Authors' Response to Reviews of

Secondary aerosol formation from dimethyl sulfide - improved mechanistic understanding based on smog chamber experiments and modelling

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RC: ***Reviewers' Comment***, AR: Authors' Response, ☐ Manuscript Text

We thank both reviewers for the constructive comments. We have addressed the comments in a point by point fashion below and modified the manuscript accordingly.

Additional Information

In relation to the accompanying paper Rosati et al. (2021b) recently published in ACS Space and Earth Chemistry (doi: 10.1021/acsearthspacechem.0c00333) there are a few aspects, which we would like to clarify.

Preliminary ADCHAM model results based on the dry experiments (DMS 2-4) were already presented in Rosati et al. (2021b). After submission of the Rosati et al. (2021b) manuscript the ADCHAM model was further modified based on an expanded experimental dataset (inluding the humid experiments DMS 6-7 and butanol experiments BUT 2-3) and the model used in this study is therefore modified compared to the model used in Rosati et al. (2021b). We have added supplementary comments to the manuscript to highlight the experiments also discussed in Rosati et al. (2021b). We have also included a short section explaining the key differences between the two model setups.

Page 3, line 57-59

Therefore, this study and the companion paper by Rosati et al. (2021b) investigate the oxidation of DMS by OH radicals performed in the AURA smog chamber at Aarhus University, using the state of the art gas and particle phase chemistry model for laboratory chamber studies (ADCHAM) (Roldin et al., 2014).

Page 3, line 71-72

Here we only give a brief overview of the smog chamber setup. For a detailed description of the setup, e.g. different instrumentations as well as results from experiments performed under dry conditions the reader is referred to Rosati et al. (2021).

Page 4, line 89-90

Table 1 provides an overview of the conditions for all AURA experiments modelled with ADCHAM. Experiments DMS 1-5 and BUT-1 are described in detail in Rosati et al. (2021) and experimental data for these experiments are adopted from Rosati et al. (2021), see also the supplementary section S2 for model details.

Table 1

Experimental (model) conditions. Experiments DMS2, DMS6 and DMS7 marked in grey are referred to as 'Dry', 'Humid' and 'Cold' in Section 4. Experiments DMS 1-5 and BUT-1 are described in detail in Rosati et al. (2021) and experimental data for these experiments are adopted from Rosati et al. (2021).

Section S2

A preliminary version of the ADCHAM model was used to present model results on the dry experiments DMS2-4 in Rosati et al. (2021). Figures S27, S28 and S29 thus includes experimental data from Rosati et al. (2021b) and similar but not identical model results. A Key difference between the two model setups includes an increase in the LWC from $3.5 \cdot 10^{-7}$ g m^{-3} utilised by Rosati et al. (2021) to 10^{-5} g m^{-3}. In Rosati et al. (2021) the model was constrained based on the non-corrected AMS particle mass. The change in LWC reflects the change in PM from the SMPS corrected AMS measurements used in this study. The large increase in LWC was partly compensated by decreasing the coefficient of eddy diffusion from 0.1 s^{-1} (used by Rosati et al. (2021)) to 0.02 s^{-1}. Furthermore, the friction velocity (u^*) and electric field strength (E_{field}) governing the wall loss of non-charged and charged particles, respectively, had to be modified in order to reproduce the SMPS corrected AMS PM. Values were decreased resulting in a smaller particle wall loss from $u^* = 0.02$ m s^{-1} and E_{field} = 10, 10 and 5 V cm^{-1} for experiment DMS 2-4 in Rosati et al. (2021), to $u^* = 0.013$ m s^{-1} and E_{field} = 3.0, 0.7 and 2.0 V cm^{-1}.

Ammonia concentrations in the AURA chamber were modelled explicitly in the new improved model setup by assuming an initial pool of dissolved ammonium-sulfate on the chamber walls, evaporating as NH_3 based on the LWC, acidity of the water film and temperature. Consequently, the influx of ammonia to the gas-phase varied in between experiments performed on different dates. This was not the case in Rosati et al. (2021b), in which we used a fixed flux of ammonia into the chamber from the chamber wall.

1. Reviewer #1

1.1. Page 1 - Line 1

RC: ***"Dimethyl sulfide (DMS) is the dominant biogenic sulphur compound in the ambient atmosphere." This statement is correct in open ocean waters.***

AR: While the emission of DMS exceeds the natural emission of sulphur compounds H_2S, CS_2, OCS, volcanic SO_2 and sulphate on a global scale (Seinfeld and Pandis, 2016), we agree that it is more precise to specify that the emission of DMS is related to marine conditions and that the atmospheric concentrating of DMS is highest in open ocean waters.

> Dimethyl sulfide (DMS) is the dominant biogenic sulphur compound in the ambient marine atmosphere

1.2. Page 3 – line 57

RC: ***"under said conditions" – what are the conditions? Please add briefly what conditions you refer to***

The phrasing "under said conditions" in the sentence "Few have studied the gas and multiphase DMS chemistry in controlled smog chamber experiments, and none have tested model predictions under said conditions.", was meant to refer to the controlled conditions of the smog chamber experiments. We recognise that the wording is imprecise and have rephrased the sentence.

> Few have studied the gas and multiphase DMS chemistry in controlled smog chamber experiments, and prior to Rosati et al. (2021b) and this work none have tested model predictions on the formation, growth and chemical composition of the aerosol particles being produced.

1.3. Page 3 - Line 75 and Page 6 – Line 135

RC: ***I suggest to use 'mixing ratio' instead of 'concentrations'. The unit ppmv is used for mixing ratios not concentrations.***

AR: This was changed in the revised manuscript.

1.4. Tables 1 and 2

RC: ***I think it is unnecessary to display "Date" (Is there any point to have 'date' in these tables? The samples already have ids/exp.). Also, I think in the discussion sections, authors refer to only 3 experiments in the tables.***

AR: The discussion section focuses on one experiment from each experimental category (dry chamber, humid chamber and cold chamber). The butanol experiments are used to motivate the presence of a water film on the Teflon bag surface. While we only present results from one experiment in each of the three categories in the main paper, the conclusion made apply to all experiments in each category (the specific results for each experiment are found in the supplementary information).

The dates can be relevant in terms of contamination in the chamber. Both for examining relevant concentrations of NH_3, NOx, etc. in Aarhus at the time of the experiment, but also in order to compare these concentrations between experiments. We expect that chamber conditions, e.g. wall contamination will be similar between experiments performed directly after each other. Also, the dates allow the reader to compare experiments mentioned in this study to the experiments mentioned in Rosati et al. (2021b).

1.5. Page 7 – Line 149

RC: ***"the leakage of NH_3(g) into the chamber become larger than the sink of NH_3(g) to the particle phase." Why? It is confusing for me. I think this paper lacks a critically evaluating the uncertainties and reporting quantitative errors on both chamber measurements and model results.***

AR: Unfortunately no direct measurements of NH_3 was made in the AURA chamber during the experiments. However, according to the study by Kirkby et al. (2011), trace amounts of ammonia are almost always present in smog chamber experiments. In our study we consider that ammonia most likely is released into the chamber in two ways. From ammonium on the chamber walls and from ammonia leaking into the Teflon bag from outside the chamber (see Page 6, line 131-142). NH_3 concentrations outside the chamber was based on measurements made at Tange (56.352222°N, 9.5875°W) located approximately 50 km from Aarhus (data available at http://ebas.nilu.no/). Also, ammonia measurements in a nearby analytical laboratory of Anders Feilberg has previously shown concentrations of ammonia in the range of 1-10 ppb.

Sensitivity runs are used to report uncertainties in the model results, since the output of the deterministic ADCHAM model is fully determined by the parameter values and the initial conditions.

In the case of the specific sentence, "the leakage of NH_3(g) into the chamber become larger than the sink of NH_3(g) to the particle phase", we refer to the modelled concentration of ammonia (see section S2.5 'Modelled NH_3 concentrations' in the supplementary information). Ammonia in the gas-phase takes part in the initial new particle formation of SA and water and therefore its concentration decreases shortly after the injection of DMS into the chamber (see supplementary figure S5). Towards the end of the experiment the SA and MSA PM formation decreases. Consequently, less NH_3 partitions to particle-phase. At the same time the leakage of NH_3 into the chamber increases in the model as the chamber bag shrinks and thus NH_3 accumulates in the gas-phase.

1.6. Page 3

RC: ***I suggest to mention what each of the sections include, at the end of the introduction.***

AR: We have added references in the introduction to the most relevant sections int the manuscript.

> A stand-alone experiment examining butanol oxidation by OH was used to quantify the effect of high and low relative humidity (RH) on the OH concentration in the AURA chamber (section 2.2). The results were used to estimate the formation of a RH dependant water film forming on the Teflon bag surface, and implemented as a means to explain the difference in DMS experiments performed at dry and humid conditions (section 3.3.1-3). Finally, we performed several sensitivity runs investigating how the new revised DMS multiphase chemistry mechanism compare with previous DMS mechanisms under different relevant atmospheric conditions (section 3.3.4).

1.7. Section 2

RC: ***This section includes Methods. You can revise the general section and sub-sections. For example, are '1.1 Chamber wall effects - gas to wall partitioning', '2.1.2 Multiphase chemistry', '2.1.3 New particle formation' and '2.1.4 Particle wall losses' all sub-sections of "2.1 ADCHAM - AURA model setup"?***

AR: We agree that section 2 and section 3 need to be restructured. An overall methods section has been made, including subsections "Smog chamber experiments", "ADCHAM - AURA model setup", "Multiphase chemistry", "New particle formation" and "Atmospheric model runs". 'Chamber wall effects - gas to wall partitioning' and 'Particle wall losses' has become subsubsections of "ADCHAM - AURA model setup".

1.8. References

RC: ***It would be useful to refer to some studies, for example HPMTF reactions (e.g. Patrick et al, PNAS, 2019) and MSIA addition reaction (e.g. Ghahremaninezhad et al., ACP, 2019).***

AR: Does the reviewer refer to the 2020 PNAS study by Patrick Veres when mentioning 'Patrick et al, PNAS, 2019'? The study by Veres et al. (2020) in PNAS is mentioned several times in the manuscript. We have added a reference to the study by Ghahremaninezhad et al. (2019).

> The importance of MSIA oxidation by OH was discussed by Glasow and Crutzen (2004) and mentioned in several other studies (Yin et al., 1990; Lucas and Prinn, 2002; Kukui et al., 2003; Ghahremaninezhad et al., 2019).

1.9. Page 24 – Line 595

RC: ***Please add reference for the Hoppel minimum (e.g. Hoppel and Frick, 1990). Also, what aerosol size are you referring as the Hoppel minimum here?***

The suggested reference has been added to the text. We refer to the aerosol size 140 nm as the Hoppel minimum proceeding the first cloud event. This information has also been added to the text.

> A distinct Hoppel minimum formed in the main growth mode at 140 nm proceeding the first cloud period (Fig. 5c) (Hoppel and Frick, 1990), becoming more profound by each cloud passage.

1.10. Quantitative results

RC: ***It is very difficult to follow the main finding of this study without quantitative results. For example: Abstract - There are some terms such as "strong dependence", "important", "a decrease in the secondary aerosol mass yield", "a strong sink" and "less important than" without any quantitative support. Line 300: "Initially the model overestimated". Line 302: "significantly underestimated". Line 331: "minor importance". There are many other examples on different sections including "Conclusions". Even if you display results on figures/tables, it would be helpful to report them in the main body of the manuscript***

AR: We agree that the conclusions made can be difficult to follow without quantitative results to support our claims. Therefore, we have added additional information in order to clarify the results obtained in this study.

> The secondary aerosol mass yield in the AURA chamber was found to have a strong dependence on the reaction of methyl sulfinic acid (MSIA) and OH causing a 58.9 percent increase in the total PM at low relative humidity (RH), while the autoxidation of the intermediate radical CH_3SCH_2OO forming hydroperoxymethyl thioformate (HPMTF) proved important at high temperature and RH decreasing the total PM by 66.2 percent.

> The effect caused a 75.0 and 92.8 percent decrease in the secondary aerosol mass yield obtained at dry

(0-12 % RH) and humid (50-80 % RH) conditions, respectively.

Model runs reproducing the ambient marine atmosphere indicate that OH comprise a strong sink of DMS in the MBL (accounting for 32.0 percent of the total sink flux of DMS), although less important than the combined effect of halogen species Cl and BrO (accounting for 25.7 and 40.4 percent, respectively).

Utilising the MCMv3.3.1 chemistry mechanism alone caused the model to slightly overestimate the sink flux of DMS by OH addition compared to proton-transfer-reaction mass spectrometry (PTR-MS) measurement made in the chamber (R^2 = 0.92 between the measured and modelled DMS concentration in experiment DMS2). ... Analogous to the DM1.0 mechanism (Hoffmann et al., 2016) the initial addition of OH to DMS was modified by implementing the DMS-OH adduct as an intermediate product, either decomposing back to DMS (Lucas and Prinn, 2002), reacting with O2 to form a stabilised peroxyl radical (RO2) or fragment into CH_3SOH. Most important was the decomposition back to DMS (not considered in MCM) that lowered the initial rate of DMS oxidation to improve the fit between the measured and modelled DMS concentration (R^2=0.95, experiment DMS2).

At the same time, MSA PM concentrations were significantly underestimated in proportion to those measured by the HR-ToF-AMS (66.7 percent on average in experiment DMS2). ... MSA, often believed to be formed solely in the abstraction pathway (MCMv3.3.1), is produced almost exclusively from the reaction of CH_3SO_3 with HO_2. However, this reaction and the pathway leading to it did not explain the yields obtained in the chamber experiments. Therefore, an alternative pathway considering oxidation of the stable intermediate MSIA by OH was implemented to increase SA and MSA production. ... The increased production of CH_3SO_2 promotes the formation of SA and MSA in the gas-phase along with PM yields in the smog chamber experiments (58.9 percent increase in the total PM during experiment DMS2).

While SO_2 is often mentioned as the most important source of SA (Barnes et al., 2006), the slow oxidation by OH and uptake to the aqueous-phase during high RH chamber conditions suggested that its contribution was less important than other sources. SO_2 comprised 34.9 percent of the SA source flux during the first 5 hours of the humid experiment DMS6, while SO_3 formed by thermal decomposition of CH_3SO_3 made up 65.1 percent. In pristine marine atmospheric conditions (see section 4.4.4), SO_2 comprised 1.8 percent of the SA source flux in the gas-phase throughout the entire simulation.

Isomerisation of $CH_3S(OO)$ to CH_3SO_2 was added to the MCM mechanism to increase the rate of SA production and hence the onset of NPF (previously too slow compared to observations in the chamber). CH_3SO_2 is the main precursor of CH_3SO_3. Consequently, the rate of $CH_3S(OO)$ isomerisation and CH_3SO_2 production affects the formation of both SA and MSA (13.1 and 16.9 percent increase in SA and MSA PM, respectively, during experiment DMS6).

Consequently, HPMTF likely played no (or an insignificant) direct part in the particle growth but remained in the gas-phase as a sulphur reservoir reducing the overall secondary aerosol yield from DMS oxidation (66.2 percent decrease in the total PM during experiment DMS6).

With the reduction in HO_2, MSA production from the CH_3SO_3+HO_2 reaction decreased correspondingly - a change from $4.53 \cdot 10^6$ cm^{-3} s^{-1} to $9.770 \cdot 10^5$ cm^{-3} s^{-1} in the MSA source flux. The reduced conversion from CH_3SO_3 to MSA favoured the decomposition of CH_3SO_3 to SO_3 and lowered the MSA/SO_4^{2-} ratio from 4.34 to 1.72 compared to experiments performed in dry conditions (Table 4).

ADCHAM reproduced the MSA (R^2 = 0.98), SO_4^{2-} (R^2 = 0.80) and NH4(+) (R^2 = 0.79) PM from HR-ToF-AMS measurements along with DMS (R^2 = 0.93) and O_3 (R^2 = 0.96) concentrations in the AURA smog chamber at 293K and high RH conditions (Fig. 3b,c). ... The model also captured trends in the PN concentration from PSM and SMPS measurements reasonably well (R^2 = 0.36) (Fig. 3a,d).

Since the oxidation of MSIA by OH was implemented as an alternative source of CH_3SO_2 (an important precursor of SA and MSA) in the gas-phase mechanism (Kukui et al., 2003), SA and MSA production and concentrations in the gas-phase were reduced in accordance with the DMSO and MSIA dissolution in the wall aqueous film (Fig. S22-23). Thus, the presence of a water film on the chamber bag surface strongly altered the DMS oxidation product ratio and total PM yield (92.8 percent total PM decrease in experiment DMS6).

MSIA oxidation by OH was essential to capture the observed onset in NPF from PSM and SMPS measurements (Fig. 3a). The reaction increases the rate of CH_3SO_2, CH_3SO_3 and hence SA production, and caused a 15.6 percent increase in the average gas-phase SA concentration during experiment DMS6.

The strong uptake of H2O2 to the water film (94.8 percent decrease in the gas-phase concentrating during experiment DMS6) likewise increased SA production and NPF by lowering HO_2 concentrations in the gas-phase, which led to a 78.4 percent decrease in the rate of the CH_3SO_3+HO_2 reaction and promoted SO_3 production from the thermal decomposition of CH_3SO_3. Consequently, SA production and hence NPF occurred faster during high RH conditions, reaching a PN concentration of 1000 molecules cm^{-3} at a 1.7 nm cut-off diameter 15 minutes earlier in experiment DMS6 compared to experiment DMS2. The total PN concentrations remained low due to the uptake of DMSO and MSIA to the water film.

The autoxidation of the CH_3SCH_2OO radical leading to the formation of HPMTF exerted a strong influence on the PM yield in the humid chamber experiments, lowering the total PM by 66.2 percent in experiment DMS6.

The H2O2 (and hence HO_2) partitioned readily to the aqueous-phase in the humid experiments but not in the dry. The difference is evident from the MSA/SO_4^{2-} PM ratio of 4.24 and 1.72 observed in dry and humid experiments, respectively (Fig. 4b)

The water film concentration was kept low at 10^{-5} g m^{-3} in accordance with the study by Svensson et al. (1987), and had less effect on the DMS oxidation compared to the humid experiments (75.0 and 92.8 percent decrease in the total PM yield obtained in dry and humid conditions, respectively).

... the increased rate of $1.0 \cdot 10^{-10}$ cm3 $molecule^{-1}$ proposed by Kukui et al. (2003) offered a good agreement with the observed PM concentration (R^2 = 0.99) (see supplementary Fig. S33).

The effect became more profound when incorporating the production of HMPTF by autoxidation (Veres et al., 2020). In this case, the rate proposed by Berndt et al. (2019) ensured a strong decrease in SA and MSA production formed via the abstraction pathway (38 percent PM decrease during experiment DMS2).

Production rates of DMSO and MSIA increased accordingly, but gas-phase concentrations remained low as both species partitioned strongly to the water film (94.1 and 99.7 percent decrease in DMSO and MSIA gas-phase concentrations, respectively, during experiment DMS6) (Fig. S24).

The autoxidation pathway leading to HPMTF formation proved less significant at 273K due to the temperature dependence on the rate determining H-shift in the CH_3SCH_2OO radical intermediate (77.2 percent decrease in rate compared to 293K).

The rate of SO_3 formation from thermal decomposition of CH_3SO_3 decreased by 91.7 percent in accordance with the decrease in chamber temperature.

Table 4 illustrates how the MSA/SO_4^{2-} ratio remains independent to changes in temperature (1.72 and 1.96 in experiment DMS6 and DMS7, respectively).

In this context, it is important to note that the presence of sea spray aerosols and consequently halogen compounds is highly dependant on wind speed. While Cl and BrO radicals comprise the main sink flux of DMS at 8 m s^{-1} their influence decrease substantially at 2 m s^{-1} (22.1 and 13.3 percent mean DMS sink flux in lowWindAtm). This effect is apparent from the lowWindAtm sensitivity run, in which OH dominates the oxidation of DMS at 55.2 percent mean DMS sink flux (see supplementary Fig. S37).

During in-cloud periods the halogen activation terminated and both bromide and chloride stayed in the aqueous-phase. Consequently, neither BrCl nor ICl was released to the gas-phase thus decreasing the sink flux of DMS by halogen species (17.0 and 9.7 percent mean DMS sink flux by Cl and BrO during cloud periods).

Besides OH the aqueous-phase oxidation of DMS by O_3 proved the main sink of DMS at 31.3 percent during in-cloud periods.

During nighttime non-cloud periods the NO_3 radical proved a small but stand-alone sink of DMS comprising 1.8 percent of the total DMS sink flux throughout the entire simulation.

The main gas-phase products comprised HPMTF ($4.2{\cdot}10^8$ molecules cm^{-3}), DMSO ($6.4{\cdot}10^8$ molecules cm^{-3}), MSIA ($2.3{\cdot}10^7$ molecules cm^{-3}) and SO_2 ($1.1{\cdot}10^8$ molecules cm^{-3}), whereas MSA ($7.1{\cdot}10^6$ molecules cm^{-3}) and SA ($8.2{\cdot}10^5$ molecules cm^{-3}) were present only in small quantities (Fig. 5a).

SA in the gas-phase formed predominantly via the SO_3 intermediate from the thermal decomposition of CH_3SO_3 , comprising 98.2 percent of the SA source flux in AtmMain. The oxidation of SO_2 by OH proved a small but insignificant source of SA (1.8 percent).

DMSO resided in the gas-phase in between cloud periods, but partitioned strongly to the aqueous-phase when clouds were present (83.2 percent decrease in gas-phase DMSO going into the first cloud-period in AtmMain).

The uptake of DMSO and subsequent oxidation to MSIA and thus MSA increased the MSA production during cloud periods and comprised 18.1 percent of the mean MSA source flux in AtmMain (see Figure S38).

Unlike the slow gas-phase oxidation, the implemented rate ensured a strong sink flux of HPMTF in the aqueous-phase ($-1.3{\cdot}10^2$ molecules cm^{-3} s^{-1} and $-8.0{\cdot}10^3$ molecules cm^{-3} s^{-1} mean HPMTF sink flux in the gas-phase and aqueous-phase, respectively).

The woCloudAtm sensitivity run demonstrated the importance of cloud chemistry in the ambient atmosphere. Semi-soluble products HPMTF and SO_2 did not partition to the deliquesced particles, and thus their conversion yields increased by a factor of 4.2 and 4.5, respectively, compared to AtmMain, as both species accumulated in the gas-phase (Table 4). SO_4^{2-} PM production decreased by 78.5 percent in consequence of the reduction in aqueous SO_2 . Unlike AtmMain, SA proved an important source of secondary aerosol mass. The increase in the SO_2 gas-phase concentration promoted SA production (40.6 percent SO_2-derived SA source flux in woCloudAtm) and thus SA derived SO_4^{2-} PM.

MSA formation remained indifferent from AtmMain and dominated in the deliquesced aerosol particles. Consequently, the MSA to SO_4^{2-} PM ratio proved higher in woCloudAtm than AtmMain (3.97 and 1.63, respectively).

The lack of reactive halogen species lowered the sink flux of DMS by 35.2 percent, causing it to accumulate in the gas-phase throughout the simulation (see supplementary Fig. S36). The total secondary aerosol yield decreased from 1.43 μg cm^{-3} to 0.29 μg cm^{-3} in accordance with the decrease in DMS decay (Table 4).

MSA PM production proved strongly reduced in woAqAtm (0.07 μg cm^{-3} at the end of the simulation) relative to AtmMain (0.85 μg cm^{-3}). ... The decrease in MSA production is evident from the decrease in the MSA/SO_4^{2-} PM ratio (1.63 and 0.40 in AtmMain and woAqAtm, respectively) (Table 4).

Analogous to woCloudAtm the SO_4^{2-} PM production was strongly reduced (66.4 percent compared to AtmMain) as SO_2 did not transform in the particle-phase.

The day and night-time DMS sink flux increased by 21.8 percent in accordance with with increased O_3 and NO2 pollution from the increase in oxidants OH, NO_3, Cl and Cl_2 (see suplementary Fig. S34). The effect is evident from the increase in the total secondary aerosol mass yield (1.43 and 1.60 μg cm^{-3} in AtmMain and PolAtm, respectively) (Table 4).

Elevated O_3 concentrations promoted SO_2 production via the CH3SO and HOOCH2SO intermediates and increased the SO_4^{2-} PM yield by 62.3 percent compared with AtmMain.

1.11. Abstract

RC: ***Define abbreviations such as MSA.***

AR: This was changed in the revised manuscript.

The observations and modelling strongly support that a liquid water film existed on the Teflon surface of the chamber bag, which enhanced the wall loss of water soluble intermediates and oxidants dimethyl sulfoxide (DMSO), MSIA, HPMTF, SO_2, methanesulfonic acid (MSA), SA and H2O2

1.12. Page 2 – Line 40

RC: ***Add space HOOCH2SCHO) - (Wu et al.,***

AR: This was changed in the revised manuscript.

1.13. Page 1 – Line 5

RC: ***Move "both" - DMS oxidation mechanism, capable of "both" reproducing smog chamber and atmospheric relevant conditions.***

AR: This was changed in the revised manuscript.

1.14. Page 2 – Line 37

RC: ***details. "mechanism remains" or "mechanisms remain" – I think the second one here is correct.***

AR: This was changed in the revised manuscript.

1.15. Page 2 – Line 50

RC: ***“MSA formation in the gas-phase does, however, remain uncertain, and early studies have suggested alternative production pathways via the MSIA intermediate.”***

AR: We have restructured the sentence.

> However, MSA formation in the gas-phase remains uncertain, and earlier studies have suggested an alternative pathway via the MSIA intermediate.

1.16. Page 3 – Line 66

RC: ***mean***

AR: This was changed in the revised manuscript.

1.17. Page 3 – Line 67:

RC: ***compares***

AR: This was changed in the revised manuscript.

1.18. Page 3 – Line 72:

RC: ***instrumentations***

AR: This was changed in the revised manuscript.

2. Reviewer #2

2.1. Page 3 line 57

RC: ***What is meaning of "model predictions under said conditions"? Do authors imply "acid conditions" or "side conditions"? Word "said conditions" appeared in numerous places. Please change this word to the clear word that can be understandable by readers. Please also check spellings and typos.***

AR: In the sentence : "Few have studied the gas and multiphase DMS chemistry in controlled smog chamber experiments, and none have tested model predictions under said conditions", 'said' (used to refer to something already mentioned or named) refers to the controlled conditions of the smog chamber experiment. The word is used as not to repeat "controlled smog chamber experiments" twice. The sentence has been restructured.

> Few have studied the gas and multiphase DMS chemistry in controlled smog chamber experiments, and none have tested model predictions on the formation, growth and chemical composition of the aerosol particles being produced.

2.2. Page 3 Line 80-85

RC: ***The authors state there is potential particles and organic contaminates from room air due to the inflow of air to the chamber during sampling. Why did not the authors use the similar setup with the humid experiments that directly use clean air added to the chamber to makeup the shrunken volume for the dry exp? The room air which contained a significant concentration of ammonia may influence an inorganic ion balance, aerosol hygroscopicity and sulfuric acid formation. In addition, some hydrocarbons can modify the gas chemistry.***

AR: The inflow of 2 lpm during humid experiments served solely to keep the RH in the chamber as constant as possible and counteract the loss of RH due to diffusion of water vapour out of the bag. Therefore, no extra inflow was used during dry experiments. The added 2 lpm during humid experiments cannot make up for the 6.9 lpm (experiment DMS6) taken out for sampling and thus affects only slightly the shrinkage of the chamber bag. The experiments presented here were meant to be in batch mode. The fact that outside air must have entered the chamber during the experiments was discovered after the experiments had been performed. At the rate of instrument sampling used in the setup, the chamber bag should have been completely empty before the end of the experiment. From observations we know that this is not the case, and therefore we assume that air from outside the chamber must have entered during the experiments. A detailed description on the gradual decrease in chamber volume is given by Rosati et al. (2021a).

Ammonia in particular may very likely have influenced the results obtained in the chamber. Especially in terms of new particle formation and particle growth. However, trace amounts of ammonia are always present in smog chamber experiments, even under extremely clean conditions as in the CLOUD chamber (Kirkby et al., 2011).

Does the reviewer by 'hydrocarbons' refer to Criegee intermediates? In that case, these should be of minor concern since we study OH reactions and not ozonolysis.

> For the humid experiments, an additional inflow of humidified particle free air with a rate of 2.0 L min^{-1} was used to keep the RH stable. This resulted in additional dilution of the chamber.

2.3. Figure 1

RC: ***1A: please add explanation for "woLWC". 1B: Is the OH concentration set to a constant number during the entire simulation period? If yes, it maybe not necessary to plot Figure 1B. Instead, explain this in the main text. 1C: cannot understand this the drawing. Which one is the Teflon film? What is the meaning of blue colored things? Is it water or moisture? Why RH is only up to 70%? Was there a horizontal gradient in RH and Temperature inside the chamber?***

AR: [1A] We agree that the term "woLWC" (without liquid water content) should have been explained in the figure caption. This has been modified in the revised manuscript. [1B] The time dependant OH concentration is estimated based on the photolysis of H_2O_2, and reaction of OH with reaction intermediates in the DMS oxidation mechanism. [1C] Figure C was meant to illustrate the effect of outside cooling on the adsorption of water onto the Teflon film, depicting different conditions in the AURA chamber. One at 5% RH and 293K, one at 70% RH and 293K and one at 70% RH and 273K (70% RH was the RH used in the experiment). At low RH and high temperature, little water would adsorb to the Teflon film, while more water would adsorb at high RH and low temperature. The Figure has been modified to clear up these misconceptions.

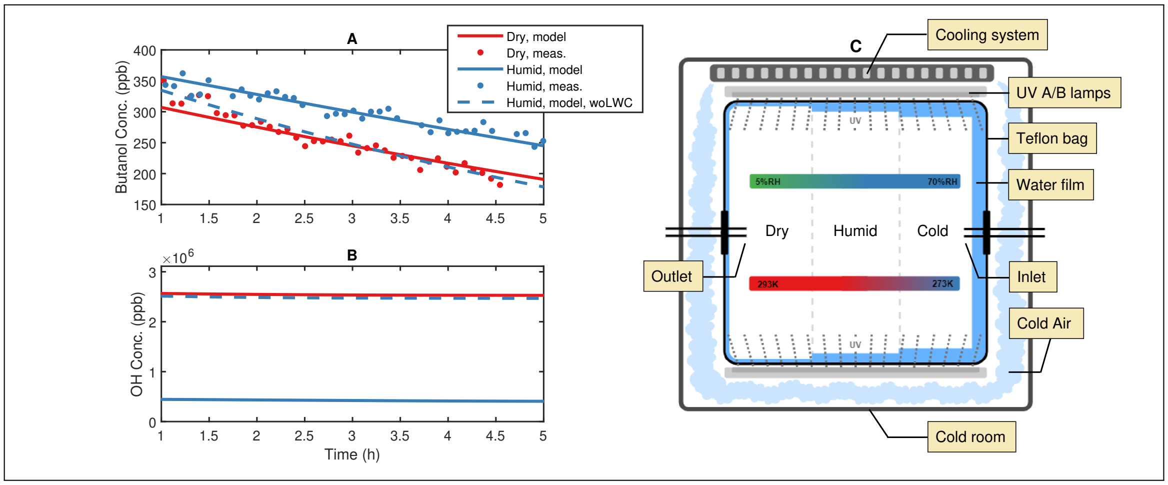

Illustration of the water film effect in the AURA chamber. Panel **A** depicts the PTR-MS butanol decay from experiments BUT1 (red) and BUT2 (blue) and **B** the OH concentration at varying RH with and without the influence of a liquid water film (woLWC : without liquid water content). The water content changed in accordance with varying temperature and RH, panel **C**. Outside cooling of the chamber may affect the water adsorption on the Teflon surface.

2.4. Table 2

RC: ***Please add necessary footnotes for the abbreviations used in the Table. It is difficult to understand the meaning of the variables because acronyms appeared later in the manuscript.***

AR: Footnotes has been added to explain the abbreviations for u^*, k_e and LWC_{wall}.

2.5. Page 5, line 109

RC: ***Butanol is hydrophilic. Is there any gaseous butanol loss to the water layer on the wall during the butanol experiments?***

AR: Based on this question we performed several sensitivity runs including the uptake of butanol to the water film in experiment But1-3 incorporating an accommodation coefficient for n-butanol based on the parameterization by Zhang et al. (2015) (2E-8, see equation 23) and a temperature dependant Henry's law solubility of 120.0*EXP(7500.0*(1.0/T-1/298.0)) (Sander, 2015). However, since butanol does not react with any of the oxidant species present in the chamber (OH, O_3, etc.) in the aqueous-phase, the uptake to the water film is limited by the equilibrium between the gas-phase and aqueous-phase and the low mass accommodation coefficient to the walls. Consequently, little butanol is lost to the chamber walls.

2.6. Page 6, line 120

RC: ***Is the unit for the water concentration on the wall correct? Should it be g per surface area of the wall?***

AR: The unit used to define the liquid water content on the wall (cw_{wall}, see Page 8, line 194-201) is reported in g m^{-3} (kg cm^{-3} in calculations) since using that unit of cw_{wall} allows one to directly obtain a dimensionless Henry's law solubility (see Jacobson (2005), Fundamentals of Atmospheric Modelling, 2ed eq. 17.99). A similar approach is used in the study by Sander (2015).

$$\begin{array}{llllllllll} H_{prim} & = & cw_{wall} & \cdot & R_{prim} & \cdot & Temperature & \cdot & H_{molec} \\ [\ \ ] & = & [kg/cm^3] & \cdot & [cm^3 \cdot atm/(mol \cdot K)] & \cdot & [K] & \cdot & [mol/(kg \cdot atm)] \end{array}$$

2.7. Page 6, line 134

RC: ***Please check if the unit for the dissolved ammonium sulfate on wall is correct. The unit of salt on the wall water could be a mass per liquid volume or the mass per air volume?***

AR: All concentrations, both in the gas-phase and aqueous-phase are given in molecules/(cm^3 air) (see Page 8, line 194-197). This is why the dimensionless Henry's law solubility is used (more information can be found in Jacobson (2005), Fundamentals of Atmospheric Modelling, 2ed chapter 17). We have elaborated this on page 6, line 134.

> To be able to capture the observed secondary ammonium mass formation and the new particle formation (Sect. 2.1.3) in all experiments, we assumed an initial pool of 100 μg m^{-3} (mass per air volume) dissolved ammonium sulfate on the chamber walls.

2.8. Page 6, line 135

RC: ***Although outdoor ammonia concentration is usually as low as 1 ppb, the indoor ammonia concentration can usually be much higher (Ampollini, Laura, et al 2019). Is the ammonia of 2 ppb from indoor environment used here reasonable? Is there any measurements of gaseous ammonia concentrations to support this value?***

AR: We agree that ammonia concentration may certainly have been higher than the 2 ppb implemented in the model setup. This estimate was based on measurements made at Tange (56.352222°N, 9.5875°W) located approximately 50 km from Aarhus (data available at http://ebas.nilu.no/). Concentrations in the range reported by Ampollini et al. (2019) (measured in an ordinary test house) would however have been unlikely to encounter in the laboratory setting surrounding the AURA smog chamber. Ammonia measurements in a nearby analytical laboratory of Anders Feilberg have previously shown concentrations of ammonia in the range of 1-10 ppb.

2.9. Page 7, line 167

RC: ***Add "," after "NO2".***

AR: This was changed in the revised manuscript.

2.10. Page 7, line 173

RC: ***Is the unit of V wrong?***

AR: Yes. This has been corrected.

> ... for a fully inflated chamber (V = 5 m^3).

2.11. Page 7, line 175-180

RC: ***Why is the concentration of ozone in some experiments (i.e., DMS1) low as 1 ppb as seen in Table 1? If the ozone concentration is lower than 1 ppb, how can the authors say that the secondary aerosol formation is most sensitive to ozone for all experiments?***

AR: The ozone values reported in Table 1 refer to the initial ozone concentration used as input in the ADCHAM model. However, as can be seen in the supplementary figures S26, S27 and S28 depicting experiments DMS1, DMS2 and DMS3 with low initial ozone concentrations, the concentration of ozone increases throughout the experiment. This relates to the NO_x contamination listed in Table 1 and described on Page 14 line 374-376, which facilitates the production of ozone. The ADCHAM model indicated that the increase in ozone affected the secondary aerosol formation (see page 14, line 353-355 and line 376-379 and page 18, line 432-434).

2.12. Page 8, line 194

RC: ***The meaning of R(g) and R(aq) is unclear. Are they represent reactions? What is their unit ?***

AR: R(g) and R(aq) denote reactions R occurring either in the gas-phase (g) or aqueous phase (aq). As the reaction R is different for each compound c in the differential equation d[c(g)] and d[c(aq)] (see Page 8, Equation 2 and 3), and incorporates multiple reactions for certain compounds (e.g. DMS undergoing both an OH-addition and OH-abstraction in the gas-phase), the term is simplified by using the notation R. We have elaborated this in greater detail in the revised manuscript.

> Eq. 2 and 3 takes into account the mass transfer between the gas-phase and aqueous phase for all compounds c_i and all relevant reactions (R_1 to R_n) in the gas (R(g)) and aqueous phase (R(aq)) ...
>
> $$d[c_i(g)]/dt = -k_{aq,i}[c_i(g)] + \frac{k_{aq,i}}{H_i^*}[c_i(aq)] + \sum R_{1,i}(g) + R_{2,i}(g) + ... + R_{n,i}(g)$$
>
> $$d[c_i(aq)]/dt = k_{aq,i}[c_i(g)] - \frac{k_{aq,i}}{H_i^*}[c_i(aq)] + \sum R_{1,i}(aq) + R_{2,i}(aq) + ... + R_{n,i}(aq)$$

2.13. Page 8 line 199

RC: ***"denote" -> "denotes". Remove ";" before "K-1".***

AR: This was changed in the revised manuscript.

2.14. Table S2

RC: ***The scientific notation in computer code (i.e., Fortran) usually uses "D" to signify double precision numbers but it is uncommon to be used in scientific documentation such as paper. It would be better to change to "E" instead of "D".***

AR: We agree that the notation should be changed to "E".

2.15. Page 9, line 213

RC: ***Why does the chemical mechanisms also include isoprene chemistry mechanisms? Is there any precursors contain isoprene species in the kinetic model?***

AR: As stated on Page 9, line 212, the majority of the reactions are only relevant for the atmospheric model simulations. This includes the MCMv3.3.1 isoprene chemistry scheme. Isoprene does not affect the DMS chemistry directly. It does however comprise a sink of oxidants in the marine boundary layer, which in turn affects the rate by which DMS is oxidised.

2.16. Page 10, line 260

RC: ***"represent" -> "represents". Line 262, "represent" -> "represents".***

AR: This was changed in the revised manuscript.

2.17. Page 11, line 283

RC: ***What is the protocol to setup the cloud conditions? Are they randomly setup?***

AR: Cloud periods are spaced 12 hours apart occurring at midday and midnight throughout the simulation. The setup is influenced by the approach of Hoffmann et al. (2016) and Braeuer et al. (2013).

> Starting at midnight the simulation included eight in-cloud periods, four during midday and four at midnight.

2.18. Section 3

RC: ***The place of this section is odd. The authors mainly discuss the simulation of ambient scenarios. However, the figure appeared in Page 22. It would be better to move the explanation to the section for atmospheric implication.***

AR: Section 3 was meant to introduce the setup of the atmospheric model runs, from which the results are presented and discussed in section 4.4.4. This was done to separate the methods concerning the smog chamber experiments (section 2) and the atmospheric simulation (section 3). We appreciate the suggestion, but would prefer to keep methods as separate sections. This should make it easier to navigate the manuscript.

2.19. Page 11, line 300

RC: ***It is not clear to use the word "Initially". When is the initial time? The early stage of experiment or the model development stage?***

AR: The sentence has been modified to specify the intended meaning of "Initially". Here we refer to a sensitivity run in which only the MCM3.3.1 chemistry was implemented in the model.

> Utilising the MCMv3.3.1 chemistry mechanism alone caused the model to overestimate the sink flux of DMS by OH addition ...

2.20. Page 12, line 303

RC: ***What is the meaning of "slow down" and "promoting" here? Does it imply the modification of mechanisms or changing experiment setup?***

This statement relates to the previous section (Page 11, line 300 to page 12, line 303), in which the use of the MCMv3.3.1 mechanism alone in the model overestimated the rate of DMS oxidation and at the same time underestimated the production of MSA. The terms "slow down" and "promoting" therefore refer to the changes made in the mechanism to explain the results obtained in the experiment. The sentence has been modified to make this clear.

> Therefore, efforts were made to reduce the rate of DMS oxidation in the addition pathway while promoting MSA production, by revising the MCMv3.3.1 mechanism.

2.21. Page 13, line 342

RC: ***"previously to slow" -> "previously too slow".***

AR: This was changed in the revised manuscript.

2.22. Page 12, section 4.1

RC: ***When authors discussed about measurements (observations), it is unclear which measurements were used and which model run it refers to. For example, Page 13, line 338: where is data for "observed and modelled SA and MSA PM"?. Do the authors perform the sensitivity test for the thermal decay rates of CH_3SO_3?***

AR: The specific example mentioned (Page 13, line 338) falls under section 4.1 (Gas-phase DMS oxidation), which involves the development of the DMS oxidation mechanism in the gas-phase. The changes made in the mechanism are not related to any specific experiment, but adjusted in order to reproduce all experiments (including ones at varying DMS concentration, temperature and relative humidity). The phrase, "rates close to the value given in MCM provide the best match between the observed and modelled SA and MSA PM." was meant to indicate that the changes made in the mechanism improved the general fit between modelled and measured results in all experiments. The same goes for similar phrasing in section 4.1 (Gas-phase DMS oxidation) and section 4.2 (Aqueous-phase DMS oxidation). In accordance with the review comment 1.10 we have added quantitative results referring to specific experiments in section 4.1.

Sensitivity tests were performed for the thermal decay of CH_3SO_3, including the rate proposed by Cao et al. (2013) mentioned on Page 13, line 336-337. However, since most studies beside Cao et al. (including Hoffmann et al. (2016) and rates presented in MCMv3.3.1) agree that the rate of thermal decomposition of CH_3SO_3 lies at approx 0.1 s^{-1} (293K), we did not present these sensitivity tests in the paper.

2.23. Section 4.1

RC: ***What is the simulated mass fraction of MSA from different pathways? Which pathway is more dominant to form MSA and SA?***

In the chamber experiments, MSA was almost exclusively produced from the CH_3SO_3+HO_2 reaction (see Page 12, line 308-309), due to the high HO_2 concentrations in the chamber. SA was found to be most sensitive to the thermal decomposition of CH_3SO_3, producing SO_3 and thus SA (see Page 13, line 229-335). In ambient conditions (see section 4.4.4 on Atmospheric implication), the aqueous-phase production of SA and MSA is significantly larger than the gas-phase production. Figure S34E, S35E, S36E, S37E and S38B illustrates the source flux of MSA from various reaction pathways under various atmospheric conditions. Two important sources of MSA in those cases includes the oxidation of MSIA by ozone (dominant in the deliquesced particles in between cloud periods) and from the CH_3SO_3 ion (dominant in the cloud droplets during cloud periods). SA in the gas-phase formed predominantly via thermal decomposition of CH_3SO_3, while SO_2 proved a significant source of SO_4^{2-} in the cloud droplet aqueous-phase (see Page 23, line 538-544). In accordance with the review comment 1.10 we have added quantitative results to illustrate the source flux of SA and MSA in the manuscript text.

2.24. Page 14, line 364

RC: ***"HPMTF may oxidize in cloud droplets" -> "HPMTF may be oxidized in cloud droplets".***

AR: This was changed in the revised manuscript.

2.25. Page 14, line 366

RC: ***Does the model include partitioning of OH radicals between the gas phase and the aqueous phase? The partitioning of OH radicals is not discussed in the previous sections.***

AR: The model includes the partitioning of 50 water soluble species between the gas-phase and aqueous-phase (see Table S2 in supplementary information). This includes the OH radical, and other reactive species such as O_3, HO_2 and H_2O_2 (see Page 14, line 351-352).

2.26. Page 14, line 378-379

RC: ***How can NO_x concentrations be estimated by using ozone formation? Where was this resulted estimation shown in the manuscript? As shown in Table 1, NO_x is lower than 2 ppb. How much uncertainty is included in NO_x?***

AR: On Page 14, line 374-376, we describe how NO_2 photodissociates to form NO and ground state atomic oxygen $O(^3P)$. $O(^3P)$ reacts rapidly with O_2 to yield ozone. NO_x monitors were used throughout the experiments, but since NO_x remained close to the detection limit these measurements were classified as uncertain. Therefore, the NO_x concentration implemented in the model was based on the ozone production in the chamber. Hence, the NO_x concentration was adjusted to match the increase in ozone observed throughout the experiments (see e.g. S26, S27 and S28 in the supplementary information). For an in-depth explanation on the NOx contamination we refer the reviewer to Rosati et al. (2021b).

2.27. Section 4.3

RC: ***This section is improper to be discussed in the results section. The chamber contaminations should be discussed in the experimental section.***

AR: We have moved section 4.3 to the experimental section.

2.28. Page 16, line 407

RC: ***Does it mean the green color organic showed in Figure 3b is fully by organic contamination?***

AR: The AMS is susceptible to a multitude of potential uncertainties and biases, of which some are difficult if not impossible to correct for completely. This is especially true for quantification of aerosols sampled from simulation chambers (Drewnick et al., 2015). Improving the understanding of these uncertainties and biases is an ongoing process in the AMS community. The organic fraction (seen in Figure 3b) is especially susceptible to biases due to complex fragmentation during ionization, thus needing calculation of organic mass using a fragmentation table. This includes scalars for estimating intensities of certain fragments of organic compounds that can constitute a significant fraction of the organic mass in certain cases. These fragments are O^+, OH^+, H_2O^+ and CO^+, that cannot be measured due to interferences. These are estimated based on CO_2^+, which in turn has to be corrected for atmospheric CO_2 and is susceptible to memory effects Pieber et al. (2016). The vaporization process of the AMS is also susceptible to memory effects (Drewnick et al., 2009, 2015; Pieber et al., 2016). These small biases are usually an insignificant contribution to the total signal and thus accepted as part of the general uncertainty of AMS measurements. However, they appear very significant in this study due to the very low aerosol mass in most of the DMS experiments. As explained in Rosati et al. (2021b) we cannot determine whether the contamination was from the chamber or from deposits (memory effects) in the AMS instrument.

> The effect could not be replicated by considering condensation of DMSO and MSIA onto preexisting particles, and may originate from organic wall contaminants, inflow of air from outside the chamber caused by the continuous instrument or from deposits and related memory effects in the AMS instrument as explained in Rosati et al. (2021b).

2.29. Page 21, line 507

RC: ***"when the UV light intensity" is high?***

AR: This was changed in the revised manuscript.

2.30. Page 21, line 508

RC: ***What is the percent of DMS oxidation through OH and O_3 pathways for this simulation?***

AR: The percent of DMS oxidation through OH (both OH addition and OH initiated H abstraction) is 32 percent (see Page 22, line 526). The percent of DMS oxidation through ozone in the aqueous phase is 4 percent. The information on the sink flux of DMS by ozone has been added to the manuscript.

> Consequently, the nighttime in-cloud oxidation of DMS was solely due to aqueous-phase O_3 (4.0 percent of the total sink flux over the entire simulation).

References

Ampollini, L., Katz, E., Bourne, S., Tian, Y., Novoselac, A., Goldstein, A., Lucic, G., Waring, M., and DeCarlo, P.: Observations and Contributions of Real-time Indoor Ammonia Concentrations During HOMEChem, Environmental Science & Technology, 53, , 2019.

Braeuer, P., Tilgner, A., Wolke, R., and Herrmann, H.: Mechanism development and modelling of tropospheric multiphase halogen chemistry: The CAPRAM Halogen Module 2.0 (HM2), JOURNAL OF ATMOSPHERIC CHEMISTRY, 70, 19–52, , 2013.

Cao, J., Wang, W.-L., Gao, L.-J., and Fu, F.: Mechanism and Thermodynamic Properties of CH3SO3 Decomposition, Acta Physico-Chimica Sinica, 29, , 2013.

Drewnick, F., Hings, S., Alfarra, M., Prevot, A., and S, B.: Aerosol Quantification with the Aerodyne Aerosol Mass Spectrometer: Detection Limits and Ionizer Background Effects, Atmospheric Measurement Techniques, 1, , 2009.

Drewnick, F., Diesch, J.-M., Faber, P., and Borrmann, S.: Aerosol mass spectrometry: Particle-vaporizer interactions and their consequences for the measurements, Atmospheric Measurement Techniques Discussions, 8, 3525–3570, , 2015.

Ghahremaninezhad, R., Gong, W., Galí Tàpias, M., Norman, A.-L., Beagley, S., Akingunola, A., Zheng, Q., Lupu, A., Lizotte, M., Levasseur, M., and Leaitch, W.: Dimethyl sulfide and its role in aerosol formation and growth in the Arctic summer – a modelling study, Atmospheric Chemistry and Physics, 19, 14 455–14 476, , 2019.

Hoffmann, E. H., Tilgner, A., Schrödner, R., Bräuer, P., Wolke, R., and Herrmann, H.: An advanced modeling study on the impacts and atmospheric implications of multiphase dimethyl sulfide chemistry, Proceedings of the National Academy of Sciences, 113, 11 776–11 781, , URL `https://www.pnas.org/content/113/42/11776`, 2016.

Jacobson, M. Z.: Fundamentals of Atmospheric Modelling (2nd edition), Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA, 2005.

Kirkby, J., Curtius, J., Almeida, J., Dunne, E., Duplissy, J., Ehrhart, S., Franchin, A., Gagné, S., Ickes, L., Kürten, A., Kupc, A., Metzger, A., Riccobono, F., Rondo, L., Schobesberger, S., Tsagkogeorgas, G., Wimmer, D., Amorim, A., Bianchi, F., and Kulmala, M.: Role of sulphuric acid, ammonia and galactic cosmic rays in atmospheric aerosol nucleation, Nature, 476, 429–33, , 2011.

Pieber, S., Haddad, I., Slowik, J., Jayne, J., Platt, S., Bozzetti, C., Daellenbach, K., Fröhlich, R., Vlachou, A., Klein, F., Dommen, J., Miljevic, B., Jiménez, J., Worsnop, D., Baltensperger, U., and Prevot, A.: Inorganic Salt Interference on CO2+ in Aerodyne AMS and ACSM Organic Aerosol Composition Studies, Environmental Science & Technology, 50, , 2016.

Rosati, B., Christiansen, S., Dinesen, A., Roldin, P., Massling, A., Nilsson, E. D., and Bilde, M.: The impact of atmospheric oxidation on hygroscopicity and cloud droplet activation of inorganic sea spray aerosol, accepted, Scientific Reports, 2021a.

Rosati, B., Christiansen, S., Wollesen de Jonge, R., Roldin, P., Jensen, M. M., Wang, K., Moosakutty, S. P., Thomsen, D., Salomonsen, C., Hyttinen, N., Elm, J., Feilberg, A., Glasius, M., and Bilde, M.: New Particle Formation and Growth from Dimethyl Sulfide Oxidation by Hydroxyl Radicals, ACS Earth and Space Chemistry, 5, 801–811, , URL `https://doi.org/10.1021/acsearthspacechem.0c00333`, 2021b.

Sander, R.: Compilation of Henry's law constants (Version 4.0) for water as solvent, Atmospheric Chemistry and Physics, 15, 4399–4981, , 2015.

Seinfeld, J. H. and Pandis, S. N.: Atmospheric Chemistry and Physics: From Air Pollution to Climate Change, John Wiley & Sons, Hoboken, NJ, 3rd edn., 2016.

Veres, P. R., Neuman, J. A., Bertram, T. H., Assaf, E., Wolfe, G. M., Williamson, C. J., Weinzierl, B., Tilmes, S., Thompson, C. R., Thames, A. B., Schroder, J. C., Saiz-Lopez, A., Rollins, A. W., Roberts, J. M., Price, D., Peischl, J., Nault, B. A., Møller, K. H., Miller, D. O., Meinardi, S., Li, Q., Lamarque, J.-F., Kupc, A., Kjaergaard, H. G., Kinnison, D., Jimenez, J. L., Jernigan, C. M., Hornbrook, R. S., Hills, A., Dollner, M., Day, D. A., Cuevas, C. A., Campuzano-Jost, P., Burkholder, J., Bui, T. P., Brune, W. H., Brown, S. S., Brock, C. A., Bourgeois, I., Blake, D. R., Apel, E. C., and Ryerson, T. B.: Global airborne sampling reveals a previously unobserved dimethyl sulfide oxidation mechanism in the marine atmosphere, Proceedings of the National Academy of Sciences, 117, 4505–4510, , URL `https://www.pnas.org/content/117/9/4505`, 2020.

Zhang, X., Schwantes, R., McVay, R., Hakulinen, H., Coggon, M., Flagan, R., and Seinfeld, J.: Vapor wall deposition in Teflon chambers, Atmospheric Chemistry and Physics, 15, 4197–4214, , 2015.