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A Computationally Efficient Model to Represent the Chemistry, Thermodynamics, and Microphysics of Secondary Organic Aerosol (simpleSOM): Model Development and Application to α-pinene SOA

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Table S.1: SOA mass concentration and O:C observations from several environmental chamber studies performed on α-pinene.

Reference	***O:C Range***	***Oxidant***	***Max SOA (μg m⁻³)***
Aiken et al.[1]	0.28	O_3	~500
Shilling et al.[2]	0.29 to 0.45	O_3	0.5 to >140
Chhabra et al.[3]	0.30 to 0.43	O_3	57 to 183
Zhang et al.[4]	0.45 to 0.55	O_3/OH	125 to 250
Järvinen et al.[5]	0.23 to 0.29	O_3/OH	>600
Nah et al.[6]	0.45 to 0.52	O_3	62 to 87
Kim et al.[7]	0.33 to 0.42	O_3/OH	20 to 255
Heaton et al.[8]	0.31 to 0.37	O_3	~400

Table S.2: simpleSOM parameters to model SOA formation from photooxidation of □-pinene for four target end-of-experiment oligomer fractions, f_{olig}=0, 20%, 50%, and 80%.

f_{olig}	k_f (cm^3 molecules^{-1} s^{-1})	k_r (s^{-1})	m_{frag}	P_{loss}	Δlogc*	P_{O1}	P_{O2}	P_{O3}	P_{O4}	P_{ELVOC}
0.0	NA	NA	3.513	0.989	1.630	0.001	0.704	0.260	0.001	0.034
0.2	10^{-24}	1.5×10^{-2}	3.651	0.961	2.198	0.001	0.897	0.067	0.001	0.034
0.5	10^{-24}	2.4×10^{-3}	4.121	0.990	2.785	0.429	0.465	0.071	0.001	0.034
0.8	10^{-24}	2.5×10^{-4}	5.240	0.990	3.140	0.694	0.180	0.091	0.001	0.034

Table S.3: simpleSOM parameters to model SOA formation from photooxidation of □-pinene for three different Db values: 10^{-10}, 3×10^{-19}, and 1×10^{-21} m^2 s^{-1}.

D_b (m^2 s^{-1})	m_{frag}	P_{loss}	Δlogc*	P_{O1}	P_{O2}	P_{O3}	P_{O4}	P_{ELVOC}
1×10^{-10}	3.513	0.989	1.630	0.001	0.704	0.260	0.001	0.034
3×10^{-19}	3.673	0.976	1.679	0.001	0.719	0.246	0.001	0.034
1×10^{-21}	2.753	0.000	6.936	0.001	0.024	0.941	0.001	0.034

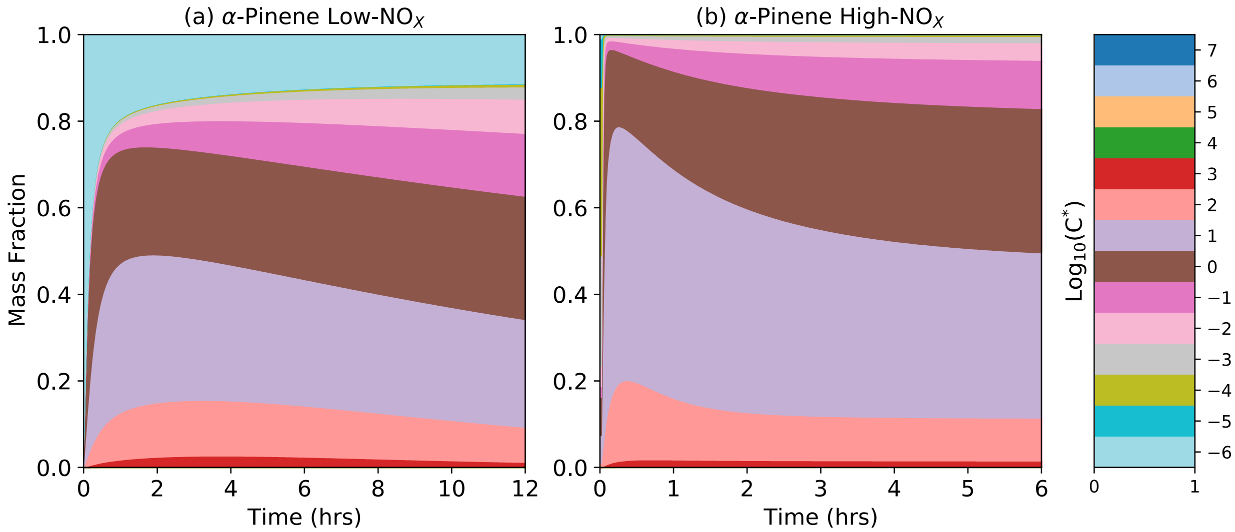

Figure S.1: Normalized, c^*-resolved contributions to SOA over time for simulations performed at (a) low NO_X and (b) high NO_X conditions. These results are from the same simulations shown in Figure 1. Lower-volatility species seem to contribute more strongly to the SOA under the low NO_X case compared to the high NO_X case during the early parts of the experiment.

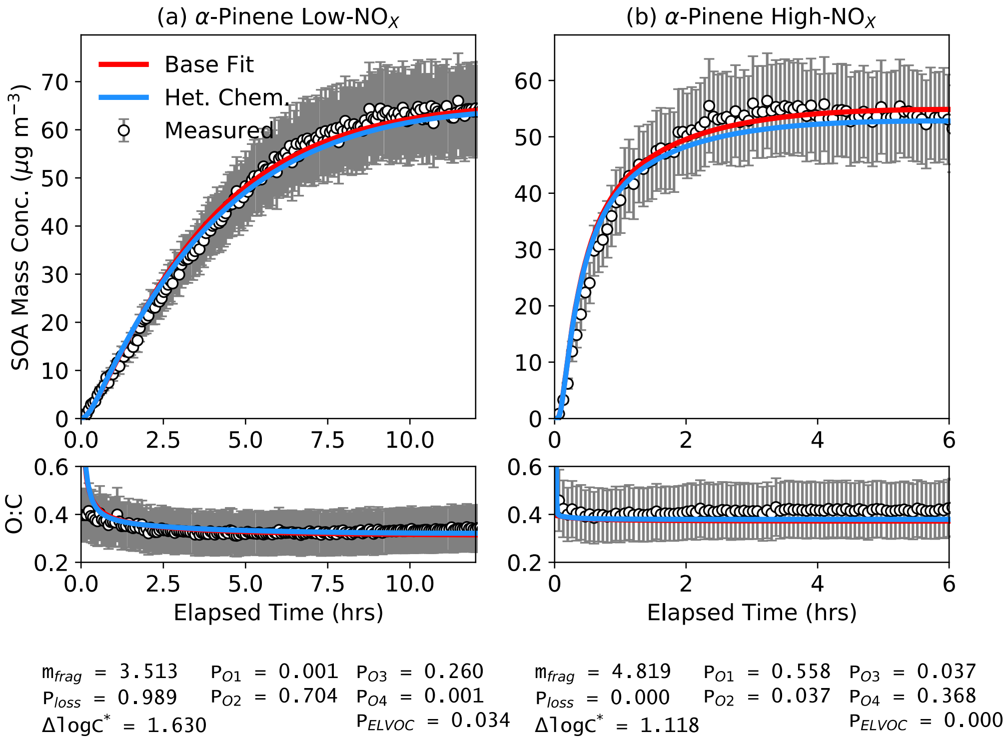

Figure S.2: simpleSOM predictions of SOA mass concentration and SOA O:C ratio compared to measurements for (a) low and (b) high NO_X photooxidation experiments performed on α-pinene. Model predictions based on fits to the SOA mass concentration and O:C are shown in solid red while those for simulations using the base fit parameters but with heterogeneous chemistry included are shown in solid blue. The fit parameters for the respective NO_X conditions are listed at the bottom of the figure.

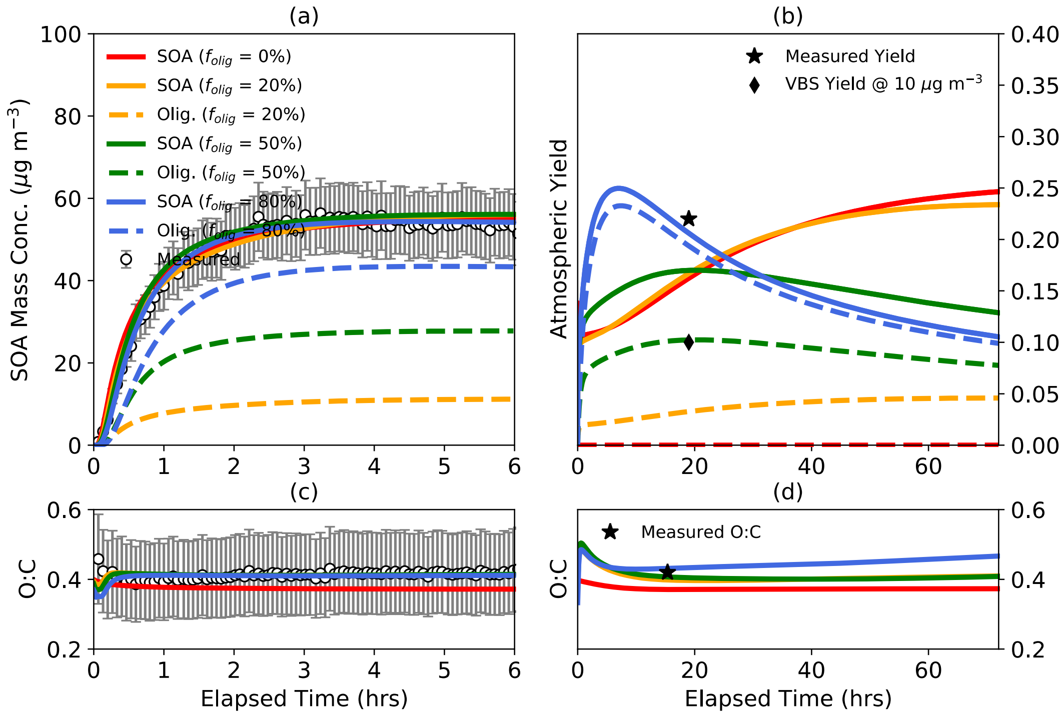

Figure S.3: Same as Figure 3 but for a high NO_X experiment. simpleSOM predictions of (a) SOA mass concentration and (c) SOA O:C ratio based on fits to the observations compared to measurements for a low NO_X photooxidation experiment performed on α-pinene for different target end-of-experiment oligomer fractions. simpleSOM predictions of (b) SOA mass yields and (d) SOA O:C ratio from atmospheric simulations performed under low NO_X conditions. Predictions of total SOA mass are shown in solid lines and the oligomer mass are shown in dashed lines.

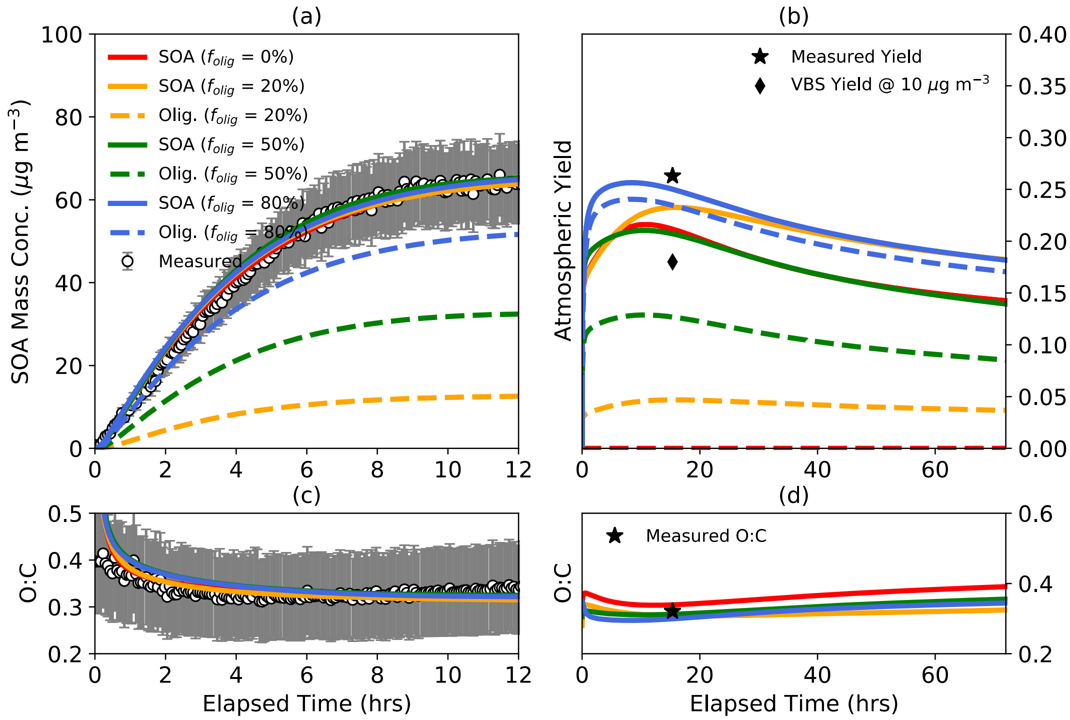

Figure S.4: Same as Figure 3 but for a k_f value of 10^{-25} cm3 molecules^{-1} s^{-1}. simpleSOM predictions of (a) SOA mass concentration and (c) SOA O:C ratio based on fits to the observations compared to measurements for a low NO_X photooxidation experiment performed on α-pinene for different target end-of-experiment oligomer fractions. simpleSOM predictions of (b) SOA mass yields and (d) SOA O:C ratio from atmospheric simulations performed under low NO_X conditions. Predictions of total SOA mass are shown in solid lines and the oligomer mass are shown in dashed lines.

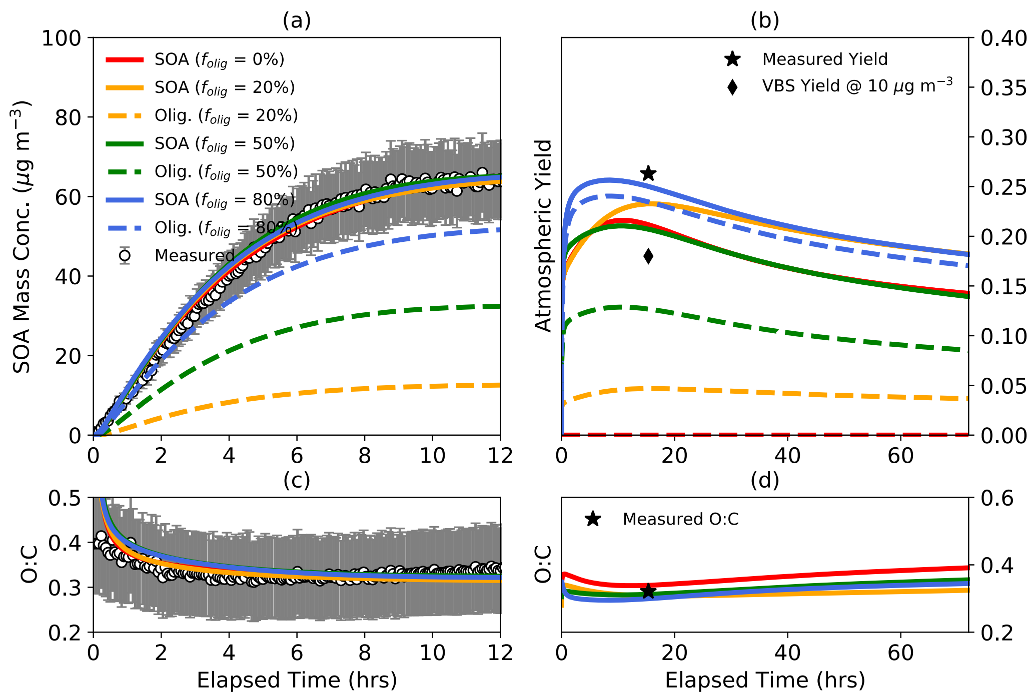

Figure S.5: Same as Figure 3 but for a k_f value of 10^{-23} cm3 molecules^{-1} s^{-1}. simpleSOM predictions of (a) SOA mass concentration and (c) SOA O:C ratio based on fits to the observations compared to measurements for a low NO_X photooxidation experiment performed on α-pinene for different target end-of-experiment oligomer fractions. simpleSOM predictions of (b) SOA mass yields and (d) SOA O:C ratio from atmospheric simulations performed under low NO_X conditions. Predictions of total SOA mass are shown in solid lines and the oligomer mass are shown in dashed lines.

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