Supplementary Information *for*

Formation of Secondary Organic Aerosol from the Heterogeneous Oxidation by Ozone of a Phytoplankton Culture

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Table of Contents:

Page 1

- 1. AMS Measurements**
 - a. Figure S1:** mass of organic, sulphate and nitrate from the AMS
- 2. AMS H:C and O:C calculations.**
 - a.** Explanation of calculation

Page 2-3

- b. Figure S2:** Mass spectrum of the model SSML, L1 growth media, and difference between the two from the AMS

Page 4

- 3. PTR Measurements**
 - a. Table S1:** Constants used for mixing ratio calculations in Equation 1.

Page 5

b. PTR-MS mixing ratios calculations

- i. **Equation S1:** Equation to calculate gas mixing ratios of measured species.

Page 6

c. PTR mass scan experiments

- i. **Figure S3:** Difference scanning mass spectrum between model SSML and L1 growth media in air.

Page 7

- i. **Figure S4:** Difference scanning mass spectrum between model SSML and L1 growth media in ozone.

Page 8

4. References

1. AMS Measurements.

Figure S1: Average mass signals of sulphate, nitrate and organics used to calculate the ratios in Figure 7. L1 growth media signal is represented by the dashed lines. Y-axis is in log scale, with a cut axis.

2. AMS H:C and O:C calculations.

The H:C and O:C ratio for the organic material in the AMS from the model SSML was calculated by detangling the organic signal from the contamination from the ammonium nitrate solution, as well as any organics formed from the oxidation of the L1 growth media with ozone.

To do this, the average high-resolution mass spectra (MS) was calculated for the organic spike from each culture. The first 5 points corresponding to the first 2.5 minutes of the experiment were averaged. The spike can be seen in that time frame in Figure 7. This average MS was calculated for the three model SSML samples, as well as the corresponding L1 growth media.

The difference in organic peaks between the model SSML MS and the L1 growth media mass spectra was calculated.

The difference spectra have similar ratios to that of the model SSML, as shown in Figure S2, which suggests that the O:C and H:C calculations are more reflective of the MS of the model SSML than L1 growth media.

The Improved-Ambient formula was used to calculate the H:C and O:C from the difference spectra.¹ The Improved-Ambient calculation of the total organics (without subtraction of the L1 growth media) is 1.690 ± 0.008 and 0.62 ± 0.03 .

Figure S2: The organic mass spectrum from the AMS for a model SSML (top), L1 growth media (middle) and the difference between the two (bottom) when exposed to ozone.

m/z	Assumed compound	S_i/S_{21}				α_i	Mixing ratio (ppb)				Reference for α_i
		<i>model SSML, air</i>	<i>model SSML, O₃</i>	<i>L1 Growth Media, air</i>	<i>L1 Growth Media, O₃</i>		<i>model SSML, air</i>	<i>model SSML, O₃</i>	<i>L1 Growth Media, air</i>	<i>L1 Growth Media, O₃</i>	
63	DMS	0.0140	0.0141	0.00852	0.0162	5.7	4.9	4.9	3.0	5.7	²
69	Isoprene	0.0146	0.0515	0.0117	0.0408	4.0	7.3	26	5.9	20	³
45	Acetaldehyde	0.318	0.653	0.105	0.765	8.4	76	1.6 x 10 ²	25	1.8 x 10 ²	³
59	Propanal/Acetone	0.124	1.45	0.0824	0.649	12.0	21	2.4 x 10 ²	14	1.1 x 10 ²	³

Table S1: The PTR signals (S_i) for a few compounds of interest, as well as the other constants necessary to calculate an estimated mixing ratio using Equation S1. S_{21} is the signal of the reagent ion (H_3O^{18+}) at m/z 21. These data were collected in full scan mode for one culture, which yields data not as precise as in selected-ion mode as presented in the main paper.

3. PTR-MS Mixing Ratios

The PTR-MS was not calibrated for these experiments, so we used previously published calibration factors on our instrument. Table S1 presents the species of interest, their normalized signals, the calibration factors (α_i), and calculated mixing ratios. The mixing ratios were calculated according to equation S1.

$$\text{Volume Mixing Ratio (ppb)} = \alpha_i^{-1} * \left(\frac{s_i}{s_{21}} \right) \left(\frac{10^6}{500} \right) \quad (1)$$

We only have unit mass resolution, so there is an assumption that the compound detected is the stated molecule at that mass to charge ratio. The species included in the table are those for which we have calibrations. Isoprene and DMS are included because they can be important as precursors for secondary aerosol formation.^{4,5}

4. PTR Scan Mass Spectra

We present the full mass range (using scanning mode) measured with the PTR-MS under the different experimental conditions for one culture only. Note that these experiments were conducted with mixing ratios of O₃ of 3.8 ppm, which is different than all the other experiments presented in this paper.

Figure S3: PTR-MS difference spectrum for the model SSML from the L1 growth media under exposure to air. All signals are normalized to the reagent ion (H_3O^{18+}) at m/z 21. These signals represent the average signal for the first 10 minutes of exposure.

Figure S4: PTR-MS difference spectrum for the model SSML from the L1 growth media under exposure to 3.8 ppm of ozone. All signals are normalized to the reagent ion (H_3O^{18+}) at m/z 21. These signals represent the average signal for the first 10 minutes of exposure.

5. References

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