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Secondary organic aerosol formation from camphene oxidation: measurements and modeling

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Table S1. Weighted fractions of total peroxy radical bimolecular reactions of each type, calculated based on SAPRC simulations.

Expt.	$[HC]_0$ (ppb)	$[HC]_0/[NO_x]_0$ (ppbv/ppbv)	SOA Yield	Total RO_2[a] (ppb)	Fraction of total RO_2 Reaction			
					NO	HO_2	NO_3	RO_2s[b]
WO1	7	7	0.15	15	0.06	0.94	0.00	0.00
WO2	9	9	0.08	18	0.04	0.96	0.00	0.00
WO3	28	28	0.27	54	0.04	0.95	0.00	0.00
WO4	57	57	0.28	99	0.05	0.92	0.00	0.03
WO5	120	120	0.27	141	0.05	0.79	0.00	0.16
WO6	223	223	0.19	165	0.04	0.66	0.00	0.30
W1	7	0.08	0.36	37	0.96	0.04	0.00	0.00
W2	25	0.18	0.33	114	0.98	0.02	0.00	0.00
W3	32	0.51	0.64	139	0.90	0.10	0.00	0.00
W4	43	5.91	0.41	110	0.49	0.50	0.00	0.01
W5	60	0.64	0.60	249	0.91	0.09	0.00	0.00
W6	131	1.33	0.59	445	0.84	0.14	0.00	0.01
W7	172	2.88	0.52	455	0.74	0.21	0.00	0.04

[a] Total RO_2 is calculated as the summation of RO_2 that undergo bimolecular reactions.

[b] "RO_2s" refers to the sum of RO_2 reacting with RO_2 and with RCO_3.

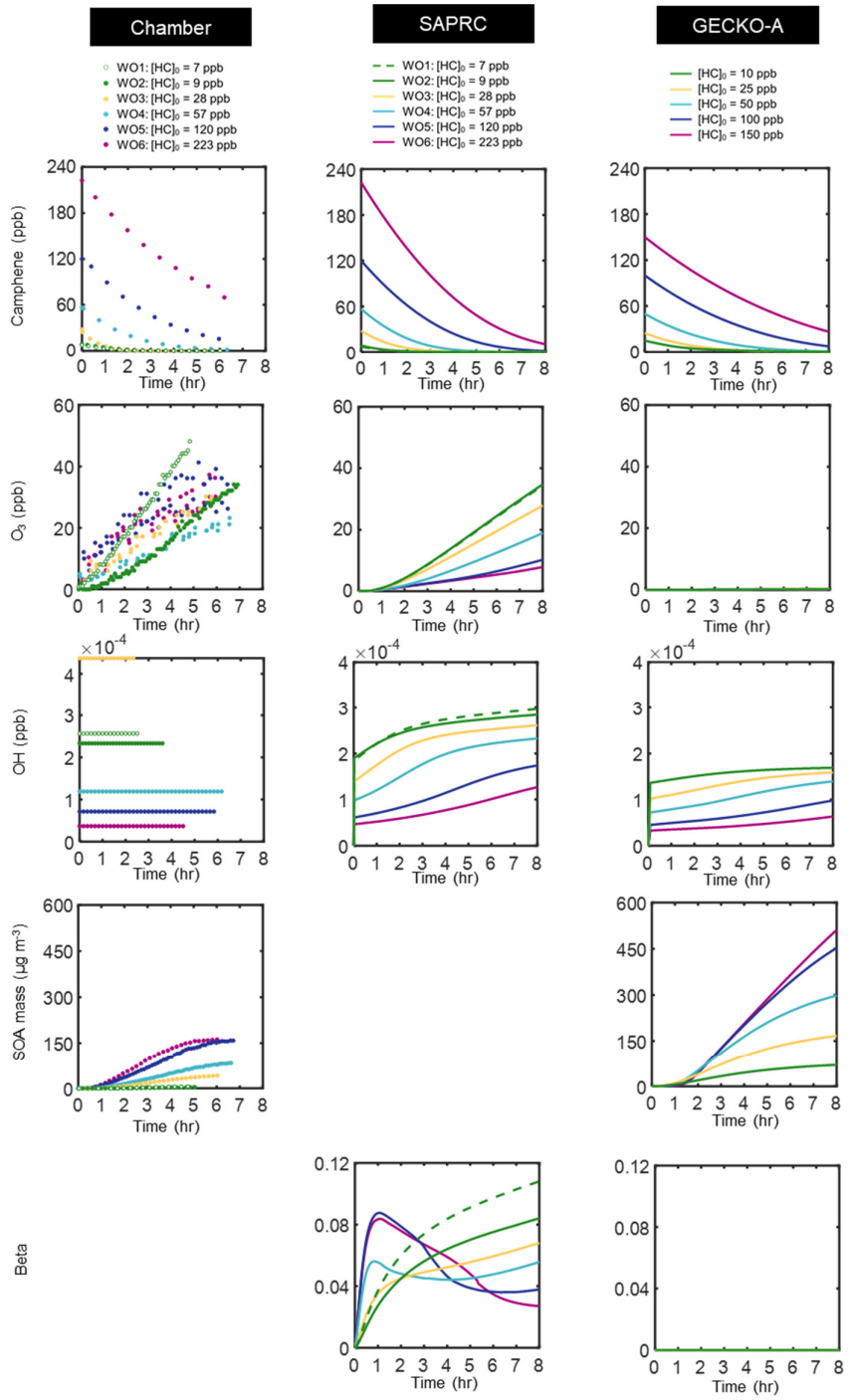


Figure S1a. Comparison of chamber data (circles) and model simulation results (lines) for the photooxidation of camphene (without added NO_x). Regarding the missing figures, the SAPRC box model used does not calculate SOA formation and measurement data are insufficient to calculate beta values. The chamber OH mixing ratio was calculated as follows:

$$[\mathbf{OH}]_{\mathbf{exp}} = \frac{\frac{d[\mathbf{cam}]_{\mathbf{exp}}}{dt} - k_{\mathbf{cam,O_3}}[\mathbf{cam}]_{\mathbf{exp}}[\mathbf{O_3}] - k_{\mathbf{cam,NO_3}}[\mathbf{cam}]_{\mathbf{exp}}[\mathbf{NO_3}]_{\mathbf{exp}}}{k_{\mathbf{cam,OH}}[\mathbf{cam}]_{\mathbf{exp}}}$$

, assuming $[\mathbf{NO_3}]_{\mathbf{exp}} \approx [\mathbf{NO_3}]_{\mathbf{sim}}$, chamber [OH] was averaged over the duration of the experiment or until consumption of camphene was complete.

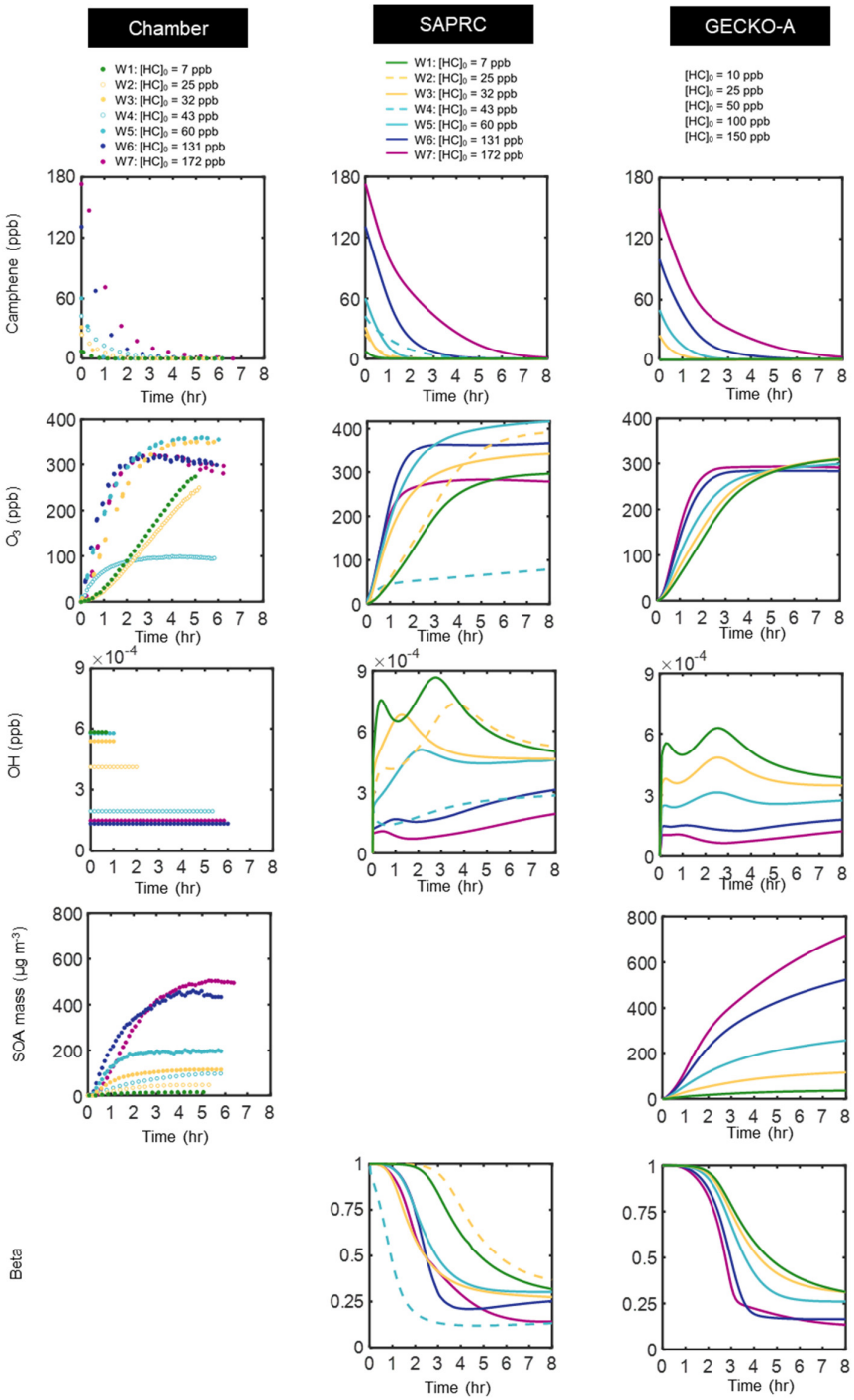


Figure S1b. Comparison of chamber data (circles) and model simulation results (lines) for the photooxidation of camphene (with added NO_x). Regarding the missing figures, the SAPRC box model used does not calculate SOA formation and measurement data are insufficient to calculate beta values. The chamber OH mixing ratio was calculated as follows:

$$[\mathbf{OH}]_{\mathbf{exp}} = \frac{\frac{d[\mathbf{cam}]_{\mathbf{exp}}}{dt} - k_{\mathbf{cam,O_3}}[\mathbf{cam}]_{\mathbf{exp}}[\mathbf{O_3}] - k_{\mathbf{cam,NO_3}}[\mathbf{cam}]_{\mathbf{exp}}[\mathbf{NO_3}]_{\mathbf{exp}}}{k_{\mathbf{cam,OH}}[\mathbf{cam}]_{\mathbf{exp}}}$$

, assuming $[\mathbf{NO_3}]_{\mathbf{exp}} \approx [\mathbf{NO_3}]_{\mathbf{sim}}$, chamber [OH] was averaged over the duration of the experiment or until consumption of camphene was complete.

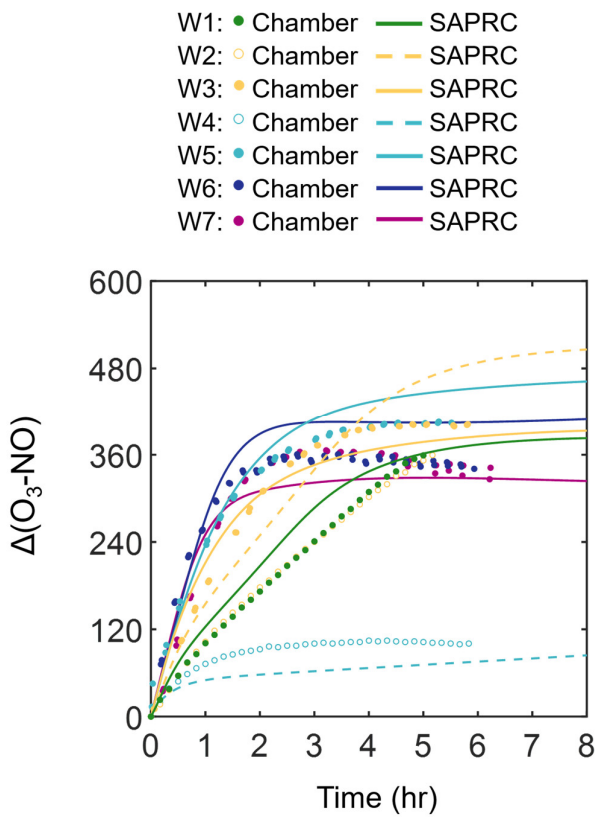
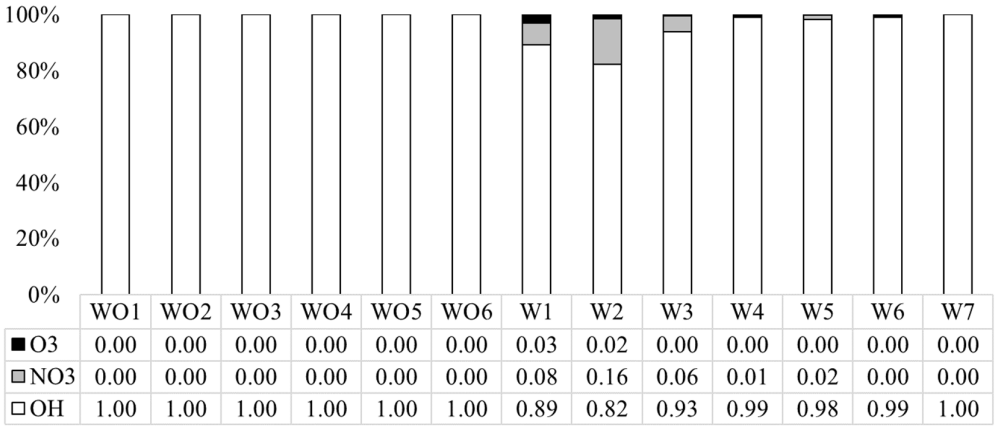
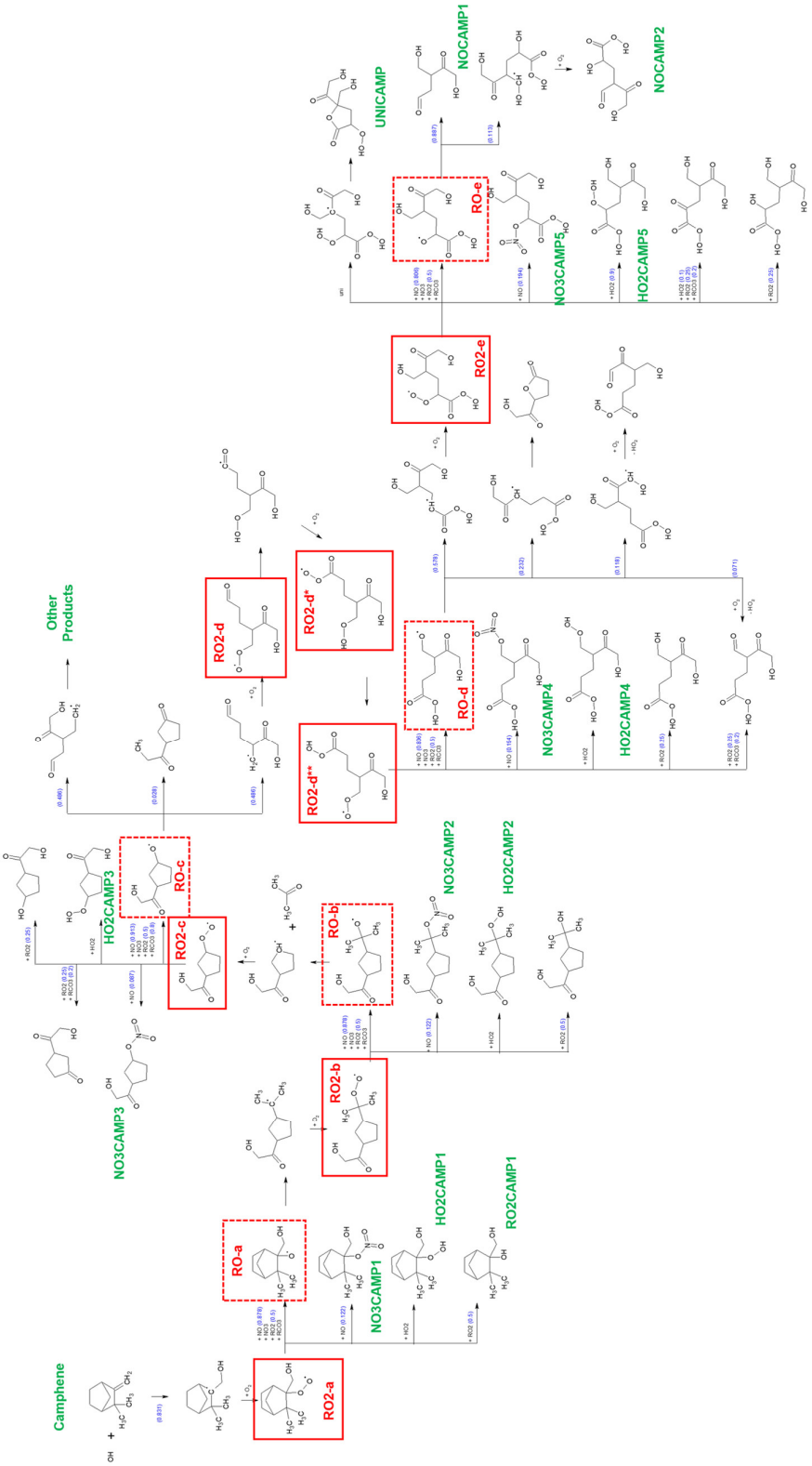


Figure S2. Comparison of the chamber data (circles) and SAPRC model simulation results (lines) for camphene photooxidation experiments with added NO_x.



	WO1	WO2	WO3	WO4	WO5	WO6	W1	W2	W3	W4	W5	W6	W7
■O3	0.00	0.00	0.00	0.00	0.00	0.00	0.03	0.02	0.00	0.00	0.00	0.00	0.00
▨NO3	0.00	0.00	0.00	0.00	0.00	0.00	0.08	0.16	0.06	0.01	0.02	0.00	0.00
□OH	1.00	1.00	1.00	1.00	1.00	1.00	0.89	0.82	0.93	0.99	0.98	0.99	1.00

Figure S3. Fractional precursor reactivity for each experiment (with added NO_x and without added NO_x) based on SAPRC simulations.



45

Figure S4. Detailed schematic of the OH-initiated oxidation of camphene at 298 K and atmospheric pressure

with added NO_x as in SAPRC.

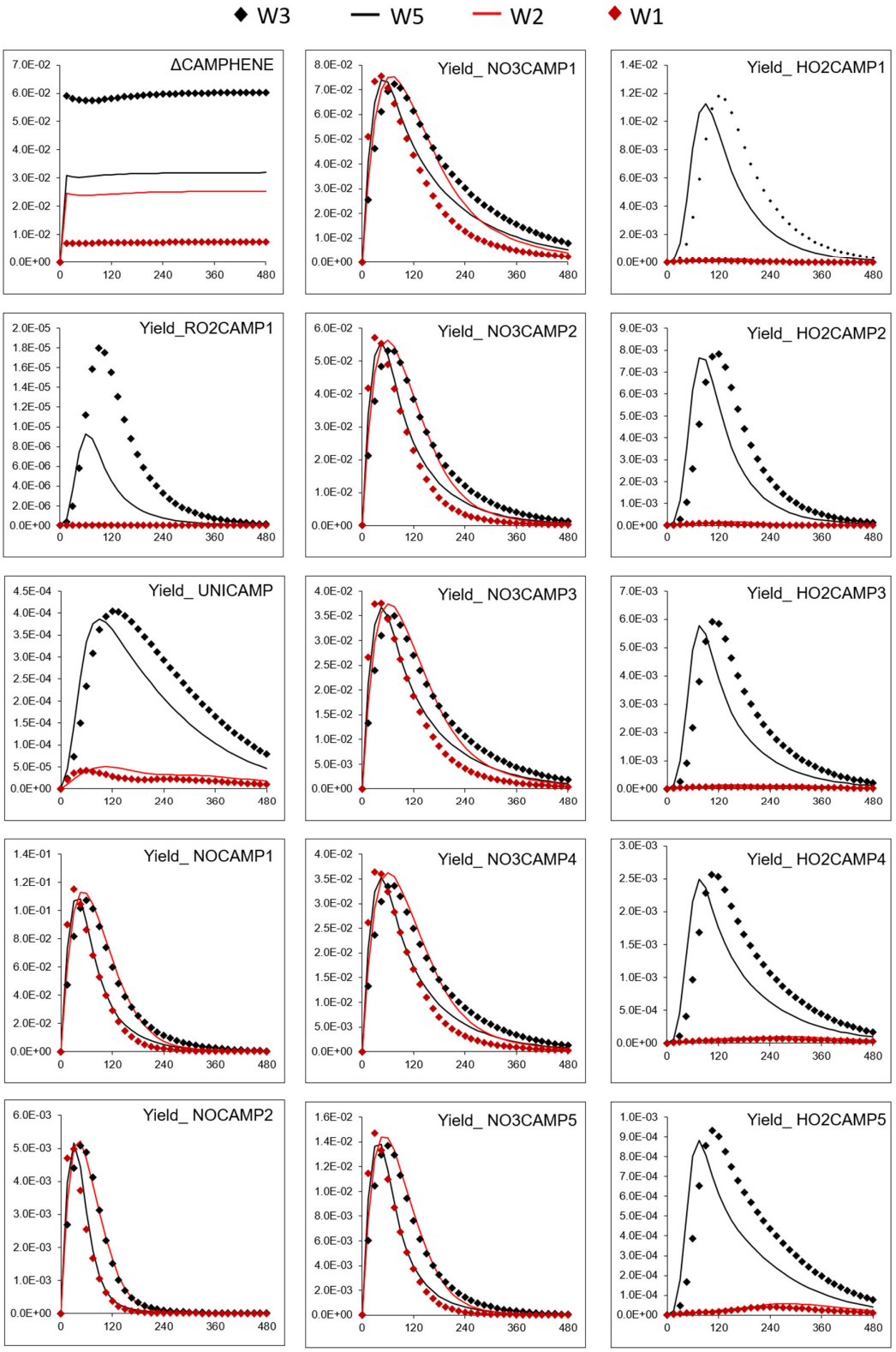


Figure S5. Time-resolved product yield distributions for W3, W5, W1 and W2 predicted by SAPRC. The yield of the product is calculated as: $\mathbf{Yield} = \Delta[\mathbf{product}]/\Delta[\mathbf{camphene}]$.

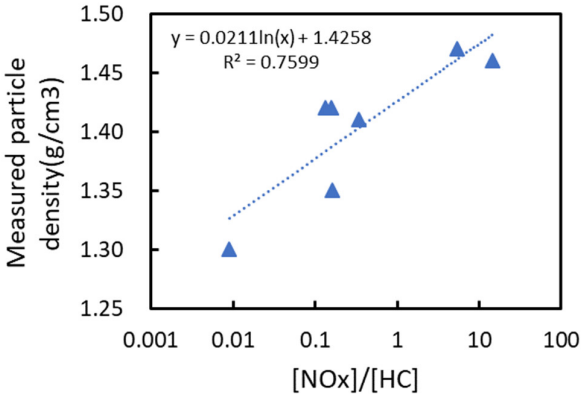


Figure S6. Fit function for measured particle density as a function of $[NOx]_0/[HC]_0$.

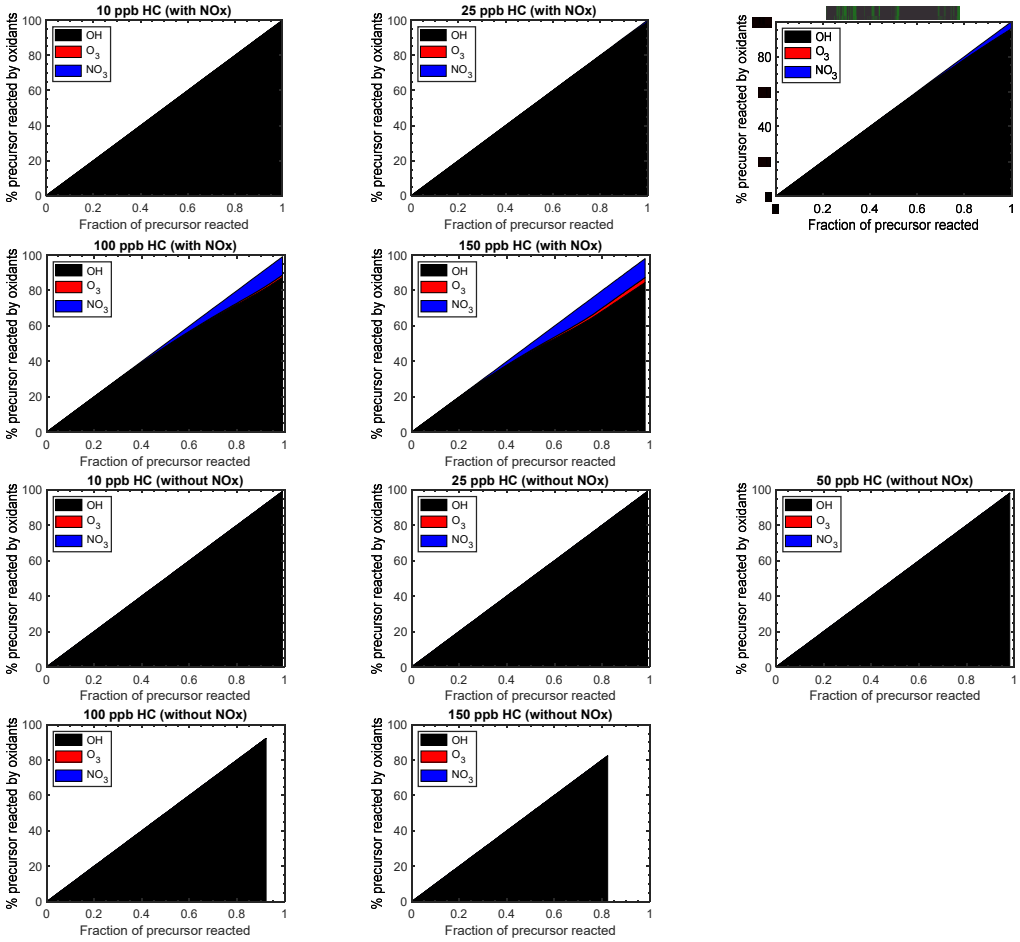


Figure S7. Fractional precursor reactivity as predicted by GECKO-A (for experiments with added NO_x and without added NO_x).

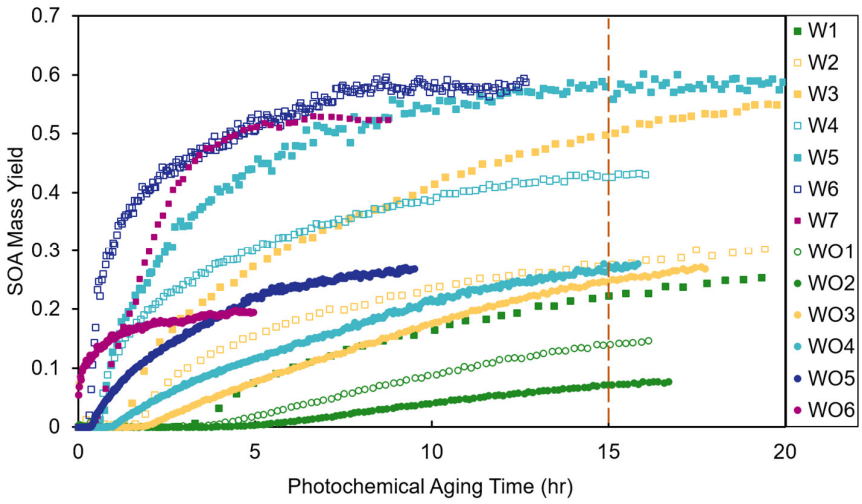


Figure S8. SOA mass yields as functions of photochemical aging time in experiments with added NO_x (squares); and experiments without added NO_x (circles) with cutoff line at 15 hours to highlight a single aging time across experiments.

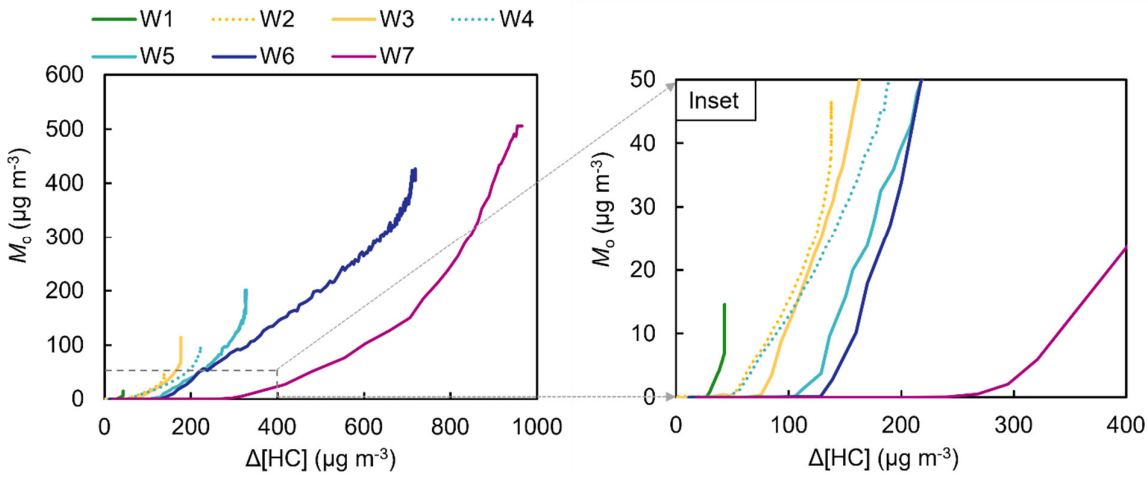


Figure S9. Measured SOA mass concentrations as a function of reacted camphene concentration with added NO_x; inset shows the lowest camphene concentrations from 0 – 400 µg m^{-3}.

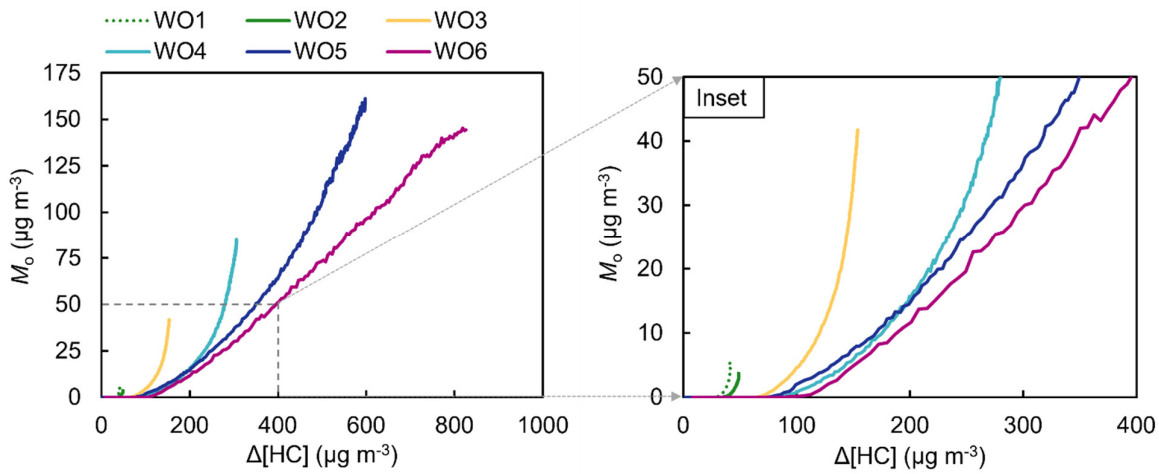


Figure S10. Measured SOA mass concentrations as a function of reacted camphene concentration without added NO_x; inset shows the lowest camphene concentrations from 0 – 400 µg m-3.