

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.

7

8

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

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

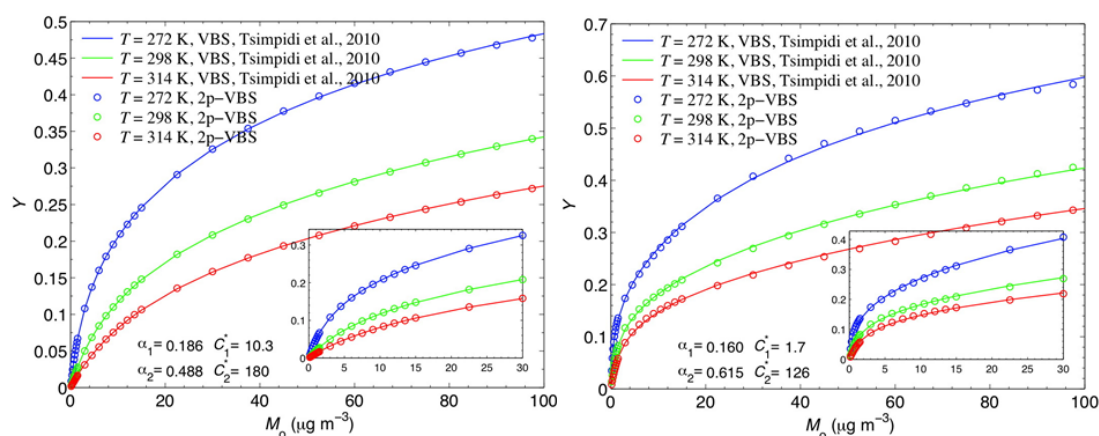
$$8 \quad V_{i,B}^* = V_{i,A}^* \Rightarrow C_{i,B}^* / \rho_B = C_{i,A}^* / \rho_A$$

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

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 NO_x TOL/ARO1.

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

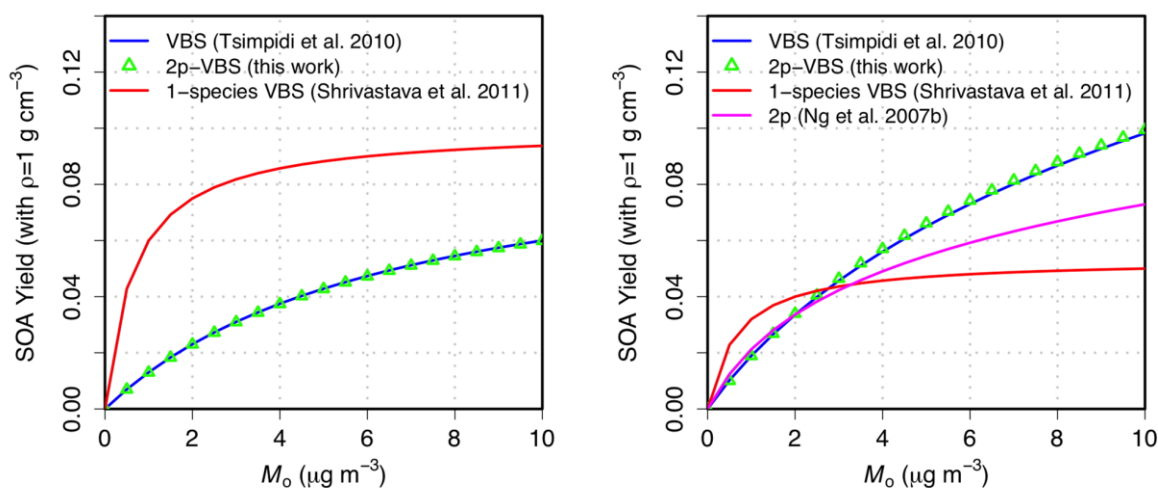
3 Figure S1. SOA Yield curves for VBS parameters (Tsimpidi et al., 2010) and 2p-VBS
4 parameters at three temperatures: for high NO_x toluene/ARO1 (panel a), and low NO_x
5 lumped monoterpenes (panel b).

6 As illustrated in Figure S1, the 2p-VBS parameters represent SOA formation with the same
7 degree of uncertainty as the VBS parameters across the range of ΔHC and M_o data. The
8 ability of any individual parameterization to accurately predict SOA formation depends on the
9 quality of the data and the chemical similarity between measured and modeled systems. In
10 this work, we start with existing VBS parameters rather than identifying atmospherically
11 relevant/irrelevant studies and fitting only data from “relevant” studies due to: 1) the
12 difficulty of determining which data are truly atmospherically relevant; and 2) the lack of data
13 in the approximate range (as discussed in this manuscript for M_o). Regarding 1, the relevance
14 of chamber experiments to the ambient atmosphere is critically important to understand in
15 developing robust parameterizations. Reacted HC concentrations and SOA mass loadings,
16 discussed in this work, are two important considerations but there are many others. As more
17 recent studies have shown (e.g., Henry et al., 2012; Eddingsaas et al., 2012), the relative
18 concentrations of gas-phase species (e.g., oxidants such as O₃, OH and NO_x) also are
19 important in determining SOA mass concentrations and physicochemical properties.
20 Regarding 2, the quality of the data at higher SOA mass loadings has been validated to some
21 extent by comparisons between experiments, including between facilities, and with ambient
22 data, and has led to considerable advances in our understanding of ambient SOA formation.
23 Experiments at low mass loadings are difficult to conduct (e.g., making accurate
24 measurements at low loadings). Furthermore, gas-phase compounds may partition

- 1 considerably to chamber walls, particularly under low mass loadings (Matsunaga and
- 2 Ziemann, 2010), making the push to more atmospherically relevant levels of
- 3 reactants/products potentially problematic.

1 Comparison with Reduced VBS

2 While implemented in different model frameworks, the reduced species “V-SOA” (1 species
3 or 1 bin) VBS parameterizations of Shrivastava et al. (2011) and the 2p-VBS
4 parameterizations in this work can be directly compared to one another and to the 4-species
5 VBS parameterizations of Tsimpidi et al. (2010), since each was intended to represent “first
6 generation” SOA formation from traditional volatile SOA precursors. Shrivastava et al.
7 (2011) used a single fixed C^* value of $1 \mu\text{g m}^{-3}$ for each precursor, corresponding to the
8 lowest volatility bin in a typical 4-species representation. The α values corresponding to $C^* =$
9 $1 \mu\text{g m}^{-3}$ were based on published VBS parameterizations, 2p parameterizations, and chamber
10 data, as reported in Shrivastava et al. (2011). For all of the traditional SOA precursors
11 evaluated in this work, the 2p-VBS parameters were better able to represent the predicted
12 SOA yield curves obtained using the Tsimpidi et al. (2010) parameters (as illustrated in
13 Figure S2 for ALK5 and TOL/ARO1).

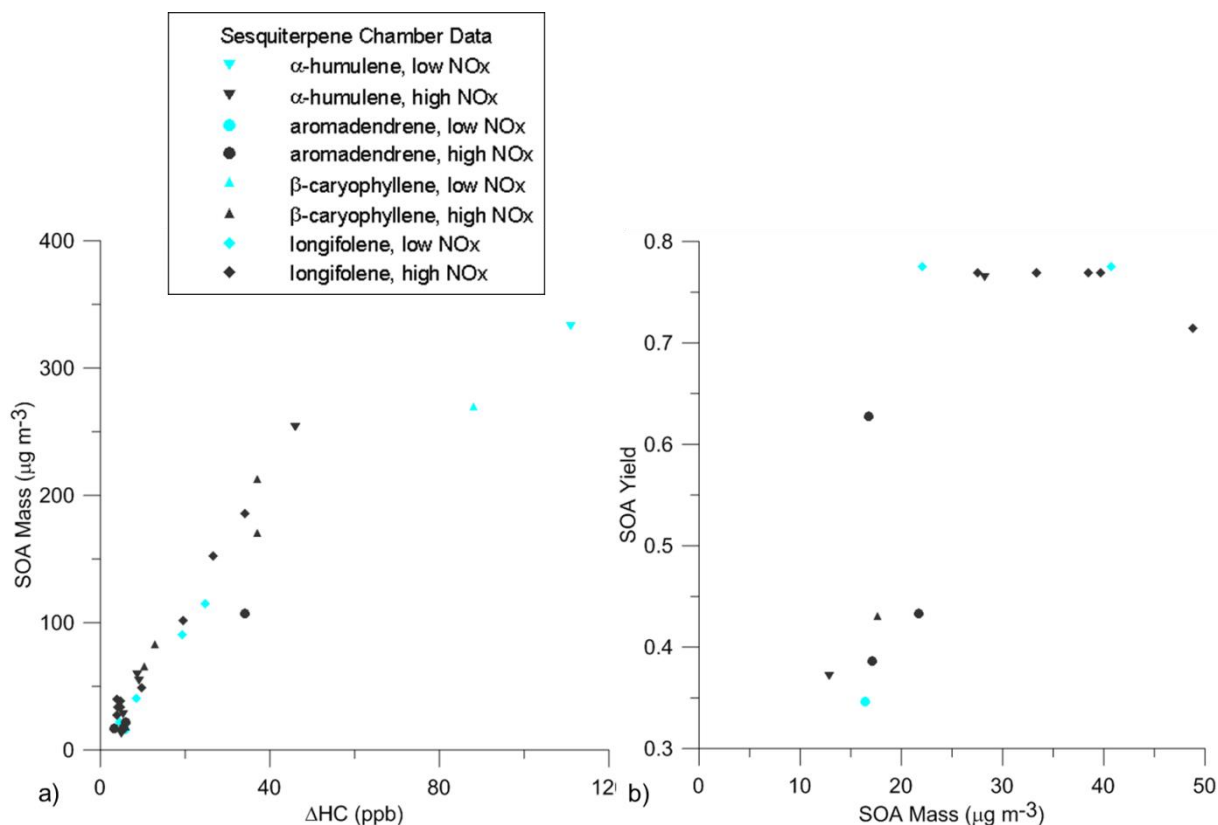


14 a) Predicted SOA yield curves for ALK5, high NOx.

b) Predicted SOA yield curves for ARO1/Toluene, high NOx.

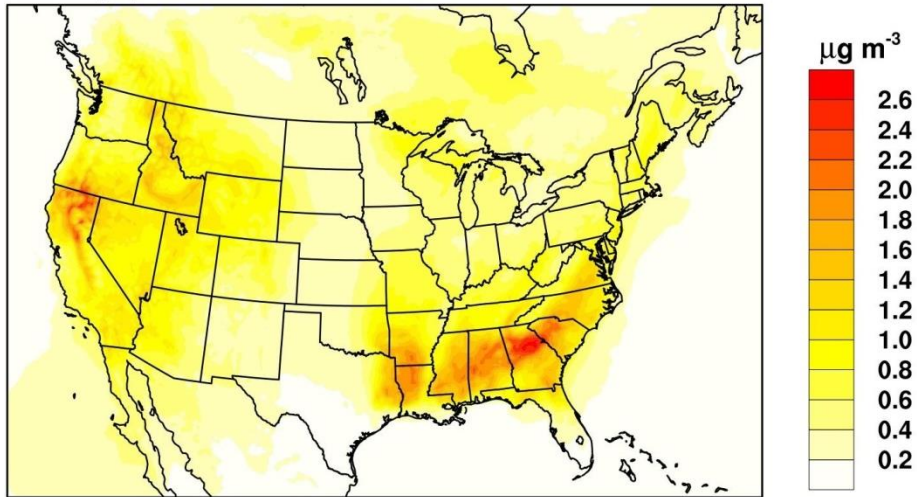
15 Figure S2. SOA yield curves for ALK5 (panel a) and ARO1/toluene/ (panel b) obtained using
16 the following SOA parameterizations: reduced 1-species VBS, Shrivastava et al. (2011); 4-
17 species VBS, Tsimpidi et al. (2010); and 2p-VBS (this work). Also shown in panel b is the
18 predicted yield curve based on Ng et al. (2007b) on which the Shrivastava et al. (2011) α
19 value was based.

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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