{\bullet}$OH oxidation of αpOS-249 are likely not sensitive to the pH under typical atmospheric conditions."

The information from **Table R1** was also added to supporting information **Table S2**:

Table S2. A summary of experimental conditions used in the series of aqueous-phase experiments.

Reactants	 **α-pinene derived organosulfate** **(αpOS-249, $C_{10}H_{17}SO_5^-$)**		
Experimental Details	**Control experiments**	**Kinetic experiments**	**Product-capture experiments**

Reactions		αpOS-249 + H_2O_2	αpOS-249 + UV	αpOS-249 + BA + $^{\bullet}$OH	αpOS-249 + $^{\bullet}$OH
Concentrations (mol L^{-1})	[αpOS-249]	5×10^{-5}	5×10^{-5}	5×10^{-5}	5×10^{-5}
	[H_2O_2]	2×10^{-3}	–	2×10^{-3}	2×10^{-3}
	[BA]	–	–	5×10^{-5}	–
	[$^{\bullet}$OH]$_{ss}$[a]	–	–	6×10^{-14}	9×10^{-14}
Measured pH values	Before oxidation	5.4 ± 0.2	5.3 ± 0.3	4.5 ± 0.2	5.4 ± 0.2
	After oxidation	5.3 ± 0.3	5.2 ± 0.3	4.5 ± 0.1	4.3 ± 0.2

2. *Similar to the last comment, ionic strength effects reactivity within aqueous solutions. Cloud water in urban areas is dominated by ammonium sulfate and ammonium nitrate, while marine NaCl. Would the presence of these salts at their atmospheric concentrations affect the rate of OH production and subsequent OS oxidation? Similar to the last comment, ionic strength affects reactivity within aqueous solutions. Cloud water in urban areas has high concentrations of ammonium sulfate and ammonium nitrate, while in marine environments, sodium chloride is the dominant salt. Would the presence of these salts at their atmospheric concentrations affect the rate of OH production and subsequent OS oxidation?*

Responses

We agree with the reviewer's comment regarding the potential influence of salts (e.g., ammonium sulfate, ammonium nitrate, and sodium chloride) on $^{\bullet}$OH production and αpOS-249 oxidation kinetics. As summarized in a previous review (Herrmann et al., 2015), the ionic strength of atmospheric fog and/or cloud droplets typically ranges from 10^{-4} to 10^{-2} mol L^{-1}. In our experimental setup, $^{\bullet}$OH radicals were generated through the photolysis of 2×10^{-3} mol L^{-1} H_2O_2 under 313 nm irradiation. Based on previous studies, the quantum yields for H_2O_2 photolysis at this wavelength are insensitive to ionic strength (Kwon and Kwon, 2010; Herrmann et al., 2015), suggesting that $^{\bullet}$OH production would not be significantly influenced by the presence of typical salt concentrations in atmospheric fog and/or cloud droplets. Moreover, in terms of how salts influence the rate of $^{\bullet}$OH oxidation of αpOS-249, it is noted that chloride ion (Cl^-) from sodium chloride can establish an equilibrium with $^{\bullet}$OH, forming $ClOH^{\bullet-}$ with an equilibrium constant of 0.7 L mol^{-1} (Jayson et al., 1973). However, this pathway is only important under strongly acidic conditions (e.g., $pH < 3$) (Jayson et al., 1973). Even when this reaction was incorporated into our model simulations with [Cl^-] ranging from 10^{-4} to 10^{-2} mol L^{-1} (**Table R2, R14**), the calculated rate constant for the $^{\bullet}$OH oxidation of αpOS-249 remain unchanged.

Regarding the impact of ionic strength on the oxidation kinetics, in cases where both reactants are charged, changes in rate constants with ionic strength are a consequence of electrostatic attractive and repulsive forces between the reactant ions and electrolyte ions in the solution (Liu et al., 2003). The influence of ionic strength on ion−neutral molecule reactions, such as the $^{\bullet}$OH reaction with *α*pOS-249, presents a challenge for prediction, given that rate constants are solely dependent on the empirical linear term, *b* ($\log k = \log k° - bI$). Here, *k* represents the observed rate constant, $k°$ is the rate constant at infinite dilution, *I* is the total ionic strength, and *b* is an empirical term derived from experimental data. This term can exhibit either a negative or positive direction (Gweme and Styler, 2024). For example, Herrmann et al. (2003) reported the positive effect of ionic strength on oxidation kinetics in reactions of $^{\bullet}$OH with acetone, 2-propanol, and 2-butanol. In contrast, Gweme and Styler (2024) observed a monotonic decrease in pseudo first-order rate constants of $^{\bullet}$OH with propyl sulfate, phenyl sulfate, and ethyl sulfate as ionic strength increased. Future studies are warranted and should systematically investigate how ionic strength modulates $^{\bullet}$OH oxidation kinetics.

Table R2. Reaction schemes and rate constants for the kinetic box model.[a]

No.	Reactions	Parameters	References
R1	$H_2O_2 + h\nu\ (\lambda = 313\ \mathrm{nm}) \rightarrow 2^{\bullet}OH$	$\Phi = 0.93$	(Herrmann et al., 2010)
R2	$2 \times {}^{\bullet}OH \rightarrow H_2O_2$	$5.5 \times 10^{9}\ M^{-1}\ s^{-1}$	(Buxton et al., 1988)
R3	${}^{\bullet}OH + H_2O_2 \rightarrow HO_2^{\bullet} + H_2O$	$3.0 \times 10^{7}\ M^{-1}\ s^{-1}$	(Christensen et al., 1982)
R4	${}^{\bullet}OH + HO_2^{\bullet} \rightarrow H_2O + O_2$	$1.0 \times 10^{10}\ M^{-1}\ s^{-1}$	(Elliot and Buxton, 1992)
R5	${}^{\bullet}OH + O_2^{\bullet-} \rightarrow OH^{-} + O_2$	$1.1 \times 10^{10}\ M^{-1}\ s^{-1}$	(Christensen et al., 1989)
R6	$H_2O \rightleftharpoons H^{+} + OH^{-}$	$pK_a = 13.999$	(Pastina and Laverne, 2001)
R7	$HO_2^{\bullet} \rightleftharpoons H^{+} + O_2^{\bullet-}$	$pK_a = 4.8$	(Buxton et al., 1988)
R8	$2 \times HO_2^{\bullet} \rightarrow H_2O_2 + O_2$	$9.8 \times 10^{5}\ M^{-1}\ s^{-1}$	(Christensen et al., 1989)
R9	$2 \times O_2^{\bullet-} + 2 \times H_2O \rightarrow H_2O_2 + O_2 + 2 \times OH^{-}$	$3.5 \times 10^{-1}\ M^{-1}\ s^{-1}$	(Judith and Bielski, 1979)
R10	$HO_2^{\bullet} + H_2O_2 \rightarrow {}^{\bullet}OH + O_2 + H_2O$	$5.0 \times 10^{-1}\ M^{-1}\ s^{-1}$	(Pastina and Laverne, 2001)
R11	$O_2^{\bullet-} + H_2O_2 \rightarrow {}^{\bullet}OH + O_2 + OH^{-}$	$1.3 \times 10^{-1}\ M^{-1}\ s^{-1}$	(Bielski et al., 1985)
R12	${}^{\bullet}$OH + *α*pOS-249 → Products	$(2.2 \pm 0.2) \times 10^{9}\ M^{-1}\ s^{-1}$	This work
R13	${}^{\bullet}$OH + BA → Products	$(5.5 \pm 0.3) \times 10^{9}\ M^{-1}\ s^{-1}$	This work
R14	${}^{\bullet}OH + Cl^{-} \rightleftharpoons ClOH^{\bullet-}$	$k_f = 4.3 \times 10^{9}\ M^{-1}\ s^{-1}$ $k_b = 6.1 \times 10^{9}\ s^{-1}$	(Jayson et al., 1973)

[a]The Model simulation was conducted at pH 5.

3. *Within this experiment the authors used a solution of apOS-249, benzoic acid (BA), and H_2O_2 to track the oxidation of apOS-249. The authors investigated the formation of fragmentation and functionalized (more oxygenated) products over time with lower carbon counts due to C-C bond cleavage during oxidation processes. Did* *authors observe any reaction products with higher carbon count numbers than C10 at early phases of the experiment that were potentially resulting from reactions between apOS-249 and BA?*

Responses

Thanks for the comments. In our experiments, we used LC-ESI-Orbitrap MS to detect the oxidation products. Throughout the entire reaction period, including early stages, we did not observe any products with C>10 under our experimental conditions. BA serves as a reference compound in the relative rate method for assessing ${}^{\bullet}$OH reaction kinetics, due to its well-established rate constants and mechanisms in aqueous-phase ${}^{\bullet}$OH oxidation. We speculate that BA typically reacts primarily with ${}^{\bullet}$OH and exhibits very limited reactivity towards target organic compounds (e.g., green leaf volatiles, nitrophenols, and aliphatic amines), as documented in previous studies (Richards-Henderson et al., 2014; Hems and Abbatt, 2018; Yang et al., 2021). Moreover, OSs are considered as relatively stable compounds (Zhang et al., 2012), with transformation pathways in the atmosphere primarily involving hydrolysis, heterogeneous oxidation, and aqueous-phase oxidation (Brüggemann et al., 2020). Thus, we do not expect significant side reactions between *α*pOS-249 and BA in our study.

4. *The authors investigated the formation of lower chain OS and inorganic sulfate due to oxidation by aqueous OH radicals. Did the authors observe any "sulfide" or "sulfonate" formation throughout their oxidation experiments? Figure S5 shows a peak at ~3.5 minutes. Is this corresponding to sulfite? Reporting these findings would be beneficial due to the potential environmental impacts of sulfite/sulfonates and sulfate/OS. This may also help close the sulfur mass balance when considering the breakdown of apOS-249.*

Responses

Thanks for the comments. We did not detect sulfonate products using LC-ESI-Orbitrap MS under our analytical conditions. As noted by Christensen et al. (2025), sulfonates typically produce a characteristic $SO_3^{\bullet-}$ (*m*/*z* = 79.96) fragment ion while lacking HSO_4^- (m/z = 96.96) in their MS^2 spectra. Neither of these signatures was observed, suggesting sulfonate formation was negligible under our conditions. In addition, sulfides could be difficult to ionize directly in ESI^- mode because they lack of acidic hydrogens that can be easily deprotonated (Christensen et al., 2025), hindering us to make definitive claims regarding their formation. The minor peak observed at RT = 3.5 mins (**Figure S5**) likely corresponds to the impact of smaller OS products. However, we believe that the formation of sulfide and sulfonate products in our study is likely insignificant given dominance of ${}^{\bullet}$OH-driven fragmentation pathways that favor OSs/inorganic sulfates production.

Minor comments:

5. *Page 3, Lines 7-9 – The authors noted that OS has profound effects on various physiochemical properties, such as surface tension and hygroscopicity. Due to the extensive discussion of OS sizes later in their findings, it will be helpful to provide more information in the introduction regarding how variations in carbon chain length can cause completely different aqueous properties of OS compounds. Reference: Bain, Alison, Man Nin Chan, and Bryan R. Bzdek. "Physical properties of short chain aqueous organosulfate aerosol." Environmental Science: Atmospheres 3.9 (2023): 1365-1373.*

Responses

Thanks for the comment, we have added the following information in the revised manuscript:

Page 3, Line 11: "In addition, atmospheric OSs possess numerous physiochemical properties including viscosity, acidity, morphology, hygroscopicity, toxicity, and surface activity, that are closely linked to their molecular structures (Hansen et al., 2015; Riva et al., 2019; Bain et al., 2023). Notably, Bain et al. (2023) demonstrated that OSs exhibit intermediate properties between inorganic sulfates (e.g., bisulfate (HSO_4^-) and sulfate (SO_4^{2-}) ions) and structurally similar alkyl organics containing functional groups other than the sulfate group (e.g., alcohols and carboxylic acids). They further reported a clear positive relationship between the carbon chain length of alkyl sulfates and surface activity. These distinctive properties ultimately govern the different environmental behaviors of OSs compared to their inorganic sulfate counterparts."

6. *Page 3, Line 32 – The phrase "retain or release inorganic sulfates" is somewhat confusing. I suggest changing it to "retain the sulfate moiety or release inorganic sulfates."*

Responses

Thank you for your comment. The following changes were made in the manuscript:

Page 4, Line 22: "The importance of OS transformation is largely contingent upon the fate of either retaining the sulfate moiety or releasing inorganic sulfates through subsequent reactions."

7. *Page 6, Line 24 – Use of NaOH as an eluent is typically done under an inert atmosphere due to the ability of carbon dioxide to partition into carbonic acid and then bicarbonate. These reactions will cause peak broadening within the system. Did the authors use any inert headspace over eluent or check to see if broadening of peaks changed over time in subsequent runs, which may have impacted peak area integration? If the same standard concentration showed a broader peak after multiple runs, concentrations of sulfate calculated by peak area might be inaccurate.*

Responses

Thanks for the comment. System stability tests were performed at the beginning of each sequence using a Na_2SO_4 standard. Across the 20-hour runs, there were no notable occurrences of peak broadening (<6 % change in peak width at half-height, **Table R3**). The analysis of our samples for sulfate quantification in IC was concluded within four hours, suggesting no expected significant impacts on peak broadening.

Table R3. Summary of peak width (50 %) information from repetitive measurements of sulfate standard at $[SO_4^{2-}] = 3.17$ ppm in IC analysis.

	Standard 1	Standard 2	Standard 3
$t = 0$	0.120 min	0.117 min	0.120 min
$t = 20$ hours	0.119 min	0.114 min	0.116 min

8. *Page 6, Line 25 – It might be helpful to include the exact retention time observed. Although the IC curves are shown in the SI, readers can compare literature and simulated elution times to those that are observed by the authors.*

Responses

Thank you for your comment. The following changes were made in the manuscript:

Page 7, Line 17: "In this work, the quantity of inorganic sulfates was measured based on its peak area in the chromatogram and quantified using a calibration curve based on Na_2SO_4 standard, with a retention time (RT) of 4.0 min."

9. *Page 9, Figure 2 – Were total intensities normalized to something, such as a reference compound, to account for instrument variations between runs at different time periods?*

Responses

Thanks for the comment. Figure 2 shows the absolute intensity, and we did not include an internal standard in our samples to avoid potential interferences. We performed system stability tests and inserted blank injections between samples to monitor baseline stability through the analysis.

10. *Page 11, Lines 4-10 –As a precaution for readers, it would be helpful if the authors could also discuss how, if this assumption was found to not be true, it would affect results.*

Responses

Thanks for the comment, we acknowledge that this simple comparison relies on the assumption that OS products have the same ionization efficiency as that of αpOS-

249. However, differences in ionization efficiency among OS products relative to the parent OS are not well understood. The results of this simple analysis should be treated with great caution. The inclusion of authentic standards is important for accurately quantifying more oxygenated C_{10} OS products and smaller OS products. Without these standards, accurate quantification becomes challenging, and both overestimation and underestimation are possible depending on the molecular structure.

We have added the following information in the revised manuscript:

Page 12, Line 6: "It is important to note that this simple comparison assumes that OS products have the same ionization efficiency as *α*pOS-249. However, differences in ionization efficiency among OS products relative to the parent OS are not well understood. As a result, the findings from this simple analysis should be interpreted with caution. Authentic standards are important for accurately quantifying more oxygenated C_{10} OS products and smaller OS products. In the absence of these standards, quantification becomes challenging, and both overestimation and underestimation are possible depending on the specific molecular structures involved."

11. *Page 13, Lines 10-12 – Did the MS^2 fragmentation patterns for any of these potentially isomeric compounds show significant differences? If significant differences are found, it would be helpful to include this information in supplemental materials.*

Responses

Thanks for the comment. While MS^2 fragmentation can help distinguish isomers, we have detected about 40 OS products with different isomeric forms, making systematic fragmentation pattern comparisons difficult for this study. Many of these isomers exhibited only subtle differences in fragmentation patterns, which were not sufficiently diagnostic for confident structural assignments.

12. *Page 14, Lines 22-23 – The authors noted the minor presence of inorganic sulfate due to hydrolysis and accounted for this in the quantification formed by oxidation. Was any kinetics data collected on this hydrolysis, as hydrolysis would likely continue alongside OH oxidation throughout the experiment? If the rate is low enough, this amount might be negligible compared to the aqueous OH oxidation. However, it is currently unclear if hydrolysis is contributing to the increased inorganic sulfate concentration during the irradiation process, even after adjustment for the initial SO_4 concentration.*

Responses

Thanks for the comment. We agree with the reviewer's comment regarding the potential formation of inorganic sulfate via hydrolysis during $^{\bullet}OH$ oxidation. Control experiments (*α*pOS-249 + UV light only and *α*pOS-249 + H_2O_2 only) were conducted and analyzed by IC analysis, and no detectable increase in inorganic sulfate was observed, only the background peak (**Figure R2**). This suggests that inorganic sulfate is primarily formed during the aqueous-phase •OH oxidation of *α*pOS-249. However, we cannot rule out the contribution of hydrolysis of OS products to inorganic sulfate formation. As discussed in **Section 3.3.3**, the sulfur conversion from *α*pOS-249 to inorganic sulfate may proceed via multiple pathways. During oxidation, more tertiary OS products are likely to form, particularly at high oxidation stages. This could increase the potential for hydrolysis-induced inorganic sulfate formation (Hu et al., 2011). Further studies are warranted to better understand the role of hydrolysis in OS transformation.

We have added the following sentence in the revised manuscript:

Page 17, Line 19: "Further studies are warranted to better understand the role of hydrolysis in OS transformation."

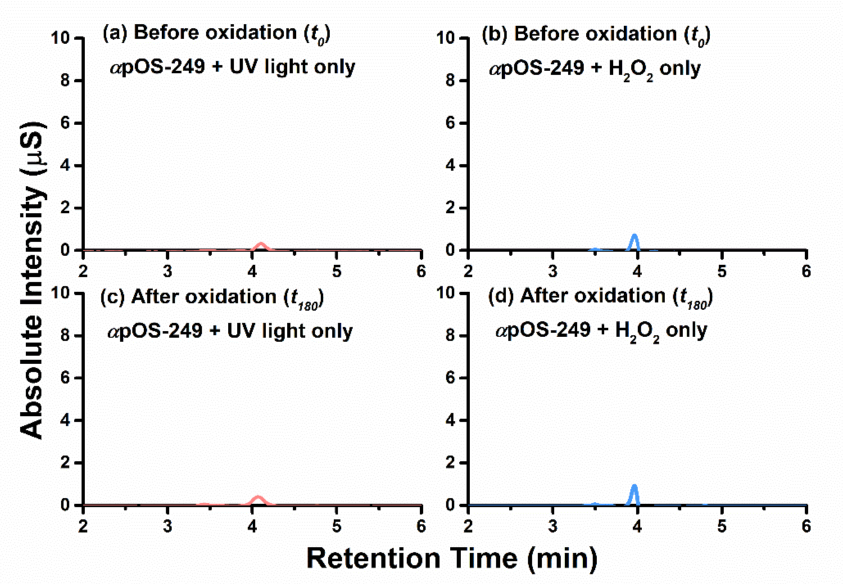


Figure R2. Ion chromatograms before (t_0) and after (t_{180}) the aqueous-phase •OH control experiments of *α*pOS-249.

13. *Page 14, Lines 29-30 – Were any control experiments performed in which UV lights remained active until no change was seen in* SO_4^{2-} *concentration? It would be interesting to see if a stagnation of inorganic sulfate concentration consumed all OS compounds in solution at these relevant concentrations of OH radicals.*

Responses

Thanks for the valuable comment. In our study, we did not maintain the lights on until a stability point was reached in the inorganic sulfate concentration. Our findings revealed that during the 3-hour aqueous-phase •OH oxidation under cloud/fog relevant •OH concentrations, about half of the sulfur present in the reacted *α*pOS-249 was transformed into inorganic sulfates. We anticipate a continuous increase in inorganic sulfate concentration when the reaction further proceeds. Future work is warranted regarding the dependence of inorganic sulfate formation on the extent of OS oxidation in the atmosphere.

We have added the following information in the revised manuscript:

Page 16, Line 4: "We anticipate a continuous increase in inorganic sulfate concentration when the reaction further proceeds. Future work is warranted regarding the dependence of inorganic sulfate formation on the extent of OS oxidation in the atmosphere."

14. *Pages 16-17, Atmospheric Implications – It would be helpful to comment on the potential influence of this finding on acidity levels due to inorganic sulfate formation, as well as the impact of trending towards smaller OS due to their different physicochemical properties than large OS, as noted in the comments above.*

Responses

Thanks for the valuable comment, we have added the following information in the revised manuscript:

Page 20, Line 1: "Furthermore, the chemical aging of αpOS-249 during aqueous-phase $^{\bullet}$OH experiments can significantly modify the composition and physiochemical properties of atmospheric aerosols and cloud droplets. For example, $^{\bullet}$OH oxidation of αpOS-249 promotes the formation of inorganic sulfates, which can enhance acidity. It also produces smaller OS products that may reduce surface activity compared with their parent αpOS-249 and larger OSs. These insights are critical for accurately evaluating the role of such atmospherically important organosulfur compounds in aerosol–cloud interactions and their potential climate impacts."

Anonymous Referee #2

General comments:

Lai et al. investigate the aqueous phase oxidation kinetics of an α-pinene-derived organosulfate by $^{\bullet}$*OH radicals, reporting a second-order rate constant of* $(2.2 \pm 0.2) \times 10^9\ L\ mol^{-1}\ s^{-1}$ *and corresponding atmospheric lifetimes ranging from minutes to two days. The study identifies a series of new OS products, including more oxygenated C10 OS compounds, smaller OS fragments, and significant amounts of inorganic sulfate. Based on the detected products and proposed mechanisms, the authors suggest that these OS species form through functionalization and fragmentation processes. Finally, a comparison with literature data reveals that most of the observed OS products have been previously detected in field studies, and some of these products exhibit previously unknown sources and formation pathways. The authors thus propose that aqueous-phase oxidation of larger OSs could explain the atmospheric presence of these OS compounds. This is a timely, well-executed study, clearly written and well-supported by the data. The findings will be of interest to ACP readers, and I think the manuscript is suitable for publication after addressing the following minor comments:*

We thank the reviewer for his/her thoughtful comments. The referee's comments are below in *italics* followed by our responses in normal font. Possible text changes or new text is given in blue.

1. *Page 3 Line 15: The statement "Various mechanisms have been proposed for OS formation" would benefit from including specific examples of these mechanisms to enhance clarity and support for the reader.*

Responses

Thanks for the comments. We have added the following information in the revised manuscript:

Page 3, Line 27: "Various mechanisms have been proposed for OS formation, with the acid-catalyzed ring-opening of epoxides in the presence of sulfate ions being the most widely recognized mechanism for OS formation from the photochemical reactions of various VOCs such as isoprene, monoterpenes (e.g., *α*-pinene, *β*-pinene, and limonene), and aromatic compounds (e.g., toluene and benzene) (Iinuma et al., 2007; Surratt et al., 2010; Zhang et al., 2012; Barbosa et al., 2017; Brüggemann et al., 2020; Jiang et al., 2022). In addition, heterogeneous reactions of gas-phase SO_2 with unsaturated hydrocarbons (e.g., oleic acid and linoleic acid) in the absence of gas-phase oxidant (e.g., O_3 and $^{\bullet}OH$) have been identified as another important contributor to OS formation in both laboratory experiments and field observations (Shang et al., 2016; Passananti et al., 2016; Zhu et al., 2019). Other proposed mechanisms include sulfate esterification reactions (Minerath et al., 2008; Perri et al., 2010), nucleophilic substitution of alcohols or epoxides with sulfuric acid (Surratt et al., 2007; Darer et al., 2011), and reactions facilitated by sulfoxy radicals (e.g., $SO_3^{\bullet-}$ and $SO_4^{\bullet-}$) (Nozière et al., 2010; Szmigielski, 2016; Wach et al., 2019)."

***2.** Page 5 Line 15: The authors need to clarify if pH affects the reaction rate. For example, please provide commentary on how the experimental results may differ under more acidic conditions.*

Responses

Thanks for the valuable comment. We agree with the reviewer that further discussion on the pH dependence of the oxidative kinetics is necessary. A similar comment has also raised by Reviewer 1 (**Comment #1**). In this study, the dissociation constants of αpOS-249 ($pK_{a1} = -3.5$ and $pK_{a2} = 12.2$) suggest that it predominantly exists in anionic form under typical atmospheric conditions (pH = −1 − 10) (Tilgner et al., 2021). We would expect insignificant variation in kinetics even under more acidic conditions, given that αpOS-249 remains in its anionic form even at low pH. However, if future studies explore extreme pH regimes (e.g., $pH < -1$), further investigation may be warranted.

We have added the following information in the revised manuscript:

Page 7, Line 28: "Furthermore, as discussed in **Section S5**, the aqueous-phase $^{\bullet}OH$ oxidation kinetics of αpOS-249 is likely insensitive to solution pH under typical atmospheric conditions."

The following information was also added in the supporting information:

Page 8, Line 74: "We acknowledge that pH can be an important factor affecting the kinetics of aqueous-phase $^{\bullet}OH$ oxidation. This phenomenon can be attributed to the pH-dependent speciation of organic compounds, which exist in different ionic forms (protonated, partially deprotonated, and deprotonated), depending on the solution acidity. These different states can alter the reaction mechanisms, potentially modifying electron transfer pathways or electronic effects, thereby influencing the overall oxidative kinetics (Chu et al., 2023). In our study, the dissociation constants ($pK_{a1} = -3.5$ and $pK_{a2} = 12.2$) of αpOS-249 (Pan et al., 2021) indicate that it predominantly exists in its singly deprotonated form across the pH range from −1 to 10. The reaction kinetics is likely not sensitive to the solution pH (Tilgner et al., 2021). Furthermore, a recent laboratory study has investigated the aqueous-phase $^{\bullet}OH$ oxidation of five atmospherically relevant OSs (methyl sulfate, ethyl sulfate, propyl sulfate, hydroxyacetone sulfate and phenyl sulfate) as a function of pH (Gweme and Styler, 2024). It was reported that the rate constants were not sensitive to pH, remaining identical within experimental error under both acidic (pH = 2) and basic (pH = 9) conditions. This stability is attributed to the fact that all the investigated OSs existed exclusively in their anionic form in the aqueous phase at these pH levels (Gweme and Styler, 2024). Taken together, the cumulative evidence suggests that the reaction kinetics of aqueous-phase $^{\bullet}$OH oxidation of αpOS-249 are likely not sensitive to the pH under typical atmospheric conditions."

3. *Page 17 Line 10: In Table 1, the use of colored cells should be avoided or removed.*
Responses

Thanks for the comment. We have revised Table 1 by removing the colors as suggested.

4. *Finally, I wonder if the authors can comment on how their findings might extend to other smaller organosulfates, particularly isoprene-derived OS. Given that isoprene-derived OS are often more abundant in the atmosphere, would you expect similar formation pathways (e.g., functionalization and fragmentation) to generate new OS products through aqueous-phase $^{\bullet}$OH oxidation? Some additional discussion on this point would help place these important results in a broader atmospheric context.*

Responses

Thanks for the valuable comment. For isoprene-derived OSs, 2-methyltetrol sulfate (2-MTS, $C_5H_{11}O_7S^-$) is one of the dominant isomers with well-defined structure, and we used it as a representative example for discussion here. Laboratory study show that aqueous-phase $^{\bullet}$OH oxidation of 2-MTS yields both more oxygenated OS products (e.g., $C_5H_{11}O_8S^-$ and $C_5H_9O_8S^-$) and smaller OS products (e.g., $C_2H_3O_6S^-$) (Harrill, 2020). These results are consistent with our observations of both functionalization and fragmentation products formed upon $^{\bullet}$OH oxidation of larger OSs (i.e., αpOS-249).

The structure-activity relationship (SAR) model was used to predict a rate constant of 2.1×10^9 L mol^{-1} s^{-1} for the aqueous-phase $^{\bullet}$OH oxidation of 2-MTS (Lai et al., 2024), corresponding to lifetimes ranging from about 3 mins in remote aerosol conditions ($[^{\bullet}OH] = 3 \times 10^{-12}$ mol L^{-1}) to approximately 2 days in urban cloud conditions ($[^{\bullet}OH] = 3.5 \times 10^{-15}$ mol L^{-1}) (Herrmann et al., 2010). In addition, Chen et al. (2020) investigated the heterogeneous $^{\bullet}$OH oxidation of 2-MTS and reported an atmospheric lifetime of 16 ± 2 days (assuming $[^{\bullet}OH] = 1.5 \times 10^6$ molecules cm^{-3}) (Chen et al., 2020). These findings suggest that aqueous-phase $^{\bullet}$OH oxidation can be a significant sink for 2-MTS, leading to both functionalization and fragmentation and producing more oxygenated and smaller OS products. Overall, we expect that similar mechanisms operate for isoprene-derived OSs in general, and that aqueous-phase $^{\bullet}$OH oxidation likely plays an important role in their atmospheric aging and transformation, especially given their high abundance.

Other Changes

1. Page 5, Line 29: "Under irradiation, a steady-state concentration of $^{\bullet}$OH ([$^{\bullet}$OH]$_{ss}$) of around $(4 - 9) \times 10^{-14}$ mol L^{-1} was generated, as calculated from the simulations using a box model (**Section S3**)."

2. Page 7, Line 31: "Relative rate method was adopted to determine the second-order rate constants for $^{\bullet}$OH oxidation of *α*pOS-249 (k_{OS}) by comparing the measured rate constants to that of a reference compound (BA) with a well-known $^{\bullet}$OH reaction rate of $k_{Ref} = (5.5 \pm 0.3) \times 10^9$ L mol^{-1} s^{-1} at a solution pH of 4.5."

3. Page 20, Line 25: "The supplement related to this article is published alongside this manuscript."

4. Page 21, Line 9: "This work is supported by The Hong Kong Research Grants Council (Ref No. 14300921: Project ID 2130791 and No. 14301922: Project ID 2130809)."

5. Page 21, Line 19: "~~Review statement.~~"

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