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Atmospheric Chemistry and Physics Discussions

Supplement of

Simulating secondary organic aerosol in a regional air quality model using the statistical oxidation model – Part 2: Assessing the influence of vapor wall losses

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The Supplemental Material consists of five figures and one table.

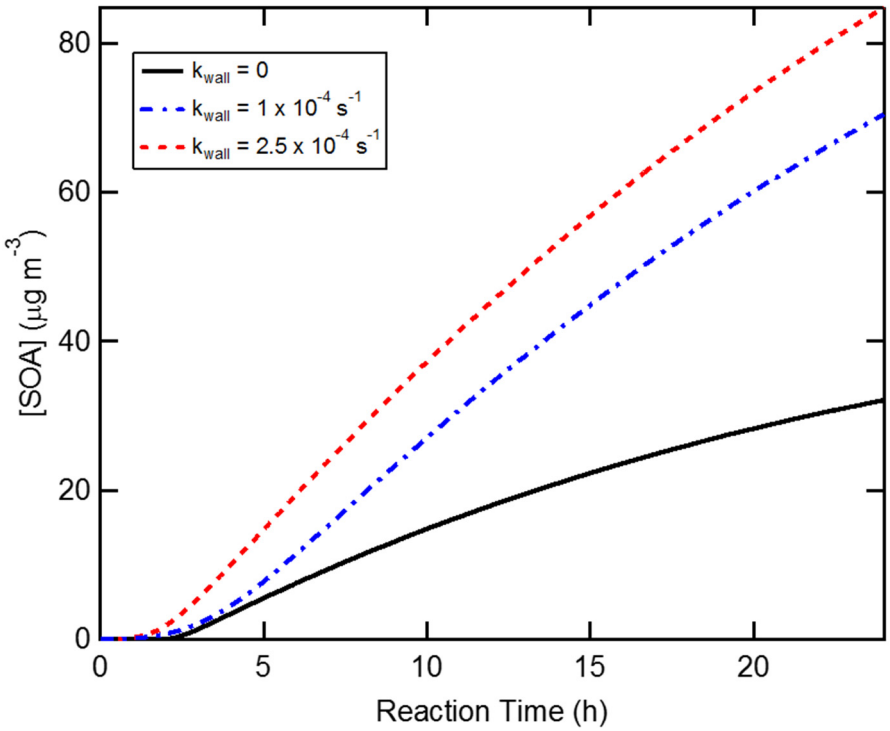

Figure S1. Box model simulations of SOA formation using SOM parameters determined from fitting low-NO_x toluene + OH SOA data assuming k_{wall} = 0, 1 x 10^{-4} and 2.5 x 10^{-4} s^{-1}, but where the simulations are run with k_{wall} = 0 s^{-1}. Reaction conditions here are $[toluene]_{t=0}$ = 100 μg m^{-3} and [OH] = 2 x 10^6 molecules cm^{-3}.

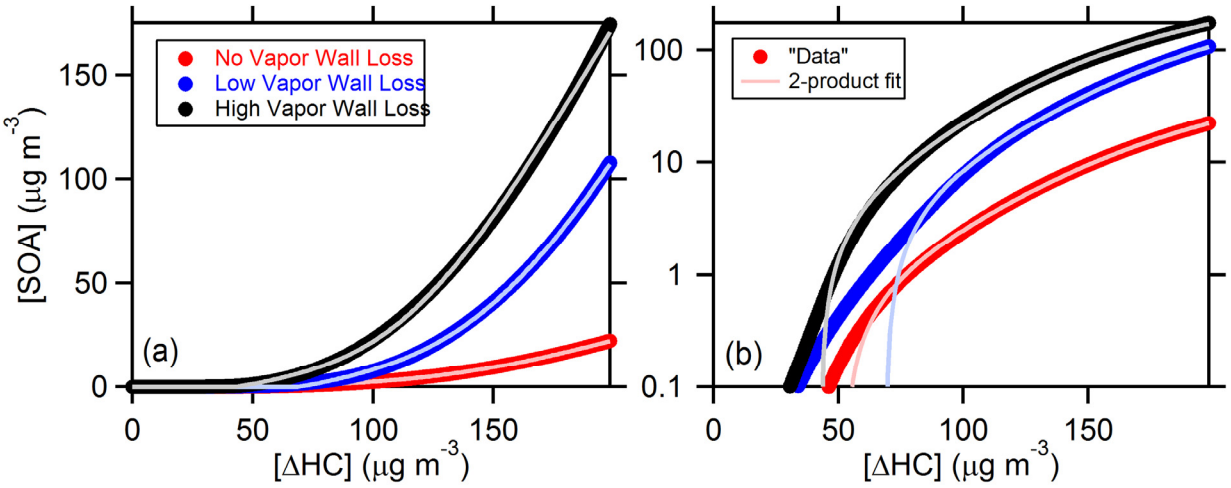

Figure S2. Example of 2-product fitting to SOA yield curves for dodecane + OH SOA formed under low-NO_x conditions. The 2-product model was fit to simulated vapor wall-loss-corrected yield curves (circles) that were generated using the SOM model. The original SOM fits were performed using variable k_{wall} values to account for vapor wall losses, but the subsequent simulated yield curves were generated with k_{wall} = 0. The lines are colored according to the wall-loss condition used when SOM was fit to the chamber observations, no wall loss (red), low wall loss (blue) and high wall loss (black).The best 2-product fits are shown as solid lines. Panel (a) shows the curves and fits on a linear scale and panel (b) shows the same on a log scale. Note that on a linear scale the deviations between the fit curves and the "data" at low [SOA] is not visibly evident.

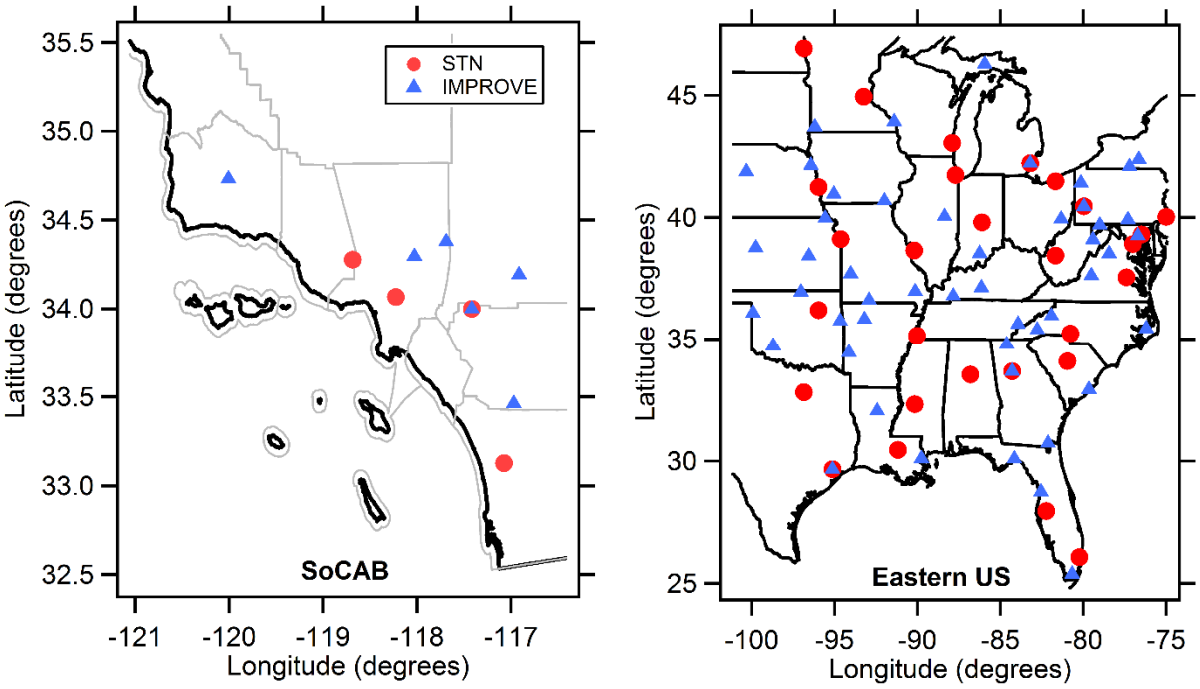

Figure S3. Map of STN and IMPROVE sites in the (left) SoCAB and (right) eastern US. STN sites are shown as red circles and IMPROVE sites as blue triangles.

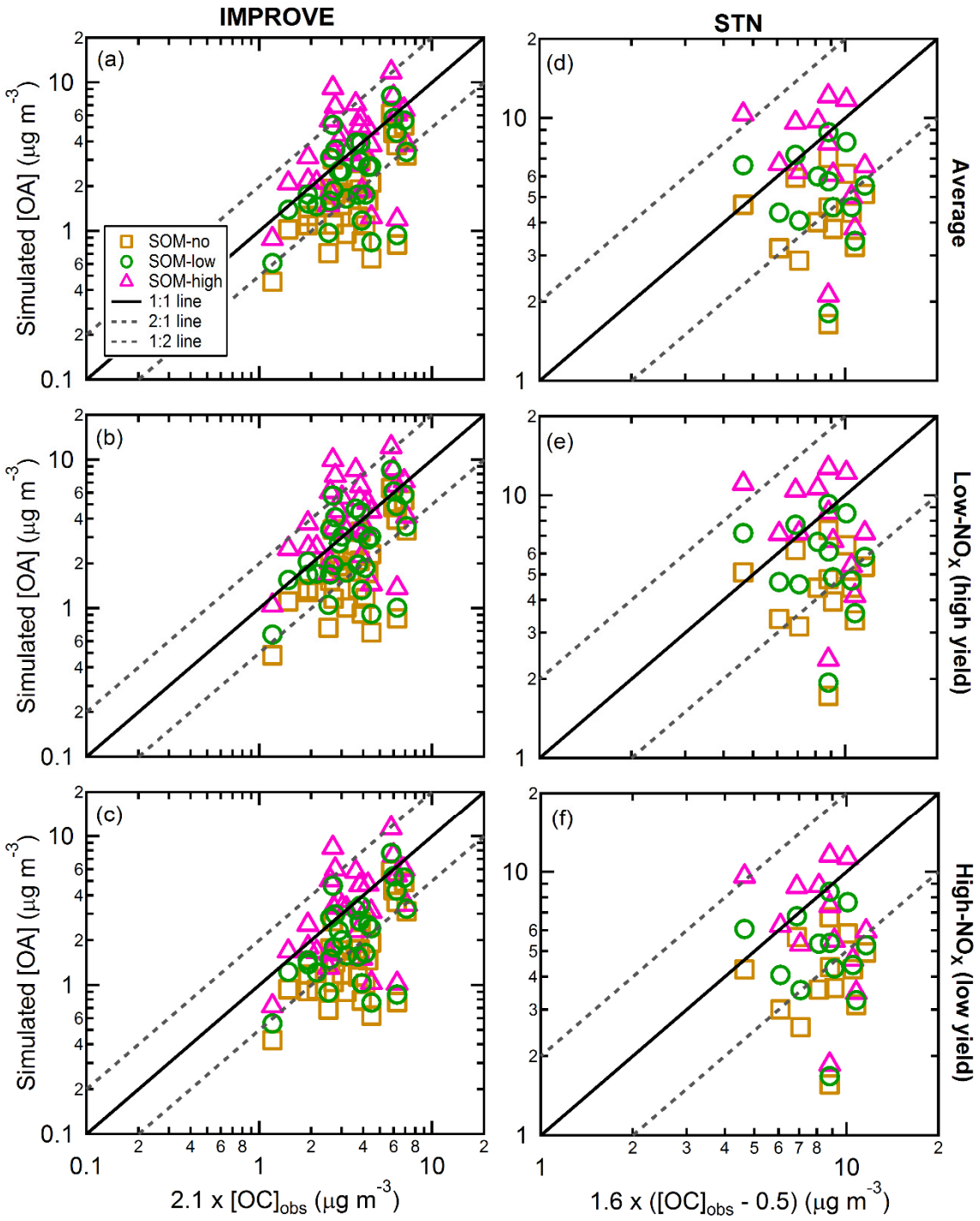

Figure S4. Scatter plots of simulated versus observed total OA (SOA + POA) concentrations for SoCAB for (left panels) IMPROVE and (right panels) STN sites. Simulation results are shown for SOM-no (orange), SOM-low (green) and SOM-high (pink). Results are reported from simulations run using the (top) average, (middle) low-NO_x / high-yield, and (bottom) high-NO_x / low-yield parameterizations.

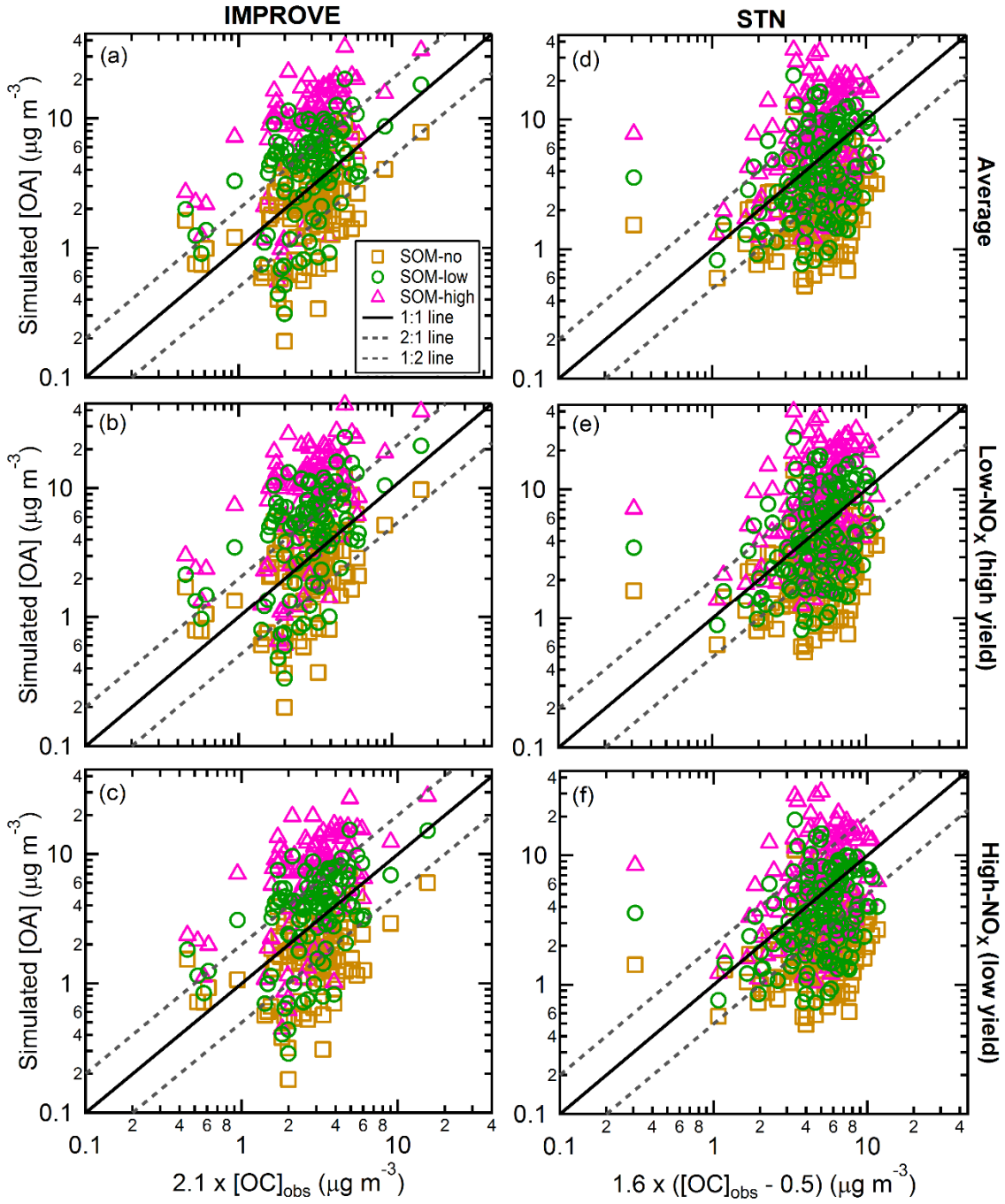

Figure S5. Scatter plots of simulated versus observed total OA (SOA + POA) concentrations for SoCAB for (left panels) IMPROVE and (right panels) STN sites. Simulation results are shown for SOM-no (orange), SOM-low (green) and SOM-high (pink). Results are reported from simulations run using the (top) average, (middle) low-NO_x / high-yield, and (bottom) high-NO_x / low-yield parameterizations. Only every other data point (one-in-two) is shown for visual clarity.

Table S1. List of best-fit SOM parameters determined by fitting SOM to experimental observations of SOA formation in the Caltech environmental chamber assuming that k_{wall} = 1 x 10^{-4} s^{-1} or 2.5 x 10^{-4} s^{-1}.

VOC Precursor Class	SAPRC-11 Species Name	VOC Surrogate	NO_x	m_{frag}	ΔLVP	p_{1O}	p_{2O}	p_{3O}	p_{4O}	Ref.^
				k_{wall} = 1 x 10^{-4} s^{-1}						
Long Alkanes	ALK5*	dodecane	low	0.677	1.57	0.97	0.023	0.003	0.004	(Cappa et al., 2013; Loza et al., 2014)
			high	0.186	1.45	0.961	0.001	0.002	0.036	
Benzene	Benzene	benzene	low	0.01	2.31	0.324	0.001	0.607	0.068	(Ng et al., 2007b)
			high	0.73	1.47	0.018	0.001	0.981	0.001	
Toluene	ARO1	toluene	low	0.843	1.70	0.066	0.001	0.106	0.827	(Zhang et al., 2014)
			high	5	1.37	0.865	0.001	0.065	0.069	
m-xylene	ARO2	m-xylene	low	0.236	1.97	0.001	0.123	0.8	0.075	(Ng et al., 2007b)
			high	0.0389	1.46	0.001	0.001	0.905	0.093	
Isoprene	Isoprene	isoprene	low	0.01	2.20	0.097	0.13	0.748	0.025	(Chhabra et al., 2011a)
			high	0.745	2.15	0.808	0.189	0.002	0.001	
Terpenes	TRP1/SESQ	α-pinene	low	0.156	1.89	0.316	0.554	0.087	0.043	(Chhabra et al., 2011a)
			high	0.0588	1.92	0.064	0.865	0.063	0.008	
				k_{wall} = 2.5 x 10^{-4} s^{-1}						
Long Alkanes	ALK5*	dodecane	low	2	1.83	0.999	0.001	0.001	0.001	(Cappa et al., 2013; Loza et al., 2014)
			high	0.266	1.47	0.965	0.001	0.002	0.032	
Benzene	Benzene	benzene	low	0.0807	1.97	0.637	0.001	0.002	0.360	(Ng et al., 2007b)
			high	0.824	1.53	0.008	0.001	0.991	0.001	
Toluene	ARO1	toluene	low	1.31	1.77	0.185	0.001	0.002	0.812	(Zhang et al., 2014)
			high	4.61	1.42	0.856	0.001	0.002	0.141	
m-xylene	ARO2	m-xylene	low	1.08	2.05	0.102	0.001	0.878	0.019	(Ng et al., 2007b)
			high	0.0671	1.46	0.001	0.001	0.942	0.056	
Isoprene	Isoprene	isoprene	low	0.0839	2.44	0.096	0.379	0.518	0.007	(Chhabra et al., 2011a)
			high	5	1.78	0.874	0.039	0.085	0.001	
Terpenes	TRP1/SESQ	α-pinene	low	0.305	1.97	0.419	0.426	0.140	0.014	(Chhabra et al., 2011a)
			high	0.16	1.91	0.500	0.422	0.070	0.008	

^These are the primary references for the experimental data. The data for the specific experiments used are presented in the supplemental material of Zhang et al.(Zhang et al., 2014)

*For SOM, the ALK5 class is separated into long alkane species grouped according to carbon number. See (Jathar et al., 2015a) for details.