

1 **Analyzing Experimental Data and Model Parameters:**
2 **Implications for Predictions of SOA Using Chemical**
3 **Transport Models**

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5

6 **Supplementary Material**

7 **S.1. Compilation of Experimental Data**

T (K), RH (%)	ΔHC (ppb)	ΔM_o ($\mu\text{g m}^{-3}$)	Yield (T)	Yield ^a (298K)	$[\text{NO}_x]_0$ (ppb)	$[\text{VOC}]_0 /$ $[\text{NO}_x]_0$ (ppbC/ppb)	Reference
<i>α-pinene+O₃, dark</i>							
303-310, ~5%	17-65	7-65	0.08-0.19	0.10-0.22	NR		Griffin et al. (1999)
301-302, <2%	23-144	10-190	0.15-0.24	0.16-0.25	<2		^b Cocker et al. (2001a)
295, NR	15-210	7-346	0.08-0.29	0.08-0.28	9-30	17-240	^c Presto et al. (2005)-low NO _x
295, NR	24-235	1-212	0.01-0.16	0.01-0.15	188-525	1.3-4.5	Presto et al. (2005)-high NO _x
295, NR	6-135	3-192	0.08-0.25	0.08-0.24	5-6	11-214	Presto and Donahue (2006)- low NO _x
295, NR	12	0.7	0.01	0.01	41	2.8	Presto and Donahue (2006)- high NO _x
298, 5-6%	14-48	29-121	0.38-0.46	0.38-0.46	0		Ng et al. (2007a)- low NO _x
296-298, 4-6%	13-47	5-41	0.06-0.16	0.06-0.16	930-968		Ng et al. (2007a)- high NO _x
285-313, NR	4-116	0.3-293	0.01-0.44	0.009-0.37	NR		Pathak et al. (2007)
301, <2%	6-82	4-167	0.12-0.37	0.13-0.39	<1		Song et al. (2007)
298, ~40%	0.3-14	0.1-7	0.05-0.15	0.05-0.15	<1		Shilling et al. (2008)
<i>photo-oxidation individual terpenes (Δ^3-carene, β-pinene, sabinene, limonene)</i>							
308-316, ~5%	29-104	3-100	0.02-0.18	0.02-0.22		~5	Griffin et al. (1999)

<i>photo-oxidation of isoprene</i>						
293, 40-50%	25-500	0.4-22	0.008-0.02	n/a	202-280	Kroll et al. (2005)
298-302, <10%	12-90	0.2-7	0.08-0.03	n/a	<1	Kroll et al. (2006)-low NOx
301, <10%	42-49	1-5	0.01-0.04	n/a	78-745	Kroll et al. (2006)-high NOx
293-295, 9-11%	33-523	3-65	0.02-0.005	n/a	822-1175	Chan et al. (2010)
NR, 5%	49-91	3-8	0.02-0.04	n/a	<det.	Chhabra et al. (2010)-low NOx
NR, <10%	81-286	1-8	0.01-0.004	n/a	892-1025	Chhabra et al. (2010)-high NOx
<i>photo-oxidation of individual sesquiterpenes (α-humulene, aromadendrene, β-caryophyllene, longifolene)</i>						
306-309, ~5%	5-13	13-82	0.3-0.8	0.4-1.0	0.5-8	Griffin et al. (1999)
297-299, ~5-10%	5-25	16-115	0.3-0.8	n/a	0	Ng et al. (2007a)- low NOx
297-299, ~5-10%	4-27	16-153	0.4-0.8	n/a	101-978	Ng et al. (2007a)- high NOx
<i>photo-oxidation of toluene and other "ARO1" (high gas-phase yield aromatics)</i>						
303-315, NR	252-381	68-171	0.07-0.1	0.09-0.1	253-793	Odum et al. (1997)-toluene
297-298, ~5%	30-80	7-31	0.07-0.2	n/a	941-947	^d Ng et al. (2007b)-toluene
285-304 ~15-20%	8-44	10-20	0.06-0.3	0.05-0.3	270-1300	^d Hildebrandt et al. (2009)-toluene
301-312, NR	103-739	13-394	0.03-0.1	0.03-0.1	304-1449	Odum et al. (1997)-other ARO1
297-298, ~5%	39	29	0.2	n/a	169	^d Ng et al. (2007b)-other ARO1
<i>photo-oxidation of naphthalene, xylene and other "ARO2" (low gas-phase yield aromatics)</i>						
293-294, <2%	59-394	11-231	0.04-0.2	0.04-0.1	144-650	^b Cocker et al. (2001b)-xylene
300, <2%	34-385	1-131	0.004-0.08	0.004-0.08	240-586	1-6 ^d Song et al. (2005)-xylene
297-298, ~5%	28-133	3-31	0.02-0.04	n/a	943-945	^d Ng et al. (2007b)-xylene
285-305 ^e , >20%	29-83	1-21	0.007-0.05	0.005-0.05	73-412	Zhou et al. (2011)-xylene

301-315, NR	58-446	13-208	0.02-0.1	0.02-0.1	143-1046		Odum et al. (1997)-other ARO2
299, 5-8%	8-18	5-19	0.1-0.2	n/a	377-494		^d Chan et al. (2009)- naphthalene
298-301, <20%	5-40	4-51	0.2	n/a	567-776		^d Kautzman et al. (2010)- naphthalene
295	5-26	2-7	0.06-0.1	0.05-0.1		4-11	Shakya and Griffin (2010)- naphthalene
<i>photo-oxidation of individual alkanes, C7-C17 (4 normal, 3 cyclic, 7 branched)</i>							
298, <1%	369-823	132- 2406	0.01-0.9	n/a		NR	Lim and Ziemann (2009)-normal
295, <20%	2-68	6-10	0.09-0.4	0.09-0.4		<1	Presto et al. (2010)
298, <1%	459-834	566- 4865	0.1-0.8	n/a		NR	Lim and Ziemann (2009)-cyclic
298, <1%	397-797	21-1206	0.008-0.2	n/a		NR	Lim and Ziemann (2009)-branched

1 Values normalized to $\rho = 1.0 \text{ g cm}^{-3}$, all data points are not included in figures (if outside selected
2 ranges for axes). NR = not reported. ^aYields were normalized to $T = 298 \text{ K}$ based on Pathak et al.
3 (2007), $\pm 1.6\%$ /degree K, unless otherwise noted. This temperature correction is in relatively good
4 agreement with observations by Takekawa et al. (2003) for anthropogenic presursors. ^bData from dry,
5 neutral-seed experiments only. ^cData from dark experiments only. ^dData from high-NO_x experiments
6 only. ^eRepresents the middle of the reported ranges.

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1 Derivation of Density Correction

2 In determining SOA yields from measurements, knowledge of the particle density is needed
3 to converted aerosol volume to aerosol mass. While the effective density can determined
4 from measurements (e.g., using a combination of Aerosol Mass Spectrometer (AMS) and a
5 Differential Mobility Analyzer (DMA)), such measurements were not always available at the
6 time SOA parameters were derived. As such, even for the same precursor compounds,
7 studies report SOA yield and/or parameters based on different assumptions of density. In
8 Table 3, we report the 2p-VBS parameters at densities matched to the assumptions of the
9 CMAQ model. We first perform parameter fitting at densities reported for the VBS
10 parameters (see Section 2.1). We then adjust the 2p-VBS parameters to the density assumed
11 in CMAQ according to the following equations:

$$12 \quad \alpha_{i,B} = \alpha_{i,A} \left(\frac{\rho_B}{\rho_A} \right) \quad (S1a)$$

$$13 \quad C_{i,B}^* = C_{i,A}^* \left(\frac{\rho_B}{\rho_A} \right) \quad (S1b)$$

14 where the ρ_A (g m^{-3}) is the density reported for the VBS parameters and ρ_B is the density
15 assumed by CMAQ.

16 To prove the validities of the equations above, we start with the definition of aerosol
17 yield Y :

$$18 \quad Y_{\text{measured}} = \frac{C_{\text{oa,measured}}}{\Delta\text{HC}_{\text{measured}}} = \frac{V_{\text{oa,measured}} \rho}{\Delta\text{HC}_{\text{measured}}} \quad (S2)$$

19 $V_{\text{oa,measured}}$ ($\text{m}^3 \text{m}^{-3}$) is the volumetric concentration of organic aerosol (e.g., as measured by a
20 DMA), $C_{\text{oa,measured}} = V_{\text{oa,measured}} \rho$ is the mass concentration in $\mu\text{g m}^{-3}$ assuming particle
21 density of ρ (g m^{-3}), and $\Delta\text{HC}_{\text{measured}}$ ($\mu\text{g m}^{-3}$) is the change in precursor hydrocarbon
22 concentration. To fit the data using a two-product model and assuming a particle density of
23 ρ_A , we get

$$24 \quad Y_{\text{measured,A}} = \frac{V_{\text{oa,measured}} \rho_A}{\Delta\text{HC}} = \frac{\alpha_{1,A}}{1 + V_{1,A}^* / V_{\text{oa,measured}}} + \frac{\alpha_{2,A}}{1 + V_{2,A}^* / V_{\text{oa,measured}}} \quad (S3)$$

25

1 where $V_{1,A}^*$ is the saturation concentration of lumped product i in units of $\text{m}^3 \text{m}^{-3}$. Similarly,
 2 if we assume a density of ρ_B instead of ρ_A , we can write

$$3 \quad Y_{\text{measured, B}} = \frac{V_{\text{oa,measured}} \rho_B}{\Delta \text{HC}} = \frac{\alpha_{1,B}}{1 + V_{1,B}^* / V_{\text{oa,measured}}} + \frac{\alpha_{2,B}}{1 + V_{2,B}^* / V_{\text{oa,measured}}} \quad (\text{S4})$$

4 Combining Equations S3 and S4 we get

$$5 \quad Y_{\text{measured, A}} = \left(\frac{\rho_B}{\rho_A} \right) Y_{\text{measured, B}} \quad (\text{S5})$$

$$\Rightarrow \sum_{i=1}^2 \frac{\alpha_{i,B}}{1 + V_{i,B}^* / V_{\text{oa,measured}}} = \frac{\rho_B}{\rho_A} \sum_{i=1}^2 \frac{\alpha_{i,A}}{1 + V_{i,A}^* / V_{\text{oa,measured}}}$$

6 Knowing $\alpha_{i,A}$ and $C_{i,A}^*$, one possible solution to Equation S5 is

$$7 \quad \alpha_{i,B} = \alpha_{i,A} \left(\frac{\rho_B}{\rho_A} \right) \quad (\text{S6a})$$

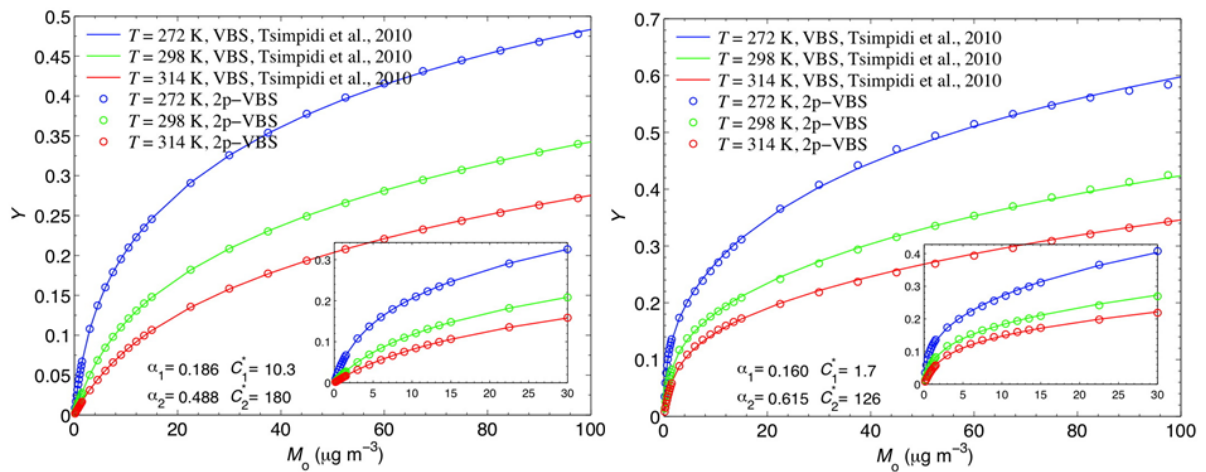
$$8 \quad V_{i,B}^* = V_{i,A}^* \Rightarrow C_{i,B}^* / \rho_B = C_{i,A}^* / \rho_A$$

$$\Rightarrow C_{i,B}^* = C_{i,A}^* \left(\frac{\rho_B}{\rho_A} \right) \quad (\text{S6b})$$

9 Equations S6a and S6b are the same as Equations S1a and S1b, respectively.

10

1 2p-VBS Fits



2 a) 2p-VBS fits for high NOx TOL/ARO1.

b) 2p-VBS fits for low NOx terpenes.

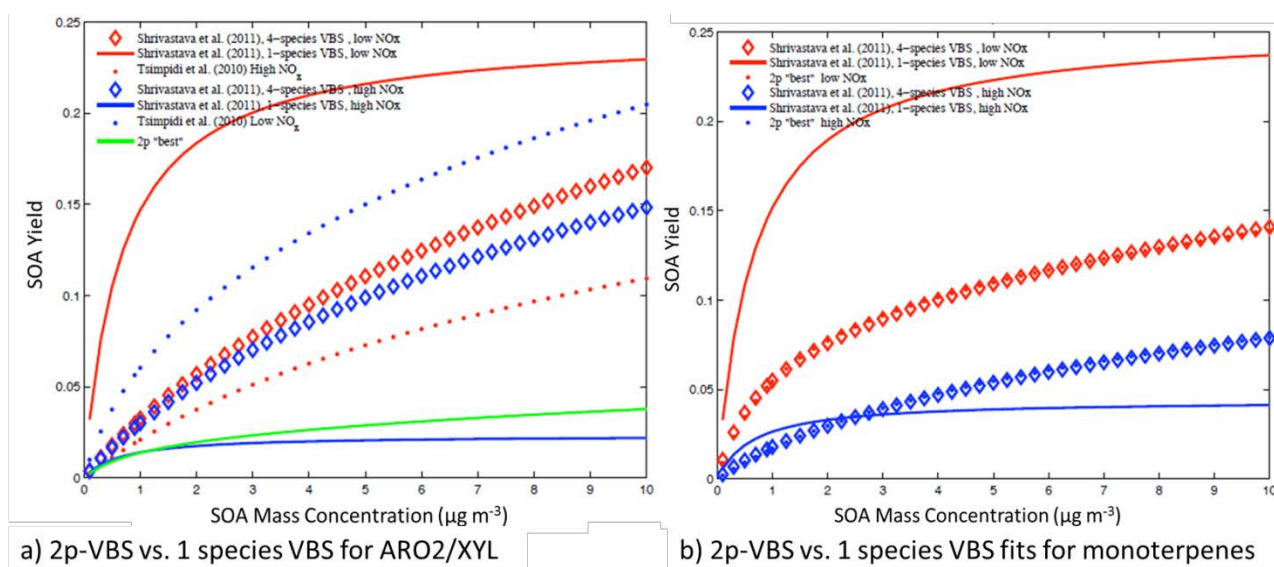
3 Figure S1. SOA Yield curves for VBS parameters (Tsimplidi et al., 2010) and 2p-VBS
 4 parameters at three temperatures: for high NOx toluene/ARO1 (panel a), and low NOx
 5 lumped monoterpenes (panel b).

6

1 Comparison with Reduced VBS

2 Consistent with the VBS fitting approach, Shrivastava et al. (2011) assigned fixed C^* values
3 for two species, POA and SOA. POA was represented by two C^* values, 10^{-2} and $10^5 \mu\text{g m}^{-3}$,
4 while traditional SOA (SOA from oxidation and condensation of volatile precursors) was
5 represented by a single C^* value of $1 \mu\text{g m}^{-3}$. The traditional SOA C^* value corresponds to
6 the lowest volatility bin in a typical 4-species representation (e.g., Tsimpidi et al. (2010)).
7 The α values were based on published VBS and 2p model parameters (rather than refit to
8 chamber data using the assumed C^* value). Because only a single C^* bin is used, the
9 condensed VBS parameterization of Shrivastava et al (2011) results in larger deviation than
10 the 2p-VBS parameterization from the original 4-species VBS parameterization for traditional
11 SOA.

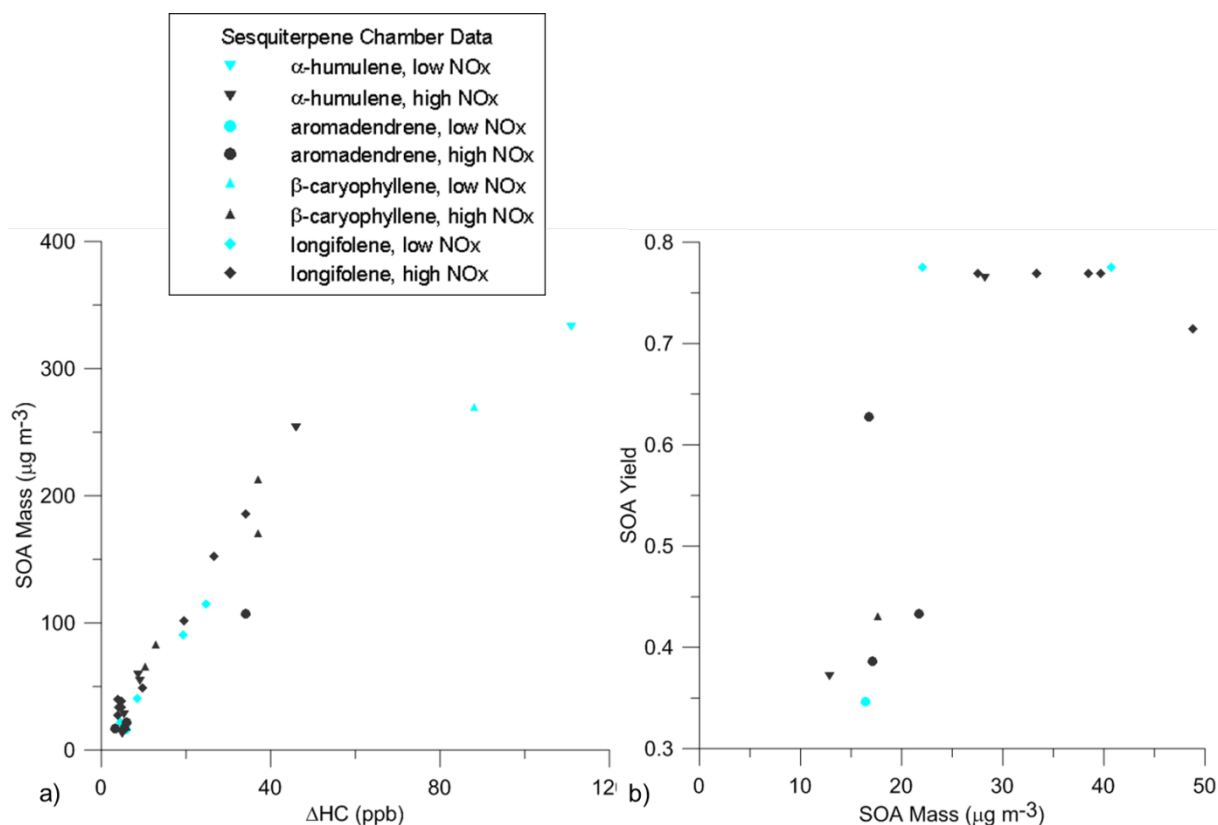
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14 Figure S2. SOA Yield curves for ARO2/xylene (panel a) and lumped monoterpenes (panel b)
15 comparing 1- and 4-species VBS parameterizations (Shrivastava et al., 2011) and “best
16 available” parameters (this work).

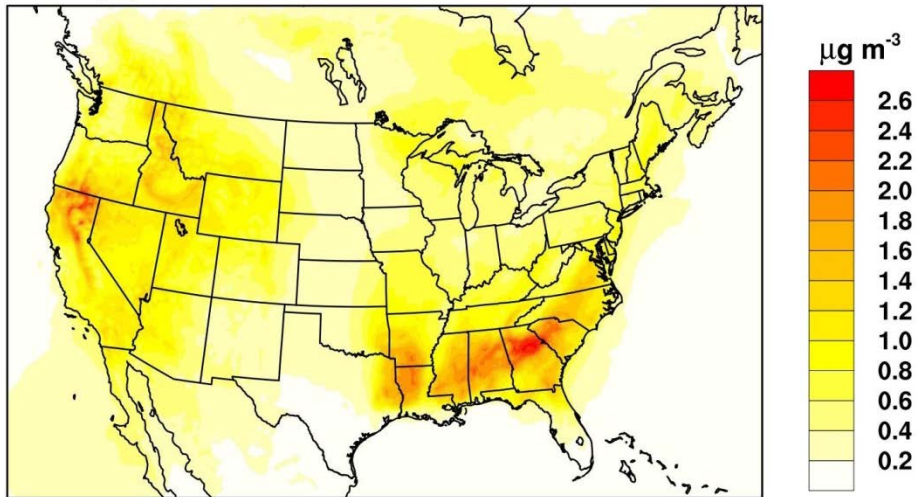
1 Sesquiterpene SOA Yields



2 Figure S3. Sesquiterpene photo-oxidation chamber data (Griffin et al., 1999; Lee et al., 2006;
3 Ng et al., 2006, 2007a): panel a) SOA mass concentration vs. level of reacted hydrocarbon,
4 ΔHC ; and panel b) SOA yield vs. SOA mass concentration. Higher SOA yields for high
5 (black symbols) vs. low (cyan symbols) NO_x experiments, as observed by Ng et al. (2007a)
6 are apparent over the large SOA mass and ΔHC range (panel a). Over a smaller SOA mass
7 range (panel b), the dependency of yield on NO_x concentration is less apparent and identity of
8 parent sesquiterpene appears to play a greater role in determining yield; for example,
9 longifolene experiments under high and low-NO_x conditions have higher SOA yields than
10 aromadendrene experiments under high and low-NO_x conditions.

11

1 **Biogenic SOA (low NO_x)**



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3 Figure S4. Difference in total biogenic SOA averaged over July 15-31, 2006 between the best
4 available simulation using the low-NO_x 2pVBS monoterpene parameters and the default
5 CMAQ simulation.

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